Integrability and non-integrability in the Ising model

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Abstract of the Dissertation

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The Ising model at magnetic field $H = 0$ is one of the most important exactly solved models in statistical mechanics, solved on the square lattice in 1944 by Onsager, and later by others on the triangular lattice; its magnetic susceptibility at $H = 0$ continues to be an unsolved aspect of the model, however. The susceptibility can either be viewed as a sum over all correlation functions of the integrable model at $H = 0$, or else as a second derivative of the free energy of the non-integrable Ising model in a field. Therefore, its analytic properties, though derived from the non-integrable model, can be studied through series expansion of the integrable correlation functions. We begin this process by analyzing the first four terms in the form factor expansion of the diagonal correlation functions, and after summing over the diagonal form factor expansion, the first four terms of the diagonal susceptibility expansion. We have been able to reduce the form factor and susceptibility expansion terms, given as multi-dimensional integrals, to closed-form functions in all cases.

Under the limit of $H \to \infty$ with the interaction energy $E \to -\infty$, the isotropic Ising model becomes a hard particle lattice gas model, with exclusion of nearest neighbor lattice sites. In this limit, the triangular lattice Ising model becomes the exactly solved hard hexagon model, while the square lattice becomes the non-integrable hard squares model. We study in detail these models for finite lattice sizes in order to understand the differences between integrable and non-integrable models. We consider the partition functions zeros and their density for different boundary conditions, and find notable differences in the density which is attributed to an extra factorization in the transfer matrices of hard hexagons which is absent in hard squares. We also study the special point at fugacity $z = -1$ of hard squares where all eigenvalues of the transfer matrix are equimodular and where the grand partition function's value depends on boundary conditions.

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Chapter 1

Introduction

1.1 History

The 2D Ising model is certainly the most celebrated of the exactly solved models in statistical mechanics [161, 163], the subject of continuous ongoing research since the famous solution in 1944 by Lars Onsager of the two-dimensional zero field Ising model on the square lattice [176]. In the intervening decades, many detailed aspects of this integrable model, where the free energy is given in closed form, have been studied, such as the correlation functions [140, 168, 253, 254, 156], spontaneous magnetization [259, 72, 184, 168], and the magnetic susceptibility [93, 20, 254, 234, 256, 257, 157, 160, 158, 171, 172, 261, 263, 266, 264, 265, 55, 56, 59, 60, 58, 50, 47, 45, 51, 170, 48, 46, 52, 44, 53, 14, 69, 236]. However, even after 70 years of study there remain outstanding questions that have eluded simple answers, such as the analytic structure of the magnetic susceptibility and the Ising model in the presence of a magnetic field.

In 1999, Nickel discovered that there appears to be an accumulation of singularities in the magnetic susceptibility along the curve describing the phase transition of the model [171, 172], giving a natural boundary in the complex plane of the magnetic susceptibility beyond which the susceptibility cannot be analytically continued. The susceptibility can be derived either from the sum over all the two-point correlation functions of the integrable Ising model at zero magnetic field, or else from a second derivative of the free energy of the non-integrable Ising model in a magnetic field. Therefore, the natural boundary connects a non-integrable model with an integrable model, and it remains unknown whether natural boundaries can arise more generally in integrable models. In this respect, studying the natural boundary offers the opportunity to illuminate differences between integrable and non-integrable models. Ongoing attempts have been made to investigate the accumulation of singularities in the susceptibility by studying the singularities that arise in the expansion of the susceptibility in terms of n-fold integrals [263, 266, 264, 265, 55, 56, 59, 60, 58, 50, 47, 45, 51, 170, 48, 46, 52, 44, 53]. We have studied the diagonal form factor expansion of the correlation functions in detail and conjecture its analytical form [12]. By summing over the form diagonal factor expansion, we have also given closed form solutions to the diagonal susceptibility n-fold integrals for $n = 3, 4$ and studied their singularity structures, which differ from those of the form factor expansion.

Another alternative to study integrability and the phenomena of the natural boundary in the Ising model is to consider the limit of the magnetic field $H \to \infty$ while taking the interaction energy $E \to -\infty$, keeping their product fixed. This leads to the hard particle lattice gas limit; in the case of a triangular lattice it leads to the hard hexagon model and in the case of a square lattice it leads to the hard square model. Even though the Ising model at zero magnetic field has been exactly solved on both the square [176] and triangular lattices [118, 231, 115, 232, 240, 169, 258, 227], the hard particle limit produces an integrable model only for the case of hard hexagons [29, 30, 133]. Therefore, the hard particle limit provides a natural platform to study the relationship between integrable and non-integrable models. So far no evidence of a curve of singularities has arisen in the study of hard hexagons; we report, however, possible evidence for such a curve on a segment of the negative real fugacity axis for hard squares. The exclusion of a similar curve for hard hexagons appears to be caused by an extra symmetry in the model which causes its transfer matrices to have an extra factorization and the roots of their characteristic polynomials to be double roots. We also study the curious point at fugacity $z = -1$ for hard squares, where the free energy may have a boundary condition dependence and where the eigenvalues of the transfer matrices have special properties. No such special point has been identified in hard hexagons. However, the existence of such a special point in hard squares does not seem generic; in fact, many of the noted properties require a special symmetry at precisely $z = -1$ to cause massive cancellations. Therefore, the existence of a global extra symmetry in the hard hexagon transfer matrices appears to be the clearest property distinguishing integrability in the two models.

1.2 Ising Model Definition

The Ising model is a spin model that can be defined on any graph. An atom is assumed to lie on each vertex of the graph and have a spin of either $\sigma = +1$ or $\sigma = -1$. Atoms are allowed to interact only with their nearest neighbors on the graph as well as with an external magnetic field H. For concreteness, we consider only two regular lattices, the square and triangular lattices.

If the interactions of an atom with its nearest neighbors is independent of direction, the model is called *isotropic*; otherwise, when the interaction energy depends on the direction of the neighbor, such as its horizontal versus vertical neighbors, the model is called *anisotropic*. If, furthermore, the interaction energies vary throughout the lattice, the model is called *inhomogeneous*. We only consider *homogeneous* Ising models, where the interaction energies are independent of the location of the atoms in the lattice.

The anisotropic interaction energy of the Ising model on the square and triangular lattices, $\mathcal{E}_{\rm sq}$ and $\mathcal{E}_{\rm tr}$, respectively, are defined as

$$\mathcal{E}_{\rm sq} = -E_h \sum_h \sigma_i\sigma_j - E_v \sum_v \sigma_i\sigma_j - H \sum_i \sigma_i \tag{1.1}$$

where the first and second sums are over all horizontal and vertical nearest neighbor pairs, respectively, and

$$\mathcal{E}_{\rm tr} = -E_h \sum_h \sigma_i\sigma_j - E_v \sum_v \sigma_i\sigma_j - E_d \sum_d \sigma_i\sigma_j - H \sum_i \sigma_i \tag{1.2}$$

where the third sum is over all nearest neighbor pairs along the third direction in the triangular lattice. When $E_i > 0$ the model is called *ferromagnetic* and when $E_i < 0$ the model is *antiferromagnetic*. For the isotropic Ising model, the interaction energies E_i are all equal to each other, denoted by E.

The canonical partition function Z of the Ising model is then defined by

$$Z = \sum_{\sigma} e^{-\mathcal{E}/k_B T} \tag{1.3}$$

where the sum is over all configurational choices of all spins on the lattice.

The thermodynamic limit is the limit where the size of the lattice grows without bound in all directions. The free energy f is then defined by

$$f = -\lim_{\mathcal{N}\to\infty} \frac{k_B T}{\mathcal{N}} \ln(Z) \tag{1.4}$$

where $\mathcal{N}$ is the total number of atoms in the lattice. In the thermodynamic limit, the free energy of the Ising model is independent of the boundary conditions of the lattice. However, for the finite lattice, we consider various boundary conditions, such as toroidal and cylindrical, in order to understand the approach to the thermodynamic limit from multiple perspectives.

The 2D Ising model is celebrated as the first exactly solved model in statistical mechanics to feature a non-zero temperature T_c where a continuous phase transition occurs [176]. For the square lattice Ising model, this critical temperature occurs at the temperature T_c that solves the following equation

$$k = 1 \tag{1.5}$$

where

$$k = \sinh(2E_h/k_B T)\sinh(2E_v/k_B T) \tag{1.6}$$

For the isotropic lattice in the thermodynamic limit, the critical temperature occurs at

$$T_c = \frac{2E}{k_B \ln(1+\sqrt{2})} \tag{1.7}$$

Starting at this temperature, as the temperature decreases the ferromagnetic spontaneous magnetization $\mathcal{M}_0$, defined by

$$\mathcal{M}_0 = \lim_{H\to 0^+} \frac{1}{\mathcal{N}} \sum_i \sigma_i \tag{1.8}$$

becomes non-zero and positive, becoming $\mathcal{M}_0 = 1$ in the limit $T \to 0$. The proof of the functional form of the ferromagnetic spontaneous magnetization has a long history [202, 259, 72, 184, 168, 214, 237, 3, 154, 28], and in the thermodynamic limit it is given by the following expression

$$\mathcal{M}_0 = \begin{cases} (1-k^{-2})^{1/8} & T \le T_c \\ 0 & T > T_c \end{cases} \tag{1.9}$$

For the antiferromagnetic Ising model, the spins favor anti-aligning while the magnetic field biases the spins toward either $\sigma = \pm 1$ depending on the sign of H. As $H \to 0$, the average magnetization will be go to 0 for all temperatures, and a spontaneous magnetization will not be seen. However, as $T \to 0$ the antiferromagnet will exhibit an increase in ordering corresponding to anti-aligned spins. If the lattice is bipartite, the lowest energy configuration at $T = 0$ will correspond to spins on each sub-lattice being equal and opposite the spins of the other sub-lattice. Therefore, for the antiferromagnetic Ising model on a bipartite lattice, we define the staggered spontaneous magnetization $\mathcal{M}_0^*$ as

$$\mathcal{M}_0^* = \lim_{H \to 0^+} \frac{1}{\mathcal{N}^*} \sum_i \sigma_i^* \tag{1.10}$$

where $\mathcal{N}^*$ corresponds to the number of spins σ^* on one of the sub-lattices. The staggered spontaneous magnetization for the antiferromagnetic Ising model on a square lattice in the thermodynamic limit is given by

$$\mathcal{M}_0^* = \begin{cases} (1 - k^{-2})^{1/8} & T \leq T_c \\ 0 & T > T_c \end{cases} \tag{1.11}$$

For the square lattice at $H = 0$, the critical temperature is the same for both the ferromagnetic and antiferromagnetic cases, since Equations 1.5 is invariant under the transformation $E_i \to -E_i$. Likewise, the spontaneous magnetization is the same for both cases, accounting for the staggered order. The square lattice Ising model's invariance under this transformation is not limited to the location of the critical temperature and spontaneous magnetization. The free energy is invariant as well. The underlying cause of the square lattice invariance is due to the fact that the square lattice is bipartite, that is, the lattice can be divided into two sub-lattices A and B such that each spin on one sub-lattice only interacts with spins on the other sub-lattice. Therefore, the interaction energy in Equation 1.1 can be rewritten in terms of spins distinguished by which sub-lattice they belong to,

$$\mathcal{E}_{\text{sq}} = -E_h \sum_h \sigma_i^A \sigma_j^B - E_v \sum_v \sigma_i^A \sigma_j^B - H \sum_i \sigma_i^A - H \sum_j \sigma_j^B \tag{1.12}$$

At $H = 0$, we can re-arrange the interaction energy further

$$\mathcal{E}_{\text{sq}} = E_h \sum_h \sigma_i^A (-\sigma_j^B) + E_v \sum_v \sigma_i^A (-\sigma_j^B) \tag{1.13}$$

Therefore, when $E_i \to -E_i$, the interaction energy goes to a ferromagnetic interaction energy of a model where each spin in the B lattice is defined to be the negative of its definition for the ferromagnetic case. However, since the partition function is the sum over all spin configurations, it will be invariant under the operation $\sigma_j^B \to -\sigma_j^B$, so that for the square lattice at $H = 0$, the free energy is invariant under the change from ferromagnetism to antiferromagnetism.

The triangular lattice, however, is not bipartite, and its interaction at $H = 0$ cannot be written in terms of spins on sub-lattices. Therefore, the free energy depends on the choice of sign for the E_i. For the ferromagnetic triangular Ising model, the critical temperature occurs at the solution of

$$k_{\mathrm{tr}} = 1 \tag{1.14}$$

where

$$k_{\mathrm{tr}} = \frac{(1-v_1^2)(1-v_2^2)(1-v_3^2)}{4[(1+v_1v_2v_3)(v_1+v_2v_3)(v_2+v_3v_1)(v_3+v_1v_2)]^{1/2}} \tag{1.15}$$

where $v_i = \tanh(E_i/k_BT)$. In the isotropic case, this gives

$$T_c = \frac{4E}{k_B \ln(3)} \tag{1.16}$$

The spontaneous magnetization for the ferromagnetic case has the following form [184, 103, 227]

$$\mathcal{M}_0^{\mathrm{tr}} = \begin{cases} (1-k_{\mathrm{tr}}^{-2})^{1/8} & T \leq T_c \\ 0 & T > T_c \end{cases} \tag{1.17}$$

The antiferromagnetic square Ising model has two unique ground states at $T = 0$, both of which have staggered order and which are related to each other by inversion of all spins. The triangular antiferromagnetic Ising model, however, has a countable number of ground states at $T = 0$ which are not simply related to each other under inversion of all spins [240, 86]. This countable number of ground states gives the triangular antiferromagnetic Ising model non-zero entropy at $T = 0$. Therefore, there is disorder at all temperatures, so that no phase transition occurs in the antiferromagnetic triangular Ising model at $H = 0$.

1.3 Hard Particle Lattice Gas Correspondence

Lattice gases are a discrete approximation of gases where each molecule is confined to lie on vertices of a lattice. Hard particle lattice gas models in particular are lattice gas models where the molecule is assumed to be infinitely repulsive in a small area around it, typically nearest neighbor sites, while farther away it does not interact with other molecules. We only consider the case where at most one molecule is allowed to occupy a site. Lattice gases are typically studied on regular 2D lattices, such as the triangular and square lattices, and a molecule is given an occupation number at the site of a vertex, $\sigma = 0$ if the site is vacant and $\sigma = 1$ if it is being occupied. The interaction potential energy for hard particle lattice gas models is then given by

$$U(\sigma_i, \sigma_j) = \begin{cases} \infty & \text{if } \sigma_i,\ \sigma_j \text{ are nearest neighbors} \\ 0 & \text{otherwise} \end{cases} \tag{1.18}$$

so that the grand partition function becomes

$$\Xi(z; \mathcal{N}) = \sum_{\sigma_i} z^n e^{-\beta U(\sigma_i, \sigma_j)} \tag{1.19}$$

where the sum is over all site occupancies σ_i on the lattice, where n is the total number of occupied lattice sites for a given configuration of σ's, where z is the fugacity, and where $\mathcal{N}$ is the total number of lattice sites and the thermodynamic limit corresponds to the limit $\mathcal{N} \to \infty$. From the infinite potential, the sum only counts configurations where there are no nearest neighbors.

Since the infinite repulsion precludes two hard particles from being neighbors on a lattice, the area carved out around a particle forms a shape characteristic of that lattice, a shape attributed as the shape of the molecule. On the square and triangular lattices, for example, the hard particle lattice gas models take the names hard squares and hard hexagons, respectively.

Hard squares and hard hexagons can be related to the Ising model by the following correspondence. For the isotropic Ising model in a field, we define

$$u = e^{-4J/k_BT} \tag{1.20}$$

$$x = e^{-2H/k_BT} \tag{1.21}$$

Then for hard squares we define

$$y = ux^{1/2} \tag{1.22}$$

and for hard hexagons

$$y = ux^{1/3} \tag{1.23}$$

Now in the limit $J \to -\infty$ and $H \to \infty$, so that $u \to \infty$ and $x \to 0$, while keeping y fixed ($H/J = 4$ for hard squares and $H/J = 6$ for hard hexagons), the partition function for the Ising model becomes the respective hard particle grand partition function, with the fugacity defined by

$$z = y^2 = u^2x \tag{1.24}$$

for hard squares and

$$z = y^3 = u^3x \tag{1.25}$$

for hard hexagons.

From the grand partition function, the hard particle lattice gas pressure $p(z;\mathcal{N})$ and density $\rho(z;\mathcal{N})$ can be found through the relations

$$\frac{p(z;\mathcal{N})}{k_BT} = \frac{1}{\mathcal{N}} \ln[\Xi(z;\mathcal{N})] \tag{1.26}$$

and

$$\rho(z;\mathcal{N}) = \frac{1}{\mathcal{N}} z \frac{d}{dz} \ln[\Xi(z;\mathcal{N})] = z \frac{d}{dz} \frac{p(z;\mathcal{N})}{k_BT} \tag{1.27}$$

and in the thermodynamic limit we choose the notation $p(z;\mathcal{N}) \to p(z)$ and $\rho(z;\mathcal{N}) \to \rho(z)$.

A universal feature of positive potential models, such as hard particle lattice gases, is the existence of a singularity on the negative real fugacity axis, which follows from Groeneveld's theorem on the alternation of sign of cluster integrals [104]. For the cluster expansion of the pressure $p(z)$

$$\bar{p}(z) = \frac{p(z)}{k_B T} = \sum_{n=1}^{\infty} b_n z^n \tag{1.28}$$

and density $\rho(z)$

$$\rho(z) = \sum_{n=1}^{\infty} n b_n z^n \tag{1.29}$$

where the b_n are the reduced cluster integrals, Groeneveld's theorem states that the b_n must alternate in sign. Therefore, the radius of convergence of these series will be determined by an unphysical singularity on the negative real axis at z_d. For hard hexagons, z_d has been proven to be at exactly at $z_d = (11 - 5\sqrt{5})/2$ [29, 30], while for hard squares its location has been numerically evaluated to be at $z_d = -0.11933888188(1)$ [233], where the parenthesis indicates the uncertainty in the last digit.

Expanding the pressure about z_d, we expect the following form in general

$$\bar{p}(z) = \sum_{n=0}^{\infty} c_n(z - z_d)^n + (z - z_d)^{\phi} \sum_{n=0}^{\infty} d_n(z - z_d)^n + (z - z_d)^{\phi+\theta_1} \sum_{n=0}^{\infty} e_n(z - z_d)^n + \dots \tag{1.30}$$

where ϕ is the critical exponent at z_d and θ_1 is the first correction to scaling exponent, and ϕ and θ_1 are not expected to be integers. From these definitions, the critical exponent of the density $\rho(z)$ will be $\phi - 1$. It had long been observed that many models in statistical mechanics of purely positive potentials all share the same critical exponent ϕ at their respective unphysical singularity z_d, depending only on the dimension of the lattice. For 2D lattices, it was found that $\phi \simeq 5/6$, holding exactly for the solved hard hexagon model [19, 84, 85, 147, 17]. This was finally proven to be the case, even for the more general case of repulsive-core potentials with an attractive component, in 1999 by Park and Fisher, by proving its correspondence with the Yang-Lee edge singularity [178]. For hard hexagons, the following exponents also hold: the order parameter exponent $\beta = 1/9$, the specific heat exponent $\alpha = 1/3$, and the correlation length exponent $\nu = 5/6$.

1.4 Transfer Matrices

A useful method of analyzing models in statistical mechanics is through the use of transfer matrices T [111, 142, 166, 148, 167, 145], which can be viewed as building up the lattice one row at a time. The basis of the rows and columns of the matrix correspond to the valid possible configuration states of a single row of states. Each matrix element, then, gives the contribution to the partition function from two consecutive rows corresponding to the configuration states of the matrix element's row and column. Depending on the boundary conditions of the lattice along the row, the transfer matrix may be considered to have free or cylindrical boundary conditions, T_F and T_C respectively, which can affect the number of configurational states per row and the matrix entries.

Part of the appeal of the transfer matrix method stems from the fact that the sum over configurational states in the definition of the partition function in Equation 1.3 can be performed simply through matrix multiplication of the transfer matrix with itself an appropriate number of times. Given an $L_h \times L_v$ square lattice, periodic in the L_v direction, for example, the partition function is given by the following expression

$$Z = \mathrm{Tr}\, T^{L_v}(L_h) \tag{1.31}$$

where the dependence of the transfer matrix T on L_h is explicitly shown, while for free boundary conditions in the L_v direction, appropriate boundary vectors $\mathbf{v}_B$ and $\mathbf{v}'_B$ are needed

$$Z = \langle \mathbf{v}_B | T^{L_v - 1}(L_h) | \mathbf{v}'_B \rangle \tag{1.32}$$

Twisted boundaries along the transfer direction can also be used, such as for Möbius strips and Klein bottles. The partition function can be written either using a matrix $O(L_h)$ which reflects the entries of a matrix horizontally or vertically,

$$Z = \mathrm{Tr}\, T^{L_v}(L_h) O(L_h) \tag{1.33}$$

Alternatively, the definition of the trace can be modified to sum over the anti-diagonal elements for Möbius strips and Klein bottles, or over other off-diagonals for other types of twisted boundary conditions.

As long as the transfer matrix is diagonalizable though the use of a diagonalizing matrix P, the product PP^{-1} can be inserted L_v times between each transfer matrix in the product in Equation 1.31. Then, because the trace of a matrix product is invariant with respect to cyclic permutations of the matrices in the product, the matrices P and P^{-1} can be arranged to diagonalize each T into the diagonal matrix $D = P^{-1}TP$ so that the trace of the product will equal the trace of D^{L_v}. Therefore, we can rewrite the partition function periodic in the L_v direction as a sum over powers of the transfer matrix eigenvalues λ_k,

$$Z = \mathrm{Tr}\, D^{L_v}(L_h) = \sum_k \lambda_k^{L_v}(L_h) \tag{1.34}$$

where the dependence of the eigenvalues λ_k on (L_h) is explicitly shown. For the case of free boundary conditions in the direction of transfer,

$$Z = \sum_k d_k \cdot \lambda_k^{L_v - 1}(L_h) \tag{1.35}$$

where

$$d_k = (\mathbf{v}_B \cdot \mathbf{v}_k)(\mathbf{v}_k \cdot \mathbf{v}'_B) \tag{1.36}$$

and where the $\mathbf{v}_k$ are the eigenvectors of the transfer matrix.

Twisted boundary conditions also can be written in terms of the eigenvalues of the transfer matrix. Every matrix satisfies its own characteristic polynomial p(x), by direct substitution of the matrix for the variable $x \to T(L_h)$. This gives a homogeneous linear recurrence relation for the transfer matrix for consecutive powers of the matrix, a recurrence relation of the order of the matrix. Therefore, the partition function for a given L_h but increasing L_v can be determined through the recurrence relation as a function of L_v. Every entry in the matrix will separately satisfy the linear recurrence relation, and therefore any linear function of the transfer matrix elements which is independent of L_v will also satisfy the recurrence relation. Since the trace in Equation 1.31, the dot product in Equation 1.32, and modified traces to account for twists are all linear functions of the elements of the transfer matrix independent of L_v, the partition functions for all these different boundary conditions along the transfer direction all satisfy the same linear recurrence relation. The general solution of a linear recurrence relation is the linear combination of the solutions of the characteristic polynomial,

$$Z = \sum_k c_k(L_H)\lambda_k^{L_v}(L_h) \tag{1.37}$$

where the c_k depend on the boundary conditions and can be determined by the initial conditions of the recurrence relation, that is the values of the partition function $Z(L_h)$ for different values of L_v. Once the eigenvalues λ_k and the c_k are determined, the partition function for other values of L_v can easily be computed. For periodic boundary conditions along the transfer direction, all the $c_k = 1$, and for free boundary conditions, the c_k are as given in Equation 1.35 in terms of the boundary vectors. For twisted boundary conditions along the transfer direction, the c_k can be determined through the initial conditions.

When the transfer matrix is invariant under a symmetry operation, its characteristic polynomial will factor into sectors. For example, for cylindrical boundary conditions, we can construct a set corresponding to a particular configuration of spins and those other configurations formed by rotating that configuration around the cylinder. The transfer matrix will be invariant under the transposition of rows and columns corresponding to rotating around the cylinder this constructed set of states. For each such a set of states, the transfer matrix will be invariant under transposition of rows and columns corresponding to its rotation. The symmetry in this case corresponds to the conservation of linear momentum, and it is possible to choose a linear momentum basis for the matrix. This new basis can be organized in terms of those states which transform into themselves after 1, 2, ... rotations around the cylinder, corresponding to a momentum of 0, 1, ... In this case, the characteristic polynomial will factor into sectors corresponding to particular momenta. For other or additional symmetries, the transfer matrix characteristic polynomial will further factor. The free boundary condition transfer matrix, for which momentum isn't conserved, still conserves parity and its characteristic polynomial factors into two sectors, corresponding to configurations of positive and negative parity.

When free boundary conditions along the direction of transfer are considered, so that boundary vectors are used in Equation 1.35, the ($\mathbf{v}_B$ and ($\mathbf{v}'_B$ will have positive parity, and in the case of cylindrical boundary condition transfer matrices, they will also have momentum zero. Therefore, their dot-product with the transfer matrix eigenvalues will only be non-zero whenever the eigenvalues of the transfer matrix have positive parity, as well as momentum zero for cylindrical transfer matrices. The partition function for free boundary conditions along the direction of transfer will then depend only on the eigenvalues corresponding to the reduced sector, and therefore the linear recursion relation satisfied by the partition function will be of a smaller order given by the order of the sector.

The main appeal of the transfer matrix method can be seen in taking the limit $L_v \to \infty$. When the temperature is positive, the transfer matrix will have only positive terms, so that from the Perron-Frobenius theorem [181, 95, 96, 174] it is guaranteed that the largest eigenvalue will be positive and non-degenerate. If we order the transfer matrix eigenvalues so that λ_0 is the largest magnitude eigenvalue, then we can rewrite Equation 1.34 for periodic boundary conditions along the transfer direction in the following manner

$$Z = \lambda_0^{L_v}(L_h)\left[1 + (\lambda_1(L_h)/\lambda_0(L_h))^{L_v} + \ldots\right] \tag{1.38}$$

Then, in the limit $L_v \to \infty$ when the temperature is positive, all terms except the first one go to zero so that

$$f = -\lim_{\mathcal{N}\to\infty} \frac{k_B T}{\mathcal{N}} \ln(Z) \approx -\lim_{\mathcal{N}\to\infty} \frac{k_B T L_v}{\mathcal{N}} \ln(\lambda_0(L_h)) \tag{1.39}$$

For the square lattice, the total number of sites is given by $\mathcal{N} = L_h L_v$, so that there will remain a factor of L_h in the denominator in Equation 1.39 above. As the size of the transfer matrix is increased for larger and larger rows so that $L_h \to \infty$, the free energy will be given exactly by

$$f = -k_B T \ln\left(\lambda_0^{(\infty)}\right) \tag{1.40}$$

where $\lambda_0^{(\infty)}$ is the largest eigenvalue of the transfer matrix in the limit $L_h \to \infty$. In order for a thermodynamic limit to exist, the free energy must independent of boundary conditions, so that for positive temperatures, $\lambda_0^{(\infty)}$ of the cylindrical transfer matrix T_C will be dominant and equal to the corresponding $\lambda_0^{(\infty)}$ of the free transfer matrix T_F. Another consequence is that $c_0 \neq 0$ in Equation 1.37 for any boundary conditions along the transfer direction for both T_C and T_F.

For non-positive temperatures, including complex temperatures, a consequence of a theorem by Beraha, Kahane, and Weiss [34, 35, 33, 32][1] is that for finite L_h, for all boundary conditions whose partition functions have the same linear recurrence relation, one (or more) same eigenvalue(s) at T will be dominant (or equimodular) for all boundary conditions along the transfer direction, except possibly at isolated points, as long as no two eigenvalues have the same modulus everywhere in the complex temperature plane. Therefore, for finite L_h, it is generally sufficient to consider only one boundary condition from all partition functions derived from the same sectors of the characteristic polynomial, since at most isolated points will have a boundary condition dependence. In the thermodynamic limit, however, where

[1]Sokal has generalized the theorem [226, 210] so that the $\lambda_k(L_h)$ are algebraic functions that need not be from the same characteristic equation; this extension is irrelevant for partition functions defined through transfer matrices.

$L_h \to \infty$, no theorem exists to guarantee boundary condition independence at non-positive temperatures of the free energy. Therefore, is it also not guaranteed that the limiting dominant eigenvalue for T_C at a non-positive temperature be equal to the limiting dominant eigenvalue of T_F at that temperature.

For one dimensional models, the transfer matrix is generally the simplest approach to solving a model, since there is no L_h dependence to the largest eigenvalue; diagonalization of a single transfer matrix is sufficient to solve the model. However, 1D models with short-range interactions do not exhibit a continuous phase transition [116, 195, 88]. For two dimensional models which can have phase transitions, however, the dependence of the largest eigenvalue on L_h means that a knowledge of how to diagonalize the transfer matrix for each L_h is necessary before being able to take the limit $L_h \to \infty$. It was through exactly such a determination of the largest eigenvalue of the cylindrical transfer matrix for each L_h, using periodic boundary conditions in the direction of transfer, that Onsager first solved the free energy of the 2D Ising model in 1944 [176].

1.5 Zeros and Equimodular Curves

Another approach to study models in statistical mechanics, initiated by Lee and Yang in 1952 [151], is to study the roots of the finite partition function of the model. Lee and Yang originally considered magnetic field zeros; this was generalized by Fisher [92] and others [2, 138, 175] to temperature zeros. For the isotropic Ising model at $H = 0$ or the hard particle lattice gases on a finite sized lattice, the variables u or z defined above, respectively, cast the partition function into the form of a polynomial, which can be written in the following form

$$Z = \prod_i (1 - t/t_i) \tag{1.41}$$

where $t = u$ or $t = z$ and t_i is a root of the polynomial. Therefore, the partition function is completely specified by its roots. In the thermodynamic limit, the free energy can be written, up to an additive constant, in terms of the density $g(x, y)$ of the limiting positions of the partition function roots $z_i = x + iy$ as

$$f = -k_B T \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x, y) \ln(z - x - iy) dx dy \tag{1.42}$$

where the density $g(x, y)$ is defined as the limit $\mathcal{N} \to \infty$ and $dx, dy \to 0$ of the number $\mathcal{N} g(x, y) dx dy$ of partition function roots in the area $x \pm dx + i(y \pm dy)$.

As long as the lattice is finite, so that the partition function is a polynomial, there cannot be a root on the positive real temperature or fugacity axis, since by definition the partition function is a sum of positive terms. Therefore, the complex roots of the partition function can only approach the positive real axis for a finite lattice. However, in the thermodynamic limit, the roots may converge to the positive real axis, at a location corresponding to the critical temperature T_c or critical fugacity z_c. In principle the approach of the roots to the positive real axis could be used to estimate the critical location for unsolved models, although in practice the approach is slow enough to be impracticable.

For the anisotropic square lattice Ising model at $H = 0$, the temperature roots accumulate in the thermodynamic limit to areas [230] given by the solution of the following equation

$$\cosh(2J_1/K_BT)\cosh(2J_2/K_BT) - \sinh(2J_1/K_BT)\cos(\theta_1) - \sinh(2J_2/k_BT)\cos(\theta_2) \quad (1.43)$$

In the isotropic case, the square lattice temperature roots lie on the circle given by

$$|\sinh(2J/K_BT)|^2 = 1 \quad (1.44)$$

Lu and Wu [155] have determined the density of roots along the circle to be

$$\frac{|\sin\theta|}{\pi^2}K(\sin\theta) \quad (1.45)$$

where θ is defined by $\sinh(2J/K_Bt) = \exp(i\theta)$ and where K is the complete elliptic integral of the first kind.

For the anisotropic triangular lattice at $H = 0$ the roots accumulate to areas [230] corresponding to the solution of the following equation

$$\begin{aligned}&\cosh(2J_1/K_BT)\cosh(2J_2/K_BT)\cosh(2J_3/k_BT)\\&\quad+\sinh(2J_1/K_BT)\sinh(2J_2/K_BT)\sinh(2J_3/k_BT)\\&\quad-\sinh(2J_1/K_BT)\cos(\theta_1)-\sinh(2J_2/K_BT)\cos(\theta_2)\\&\quad-\sinh(2J_3/K_BT)\cos(\theta_1+\theta_2)\end{aligned} \quad (1.46)$$

In the isotropic case, the triagular lattice roots lie on two curves, the circle given by

$$w = \sinh(2J/k_BT)[\sinh(2J/k_BT) + \cosh(2J/k_BT)] = 1 \quad (1.47)$$

and the interval on the negative w real axis

$$\mathrm{Re}(w) = (-2, -1/2) \quad (1.48)$$

Lu and Wu [155] give the density on the circle as

$$\frac{|\sin\theta|}{\pi^2\sqrt{A(\theta)}}K(k) \quad (1.49)$$

where θ is defined from $w = \exp(i\theta)$, $A(\theta) = \sqrt{5 + 4\cos\theta}$, and where

$$k^2 = \frac{1}{16}\left[\frac{3}{A(\theta)} - 1\right][1 + A(\theta)]^3 \quad (1.50)$$

while the density on the line segment is given by

$$\frac{|\sinh\lambda|}{\pi^2 k\sqrt{B(\lambda)}}K(k^{-1}) \tag{1.51}$$

where λ is defined from $w = -\exp(\lambda)$, $B(\lambda) = \sqrt{5 - 4\cosh(\lambda)}$, and where

$$k^2 = \frac{1}{16}\left[\frac{3}{B(\theta)} - 1\right][1 + B(\theta)]^3 \tag{1.52}$$

It is not necessary that the interaction energies be anisotropic for roots to lie in areas. Matveev and Shrock were the first to show that even an integrable model with isotropic couplings can have roots which lie in areas [159].

For general ferromagnetic Ising models in a field $H \neq 0$, Lee and Yang proved that the magnetic field zeros x lie on the imaginary H axis for real temperatures T or on the circle $|e^{2H}| = 1$. Alternatively, by recasting the Ising model in a field into a lattice gas model, where the free energy f is proportional to the pressure p and the magnetization M is proportional to the density ρ, they proved that the roots of the grand partition function as a function of fugacity lie on a circle. For $T \leq T_C$, the roots form a full circle, but for $T > T_c$ a gap will open up in the circle around z_c, or alternatively, around the origin in the imaginary H axis, forming two endpoints called the Yang-Lee edge. It was also shown by Kortman and Griffiths [141] that the density of zeros at the Yang-Lee edge diverges in the thermodynamic limit, depending on the dimensionality. Calling the density of roots on the imaginary H axis $g(h)$ with edges at $h = \pm i h_0$, the density will diverge as

$$g(h) = [|h| - h_0(T)]^{\sigma} \tag{1.53}$$

where $g(h)$ is defined so that the number of roots h_i between ih and $i(h + dh)$ is $\mathcal{N}g(h)dh$. The free energy in the thermodynamic limit can then be written as

$$f = k_B T \int_{-\infty}^{\infty} g(h_i)\ln(h - ih_i)dh_i \tag{1.54}$$

The roots of the partition function can be viewed as branch cuts of the free energy, with branch points at $h = \pm i h_0$. Near the branch points, the free energy will then behave as

$$f \propto [|h| - h_0(T)]^{\sigma+1} \tag{1.55}$$

The Yang-Lee exponent σ was only known exactly in 1D and in the limit $d \to \infty$ as $\sigma = -1/2, 1/2$, respectively [151, 141]. In the limit $T \to \infty$ of Ising ferromagnets in a field in arbitrary dimension, Kurtze and Fisher proved [146] that the Yang-Lee edge singularity corresponds to the singularity on the negative real axis of a fluid of hard dimers on the same lattice, giving a relationship between the Yang-Lee edge singularity and the negative real fugacity axis singularities of this repulsive-core model. Poland noticed that the critical exponents of the negative fugacity singularities of a wide variety of repulsive-core models appeared to be universal, depending only dimensionality [183]. In 1999 Park and Fisher proved that indeed the negative real fugacity singularities for repuslive-core models all belong to the Yang-Lee edge universality class [178]. In fluid language, the free energy f is recast in terms of the pressure p of the fluid, so that the critical exponent ϕ of the pressure p or density ρ on the negative fugacity axis corresponds to the Yang-Lee quantity $\sigma + 1$. Finally, knowing the exactly solved hard hexagon model critical exponent $\phi = 5/6$ yields a Yang-Lee edge critical exponent in $d = 2$ of $\sigma = -1/6$. Furthermore, the exponent of $\sigma = -1/6$ will therefore also corresponds to the divergence of the density of the fugacity roots of any repulsive-core model at z_d, including hard squares.

Yang and Lee's circle theorem gives precise information on the location of the complex fugacity roots of fluids, a circle; however, it only applies to fluids that correspond to ferromagnetic Ising models in a field. There are several results which are less restrictive and also apply to antiferromagnetic potentials. For 1D hard particle lattice gases, Penrose and Elvey have proven that the thermodynamic limit distribution of zeros of the grand partition function lie on simply connected arcs [180]. In 2D, exact and numerical results show that partition function roots can accumulate to discrete points, curves, or else occupy areas as the size of the lattice increases, for example [208, 230, 247, 228, 229, 159, 211]. For models of dimension ≥ 2, using Pirogov-Sinai theory [182] Biskup et al have proven [38] that a large class of models which depend on one complex variable have zeros which lie on at most a countable number of simple smooth curves which begin and end at multiple points, points where multiple curves depart from, the number of multiple points in any compact set of the complex plane is finite, and they characterize the nature of the degeneracies of the roots. They also consider the case of their class of models depending on multiple complex variables [39]. In general, however, there is no single theory able to classify the nature and location of the roots of a generic model in statistical mechanics, and no result is known concerning the roots of the hard hexagon and hard square grand partition functions in the thermodynamic limit.

By way of contrast, rather than try to locate and characterize the locus of roots of a model, a theorem by Ruelle allows the rigorous exclusion of regions of the complex plane from having zeros in the thermodynamic limit [196, 197, 198]. Ruelle's theorem has been applied to hard squares [117, 201] and hard hexagons [149, 150]; however, the regions of exclusion near the origin in these two cases did not yield any new information than could already be obtained numerically.

The locations of the roots of the partition function can be at least partially understood in terms of the eigenvalues of the transfer matrix with appropriate boundary conditions. When the temperature u or fugacity z is negative or complex, the Perron-Frobenius theorem ceases to apply, and it cannot be guaranteed that the largest magnitude eigenvalue of the transfer matrix is either unique or positive. In fact, away from the positive real axis, the eigenvalue which was largest on the positive real axis may be superseded in magnitude by other eigenvalues. The locations where such a transition occurs, that is, the locations where two or more eigenvalues have equal modulus in the complex u or z plane, are called equimodular curves. In general, the physical eigenvalue which is maximum on the positive real axis will not be the maximal eigenvalue throughout the whole complex plane. Along an equimodular curve, the phase difference between the largest eigenvalues changes, and since the partition function is the sum of eigenvalues in Equation 1.34, the partition function will have at least one minima along the equimodular curve. Since the largest eigenvalues form the largest contribution to the magnitude of the partition function, the partition function will have zeros close to where the largest eigenvalues have equal magnitude and opposite phase, that is, near the equimodular curves of the transfer matrix. For finite L_h, the theorem by Beraha, Kahane, and Weiss [34, 35, 33, 32] [2] states that the limiting zeros for $L_v \to \infty$ of all partition function which obey a given linear recurrence relation converge either to isolated points, which depend on boundary conditions along the direction of transfer, or else to the equimodular curves, which are independent of boundary conditions, as long as no two eigenvalues have equal modulus everywhere in the complex plane. In particular, for the $T_F(L_h)$ transfer matrix, the roots of the partition functions of cylindrical (periodic along the L_v direction) and Möbius (twist in the L_v direction) boundary conditions for finite L_h will converge to the same equimodular curves as $L_v \to \infty$, and similarly for toroidal and Klein bottle boundary conditions for the $T_C(L_h)$ transfer matrix. The theorem is silent, though, concerning how the partition functions zeros for free-free boundary conditions relate to cylindrical (free along the L_v direction) boundary conditions, how these relate to cylindrical/Möbius boundary conditions and how any of these relate to toroidal/Klein bottle boundary conditions. Furthermore, their theorem does not apply to the thermodynamic limit where both $L_h, L_v \to \infty$; in particular, it does not guarantee that equimodular curves of T_C converge to those of T_F in the thermodynamic limit.

Since the partition function roots converge to the critical point on the positive temperature or fugacity axis in the thermodynamic limit, there will be (at least) one equimodular curve for both cylindrical and free transfer matrices T_C and T_F, respectively, that crosses the positive real axis in the thermodynamic limit at the location T_c or z_c. This (these) curve(s) will separate two different maximum eigenvalues on the positive real axis by definition, one above and one below the critical point, and the critical point will be a singularity for both eigenvalues. These two physical eigenvalues do not need to be related to each other analytically; from the exact solution of hard hexagons, for example, it is known that the two eigenvalues on either side of z_c (to be precise, the limit $L_v, L_h \to \infty$ of $\lambda_0^{1/L_v L_h}(L_h)$ for both $\lambda_0(L_h)$) satisfy different algebraic equations [133].

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[2]See footnote on page 11. Also, Wood appears to have independently thought of using equimodular curves to study limiting locations of partition function zeros [246, 248, 250]. See also [218]. Earlier than all of these, in 1967 Nilsen and Hemmer [173] presented a method for finding limiting grand partition function zeros in terms of equimodular poles of the grand pressure function, in the context of hard squares.

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Chapter 2

Summary of New Results

2.1 Paper 1: Ising Model Diagonal Form Factors

The Ising model two-point correlation functions $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ are defined by

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle = \frac{1}{Z}\sum_{\sigma}\sigma_{0,0}\sigma_{M,N}e^{-\mathcal{E}/k_B T} \tag{2.1}$$

where $\sigma_{0,0}$ is chosen because in the thermodynamic limit the correlations will be independent of location in the bulk; only relative locations between two spins matter.

The Ising model correlations have a long history, which began when Kaufman and Onsager computed the row correlation function ($M = 0$ above) in 1949 as a Toeplitz matrix [140]. A major development happened in 1963 when Montroll, Potts, and Ward [168] used the Pfaffian method to give the general correlations $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ in the thermodynamic limit as determinants of the size the length of the path chosen between $\sigma_{0,0}$ and $\sigma_{M,N}$. Their method would give the row correlations as an $N \times N$ determinant while for the diagonal correlations a $2N \times 2N$ determinant. The next year, however, Stephenson used their method on the triangular lattice, and specializing to the square lattice by taking the diagonal interaction energy to zero, the diagonal correlation was given a $N \times N$ Toeplitz determinantal form [227].

In 1984 and the next year, Ghosh and Shrock gave examples up to $N = 6$ of the correlations written in terms of the complete elliptic integrals of the first and second kind for the anisotropic case along the diagonal [99], and for the isotropic case for row [100] and off-diagonal [219] correlations.

The reduction of correlations to elliptic integrals of the first and second kind, $K(k)$ and $E(k)$, respectively, follows from writing the coefficients in the Toeplitz determinant as hypergeometric functions, taking the determinant, and then using contiguous relations to write the hypergeometric functions in terms of the basis of $K(k)$ and $E(k)$. The Toeplitz matrix entries can all be written in terms of hypergeometric functions of the form $F(\pm 1/2, n \pm 1/2; n+1; t)$, where

$$t = \begin{cases} k^2, & T < T_c \\ k^{-2}, & T > T_c \end{cases} \tag{2.2}$$

and where k is defined in Equation 1.6. These can then be related to the complete elliptic integrals by the following correspondence

$$K(t^{1/2}) = \frac{\pi}{2}F(1/2, 1/2; 1; t) \tag{2.3}$$

$$E(t^{1/2}) = \frac{\pi}{2}F(-1/2, 1/2; 1; t) \tag{2.4}$$

When M, N are large, finding the determinants of the Toeplitz matrices for the correlations $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ is not an efficient method of computation. As $M, N \to \infty$, the correlations become the spontaneous magnetization $\mathcal{M}_0$,

$$\lim_{M,N\to\infty}\langle\sigma_{0,0}\sigma_{M,N}\rangle = \mathcal{M}_0 \tag{2.5}$$

where for $T < T_c$, $\mathcal{M}_0 = (1-t)^{1/4}$, and so we can seek an expansion for the correlation functions around $M, N \to \infty$ whose first term is exactly $\mathcal{M}_0$, and further terms are corrections of order M, N. That is, for $T < T_c$

$$\langle \sigma_{0,0}\sigma_{M,N} \rangle = (1-t)^{1/4} \left\{ 1 + \sum_{n=1}^{\infty} f_{M,N}^{(2n)} \right\}, \tag{2.6}$$

and for $T > T_c$

$$\langle \sigma_{0,0}\sigma_{M,N} \rangle = (1-t)^{1/4} \sum_{n=0}^{\infty} f_{M,N}^{(2n+1)}, \tag{2.7}$$

This is the form factor expansion of the correlation functions, where $f_{M,N}^{(n)}$ are sums in the finite lattice or n-fold integrals in the thermodynamic limit. When $M = 0$ or N the expansion is called the row or diagonal form factor expansion, respectively.

The process of deriving the form factor expansion was started in 1966 in [253] for row correlations, in [81] for general correlations, and in [162, 163] for diagonal correlations. The method of [253] was carried out to all orders in [254] in the form of an exponential expansion in the thermodynamic limit,

$$\langle \sigma_{0,0}\sigma_{M,N} \rangle = (1-t)^{1/4} \exp\left(\sum_{n=1}^{\infty} F_{M,N}^{2n} \right) \tag{2.8}$$

for $T < T_c$, and for $T > T_c$

$$\langle \sigma_{0,0}\sigma_{M,N} \rangle = (1-t)^{1/4} \sum_{m=0}^{\infty} G_{M,N}^{2n+1} \exp\left(\sum_{n=1}^{\infty} \tilde{F}_{M,N}^{2n} \right) \tag{2.9}$$

where the $F_{M,N}^{2n}$, $\tilde{F}_{M,N}^{2n}$ are $2n$-fold integrals, and the $G_{M,N}^{2n+1}$ are $(2n+1)$-fold integrals. From this exponential expansion, the first few terms of the form factor expansion were given.

The exponential terms were expanded to all orders in 2007 to give the form factor expansion [156, 54], for the row and diagonal form factors, and derived independently for the row form factors in [62, 63].

The first leading term for $T > T_c$ was found in [254] to be written in terms of hypergeometric functions contiguous to the complete elliptic integrals of the first and second kinds as

$$f_{N,N}^{(1)}(t) = \lambda_N t^{N/2} F_N \tag{2.10}$$

where

$$\lambda_N = \frac{(1/2)_N}{N!} \tag{2.11}$$

$$F_N(t) = {}_2F_1(1/2, N+1/2; N+1; t) \tag{2.12}$$

and $(a)_n = a(a+1)\cdots(a+n-1)$ is the Pochhammer symbol. As an example, $f_{0,0}^{(1)} =$

$\frac{2}{\pi}K(t^{1/2}) = F_0$. The relation of the one dimensional integral to hypergeometric functions follows directly from the integral form of the hypergeometric function

$$ {}_2F_1(a,b;c;t) = \int_0^1 x^{b-1}(1-x)^{c-b-1}(1-tx)^{-a}dx \tag{2.13}$$

However, it is not obvious that in general the n-fold integrals appearing in the full expansion factor into products of one dimensional integrals related to hypergeometric functions. In 2007 in [54] it was found by means of large series expansions in Maple examples for n as high as 9 and N as high as 4 that the diagonal form factors could all be written as sums of products of the complete elliptic integrals of the first and second kinds. However, no analytic proof was found for these examples.

2.1.1 New Results

In [12] we present a new method for exactly factoring the n-fold diagonal form factor integrals into sums and products of one-dimensional integrals. We find that all the n-fold integrals can be written as sums of products of hypergeometric functions of the form ${}_2F_1(1/2, N+1/2; N+1; t)$ which occurs in $f^{(1)}_{N,N}$ and which are contiguous to the complete elliptic integrals of the first and second kinds. In particular, we prove results for $n = 2,\ 3$ give a result for $n = 4$, valid for all N, and conjecture the general form of the result for arbitrary n.

The exact results, together with the conversion of the examples up to $n = 5$ of [54] to the contiguous basis $F_N,\ F_{N+1}$ lead us to the following conjecture on the structure of the diagonal form factors

$$\begin{aligned} f^{(2n)}_{N,N}(t) &= \sum_{m=0}^{n-1} c^{(2n)}_m f^{(2m)}_{m,m}(t) + \sum_{m=0}^{2n} C^{2n}_m(N;t) F_N^{2n-m} F_{N+1}^m && (2.14)\\ t^{-N/2} f^{(2n+1)}_{N,N}(t) &= t^{-N/2} \sum_{m=0}^{n-1} c^{(2n+1)}_m f^{(2m+1)}_{m,m}(t) + \sum_{m=0}^{2n+1} C^{2n+1}_m(N;t) F_N^{2n+1-m} F_{N+1}^m && (2.15)\end{aligned}$$

where the $c^{(n)}_m$ are constants, and the $C^{(n)}_m$ are polynomials with the following palindromic structure

$$\begin{aligned} C^{(2n)}(N;t) &= t^{n(2N+1)+m}\, C^{(2n)}_m(N;1/t) && (2.16)\\ C^{(2n+1)}(N;t) &= t^{n(2N+1)+m}\, C^{(2n+1)}_m(N;1/t) && (2.17)\end{aligned}$$

and where the degrees of the polynomials are given by

$$\deg C^{2n}_m(N;t) = \deg C^{2n+1}_m(N;t) = n(2N+1) \tag{2.18}$$

While the method presented in [12] is very general and applies to all orders of the diagonal form factor expansion, the procedure becomes very cumbersome beyond $n = 4$.

2.2 Paper 2: Ising Model Diagonal Susceptibility

One of the main unresolved portions of the 2D Ising model is the magnetic susceptibility χ, defined as follows

$$\chi = -\beta \frac{\partial^2 f(H,T)}{\partial H^2}\bigg|_{H=0} = \beta \sum_{M=-\infty}^{\infty} \sum_{N=-\infty}^{\infty} \left[\langle \sigma_{0,0}\sigma_{M,N}\rangle - \mathcal{M}^2\right], \tag{2.19}$$

One method to analyze the magnetic susceptibility is to use the form factor expansion of the correlations in this double sum formula. Then, the double sums over M, N can be summed under the integral sign, to produce a high or low temperature series expansion for the susceptibility. For $T < T_c$

$$\chi = \beta(1-t)^{1/4} \sum_{n=1}^{\infty} \hat{\chi}^{(2n)} \tag{2.20}$$

and for $T > T_c$

$$\chi = \beta(1-t)^{1/4} \sum_{n=0}^{\infty} \hat{\chi}^{(2n+1)} \tag{2.21}$$

where $\hat{\chi}^{(n)}$ is an n-fold integral defined by

$$\hat{\chi}^{(n)} = \sum_{M=-\infty}^{\infty} \sum_{N=-\infty}^{\infty} f_{M,N}^{(n)} \tag{2.22}$$

Some work has been done to study the behavior of the general $\hat{\chi}^n$ for particular values of n [263, 266, 264, 265, 47]. However, a simpler problem is to only sum over the diagonal correlation functions [57], which can be interpreted physically as having the magnetic field only interact with the spins lying along the diagonal in the bulk.

$$k_B T \chi_d(t) = \sum_{N=-\infty}^{\infty} \left[\langle \sigma_{0,0}\sigma_{N,N}\rangle - \mathcal{M}^2\right], \tag{2.23}$$

Again, the sum over N can be performed under the integral sign in the form factor expansion to yield the diagonal susceptibility expansions

$$k_B T \chi_d(t) = (1-t)^{1/4} \left(1 + \sum_{n=1}^{\infty} \tilde{\chi}_d^{(2n)}(t)\right), \tag{2.24}$$

for $T < T_c$ and

$$k_B T \chi_d(t) = (1-t)^{1/4} \sum_{n=0}^{\infty} \tilde{\chi}_d^{(2n+1)}(t), \tag{2.25}$$

for $T > T_c$. The first integrals of the high and low temperature diagonal susceptibility expansion were exactly solved in [57] as

$$\tilde{\chi}_d^{(1)}(x) = \frac{1}{1-x} \tag{2.26}$$

$$\tilde{\chi}_d^{(2)}(t) = \frac{t}{4(1-t)} \tag{2.27}$$

where for odd n the variable $x = t^{1/2} = k^{-1}$ is used rather than t.

While these leading term results appear simple, the next leading terms $\tilde{\chi}_d^{(3)}(x)$ and $\tilde{\chi}_d^{(4)}(t)$ are much more involved. In [57] they were found to be solutions of linear differential equations of orders 6 and 8, respectively, both of which factor into a direct sum of three linear differential operators. In each case, the solution of the smallest direct sum factor was found to be the previous term in the susceptibility series, $\tilde{\chi}_d^{(1)}(x)$ and $\tilde{\chi}_d^{(2)}(t)$, respectively, and it has been conjectured [] that the previous term $\tilde{\chi}_d^{(n-2)}(t)$ is always in the linear combination of the solution of the term $\tilde{\chi}_d^{(n)}(t)$. Of the remaining two direct sum factors in each case, the second largest order factors were solved in terms of hypergeometric functions contiguous to the elliptic integrals of the first and second kind. However, the largest order factors in each case were left unsolved in [57].

In [47], the largest factor in the direct sum of $\tilde{\chi}_d^{(3)}(x)$ was finally solved for in terms of a ${}_3F_2$ hypergeometric function, although the linear combination of the three solutions which gives $\tilde{\chi}_d^{(3)}(x)$ was not given, nor was the singularity structure of $\tilde{\chi}_d^{(3)}(x)$ determined.

2.2.1 New Results

In [9] we completed the study of $\tilde{\chi}_d^{(3)}(x)$ and $\tilde{\chi}_d^{(4)}(t)$ by solving the remaining largest factor in the direct sum decomposition of the linear ODE for $\tilde{\chi}_d^{(4)}(x)$ and giving the linear combinations of the three solutions which produce $\tilde{\chi}_d^{(3)}(x)$ and $\tilde{\chi}_d^{(4)}(x)$. We also analytically compute the full singularity structure at all of the finite singular points of $\tilde{\chi}_d^{(3)}(x)$ and $\tilde{\chi}_d^{(4)}(t)$ by solving the connection problems.

Through the use of a pullback in the argument of the hypergeometric function we were able to write the ${}_3F_2$ hypergeometric function of the largest factor of $\tilde{\chi}_d^{(3)}(x)$ in terms of sums and products of ${}_2F_1$ hypergeometric functions contiguous to the elliptic integrals of the first and second kind. However, the third factor in the direct sum of the linear ODE for $\tilde{\chi}_d^{(4)}(t)$ gives rise to a solution which is a solution of a Calabi-Yau ODE. We have been able to express this solution in terms of a linear differential operator of order 3 acting upon a ${}_4F_3$ hypergeometric function. We were unable, however, to reduce the solution to sums and products of ${}_2F_1$ hypergeometric functions contiguous to the elliptic integrals of the first and second kind. It appears that the Ising susceptibility has a more complex analytic structure compared to the Ising model form factors, which appear to all be given in terms of elliptic integrals of the first and second kinds.

We also considered the diagonal susceptibility term $\tilde{\chi}_d^{(5)}(x)$, first considered in [57]. We were unable to perform a full direct sum decomposition of the linear differential operator due to memory constraints, although we were able to solve some of its factors in terms of ${}_2F_1$ hypergeometric functions contiguous to the elliptic integrals of the first and second kind. As was seen in $\tilde{\chi}_d^{(3)}(x)$ and $\tilde{\chi}_d^{(4)}(x)$ already, we determined that the previous diagonal susceptibility term $\tilde{\chi}_d^{(3)}(x)$ is in the linear combination of the solution of $\tilde{\chi}_d^{(5)}(x)$.

2.3 Paper 3: Hard Hexagons

Hard hexagons was first studied approximately through series expansions, starting in 1966 [200], where an approximation for z_c was found, and in [97], where an approximation for z_d was found. The free energy of the hard hexagon model was exactly solved by Baxter [29, 30] in the thermodynamic limit on the positive real fugacity axis using corner transfer matrices rather than the transfer matrices defined above. Baxter found that the hard hexagon model exhibits a continuous phase transition at the fugacity point $z_c = (11+5\sqrt{5})/2$, and he identified a low density and a high density partition function per site, κ_- and κ_+, respectively, valid below and above z_c. The $\kappa_\pm$ are defined as

$$\kappa_\pm = \lim_{L_v, L_h \to \infty} Z^{1/L_v L_h} \tag{2.28}$$

Baxter gave the partition functions per site as infinite products in terms of an auxiliary variable x, and he also gave the fugacity z as an infinite product in terms of the same x. These infinite products can be written in terms of theta functions [13, 19] and Joyce found that the auxiliary variable x can be eliminated in order to give $\kappa_\pm$ in terms of z [133]. Joyce found, in fact, that $\kappa_\pm$ are algebraic functions, which are singular at z_c, as well as at the unphysical singularity $z_d = (11 - 5\sqrt{5})/2$.

For κ_+, Joyce showed that it satisfies an algebraic equation of order 24 in κ_+ and order 22 in z. He also showed that κ_- is an algebraic function, but did not give the algebraic equation. Joyce also derived algebraic equations for the mean density in the high and low density regime, $\rho_\pm = -z\frac{d\kappa_\pm}{dz}$ [133]. The algebraic equation for ρ_+ is of order 4 in ρ_+ and order 2 in z, while the algebraic equation for ρ_- is of order 12 in ρ_- and order 4 in z.

2.3.1 New Results

For the low density regime we have found in [10] by means of a Maple series expansion computation that the low density partition function per site κ_- satisfies an algebraic equation of order 24 in κ_- and order 22 in z. We also found that the algebraic equation for the high density partition function per site given by Joyce as well as the new low density algebraic equation satisfy the following palindromic condition

$$z^{44} \cdot f_{\pm}\left(-\frac{1}{z}, \frac{\kappa_{\pm}}{z}\right) = f_{\pm}(z, \kappa_{\pm}). \tag{2.29}$$

where the $f_{\pm}$ are the algebraic equations satisfied by $\kappa_{\pm}$.

Using our new algebraic equation, we found an exact Puiseux series expansion for the mean density at the location of the unphysical singularity z_d on the negative real fugacity axis, in agreement with the exponents associated with the Yang-Lee edge, which is related by universality to hard hexagons. This series was written as the sum of six series multiplying leading exponents $-1/6$ and 0 and the corrections to scaling exponents 2/3, 3/2, 7/3, 19/6. Interestingly, the series multiplying the exponent 0 has a sign change at the 555th term.

We also study extensively the hard hexagon model on the finite $L \times L$ lattice by enumerating exactly the partition function up to $L \leq 39$ for several boundary conditions in order to locate the partition function zeros. We further calculate the transfer matrices eigenvalues for $L_h \leq 30$ in order to compute the equimodular curves for various boundary conditions.

Using both partition function zeros as well as equimodular curves we are able to explore the analytic structure of the model in the complex fugacity plane. The boundary where the high and low density partition functions per site are equimodular would correspond to the limiting location of the locus of zeros of the finite partition function in the thermodynamic limit if κ_- and κ_+ are the only two dominant eigenvalues of the transfer matrices throughout the complex plane in the thermodynamic limit. We have found, however, that there is a "necklace" of partition function zeros which accumulate in the left half-plane which do not appear to converge to the curve where κ_- and κ_+ are equimodular. Since the finite transfer matrices also give extra equimodular curves in necklace region, we conjecture that at least one new eigenvalue is dominant in the necklace region in the thermodynamic limit, and perhaps many more.

We have compared, for both partition function zeros and equimodular curves, the dependence of the curves and zeros on boundary conditions, considering both cylindrical and toroidal boundary conditions. In general, we find the zeros for different boundary conditions converging to each other, and that the equimodular curves for toroidal boundary conditions appear to be converging to the cylindrical boundary condition equimodular curves. We conjecture that the zeros and equimodular curves are converging mutually to each other, but it is still unclear at present the limiting locus of the zeros and equimodular curves in the thermodynamic limit. It is also unknown how the new eigenvalues in the necklace region may affect the analytic continuation across the zero curves, especially if the number of eigenvalues increases with increasing lattice size.

Because it is an exactly solved model, the hard hexagon model exhibits many special features which are likely not shared with non-integrable models. For example, we find that the characteristic polynomial of its transfer matrix in the translationally invariant sector factorizes and its resultant has predominantly double roots. Neither of these features are seen in other hard particle lattice gases defined on the square lattice, or other Archimedean lattices (unpublished). This has the effect that the equimodular curves do not have any gaps but are continuous.

Both the partition function roots and the equimodular curves contain a line segment on the negative real axis, whose right-most endpoint is converging towards the unphysical singularity at z_d. We have not been able to determine the limiting value of the left-most endpoint, however. At z_d we have examined for finite lattices the exponent of the divergence of the density of roots, which has the critical exponent of $-1/6$. We have found that even for $L = 39$ the divergence at z_d showed significant oscillations so that the convergence to an exponent of $-1/6$ is slow for hard hexagons. Furthermore, the $-1/6$ divergence was limited to a very small interval very close to z_d, while the density of roots in the rest of the interval on the negative real axis exhibits a different divergence exponent.

2.4 Paper 4: Hard Squares

The hard square model was first discussed in 1965 by Gaunt and Fisher as an approximation of the hard-sphere lattice gases [98], and since then it has proven an interesting unsolved model in statistical mechanics [188, 200, 173, 199, 117, 201, 26, 249, 102, 84, 246, 248, 250, 106, 179, 136, 18, 135, 105, 90, 130, 91, 131, 132, 25, 4, 70, 127, 71]. Interest in the model also stems from the correspondence that at fugacity $z = 1$, the partition function on a square lattice of size $N \times N$ is equal to the number of binary matrices of order $N \times N$, that is, square matrices whose elements are either 0 or 1 [24].

It has long been known through series expansions that the hard square model exhibits a physical phase transition on the positive real fugacity axis [98]. The best current estimation is $z_c = 3.79625517391234(4)$ [105], where the uncertainty in the last digit is indicated in the parenthesis. The value of the unphysical singularity z_d is also of interest in series expansions, since due to being closer to the origin than z_c, series expansions are dominated by effects from z_d. A precise knowledge of the location of z_d allows the use of a transformation to move the location of z_d farther away in order to give better series expansions around the physical singularity z_c. The best current estimate of z_d is $z_d = -0.11933888188(1)$ [233].

The complex fugacity zeros in the $L_v \to \infty$ limit of the grand partition function of hard squares have been located as early as 1967 by Nilsen and Hemmer [173] for $L_h = 3, 4$ and screw boundary conditions, through a method analogous to equimodular curves but for the grand pressure ensemble. They also computed the density of the roots along the curves. Using Ruelle's method, a small region of the complex plane near the origin was determined to be zero-free in the thermodynamic limit by Hubbard and Runnels in 1972 [117, 201]. Later in 1987, Wood argued that the zeros of the grand partition function should converge to the transfer matrix equimodular curves in the $L_v \to \infty$ limit and studied the equimodular curves of hard squares for $L_h \leq 6$ for toroidal boundary conditions [246, 248, 250]. Aside from numerous studies of the thermodynamic limit of the zeros z_c and z_d on the real axis, no further attempt at understanding the complex zeros was undertaken.

Recently, it was discovered by Fendley et al [90] and further investigated by Baxter [25] that the grand partition function of hard squares at the negative fugacity value of $z = -1$ depends strongly on boundary conditions, the ratio L_v/L_h, as well as the orientation of the lattice with respect to boundary conditions. Fendley et al [90] discovered that the grand partition function of hard squares with toroidal boundary conditions becomes $Z(-1) = 1$ whenever L_v and L_h are co-prime and furthermore, that all of the eigenvalues of the $T_C(L_h)$ transfer matrix at $z = -1$ are equimodular of unit modulus. They checked these results up to $L_h = 15$ and $L_v = 20$. These discoveries were subsequently proven to hold for all L_v, L_h by Jonsson in 2006 [130]. Baxter investigated other boundary conditions as well as cases where the lattice is rotated 45° with respect to the boundary conditions. Baxter found [25] that for cylindrical boundary conditions where the lattice is parallel to the boundaries, that the eigenvalues for $T_C(L_h)$ for $L_h \leq 12$ also are all of unit modulus. Jonsson noticed further [130] and subsequently proved for all L_v and odd L_h [132] that when L_h is odd, the partition function value at $z = -1$ follows one of two cases: if $\gcd(L_h - 1, L_v) = 3$ then $Z(-1) = -2$, otherwise $Z(-1) = 1$. For cylindrical boundary conditions of $T_C(L_h)$ with even L_h, Adamaszek proved [4] that $Z(-1)$ has polynomial growth in L_v and conjectured a form for the generating function of $Z(-1)$ as a funciton L_v, including a conjecture that the sequence of $Z(-1)$ as a function of L_v is only repeating for $L_h = 2 \mod 4$.

When the lattice is oriented at 45° with respect to the boundary conditions, the transfer can have eigenvalues with modulus other than unity, first noticed by Baxter [25]. For toroidal boundary conditions, Jonsson has proved [131] that if L_v, L_h are co-prime, then $Z(-1) = 2$ if $L_v L_h = 0 \mod 3$ and $Z(-1) = -1$ otherwise; also, if L_v, L_h are not co-prime but both are divisible by 3, then the $Z(-1)$ has asymptotic exponential growth in $L_v + L_h$, less than $L_v L_h$, so that the free energy is still zero in the thermodynamic limit. Jonsson further proved [131] in this case that the eigenvalues have modulus zero, unity, or else also, when $L_h = 0 \mod 3$ a modulus of the form $[4\cos^2(\pi n/L_v)]^{1/3}$. Baxter also considered cylindrical boundary conditions with the lattice oriented at 45° to the boundaries for $L_h \leq 12$. He found that for $L_h = 1 \mod 3$ that all of the eigenvalues of $T_C(L_h)$ have modulus zero so that $Z(-1) = 0$; otherwise the eigenvalues have modulus either zero or unity and he found $Z(-1) \neq 0$.

There are many remaining cases of boundary conditions, aspect ratios L_v/L_h, and orientations of the lattice for which no proven results exist. However, from the existing proofs, it appears that the free energy in the thermodynamic limit for all boundary conditions considered and where the lattice is parallel to the boundaries will have the limit $f(-1) = 0$, since the partition function is sub-exponential in $L_v L_h$ for all cases studied. When the lattice is oriented at 45° to the boundaries, the free energy in the proven cases also remains zero, but if Baxter's finding for cylindrical boundary conditions and $L_h = 1 \mod 3$ holds for all L_h, then the free energy in the thermodynamic limit can also diverge at $z = -1$. The nature of the point $z = -1$ is unclear, and it may constitute the first demonstrable point where thermodynamics, which requires boundary condition independence, does not apply. No such special point has been seen in the hard hexagon model on finite lattices, and it is not clear how universal such a feature is.

2.4.1 New Results

In [11] we perform a similar analysis for hard squares on the finite lattice as we did for hard hexagons [10], and we compare and contrast the properties of each in order to understand the relationship between integrable and non-integrable models. We also consider in detail the dependence of the partition function roots and equimodular curves on boundary conditions.

We consider the effect of boundary conditions in detail. We compute the zeros of the torus, cylinder, and plane $L \times L$ lattices. The transfer matrices can have either free or cylindrical boundary conditions for each transfer row, and considering only the largest modulus eigenvalue(s) is equivalent to a partition function infinitely long and with periodic boundary conditions along the transfer direction. The free and cylindrical transfer matrices correspond, then, to infinitely wide cylinders of finite height or infinitely wide torii partition functions. However, restricting the free transfer matrix eigenvalues to only the positive parity sector is equivalent to an infinitely long plane of finite width, while restricting the cylindrical transfer matrix eigenvalues to the zero momentum, positive parity sector 0^+ is equivalent to an infinitely long cylinder of finite radius. From the transfer matrix, we therefore have four different boundary conditions, a torus, a long tube, and wide ring, and long plane. As is expected, the roots of the torus and plane $L \times L$ partition functions lie closest to the equimodular curves of the transfer matrices corresponding to torii and planes, respectively. The roots of the $L \times L$ cylinder partition function, however, lie much closer to the transfer matrix corresponding to the wide ring, that is, periodic in the direction of transfer.

The roots and equimodular curves of hard squares exhibit much greater structure than hard hexagons. Just as was the case for hard hexagons, hard squares features a "necklace" of partition function roots and equimodular curves. However, for hard squares, the "necklace" covers a much larger area and extending farther towards z_c. It is unclear whether in the thermodynamic limit the necklace will converge to z_c or not. The hard squares equimodular curves also exhibit much greater structure. Near the special point $z = -1$, smaller and smaller loops, regions, and endpoints form with increasing transfer row size L_h. It is unclear the effect of the developing structure on the analytical behavior of the thermodynamic functions hear $z = -1$.

Roughly half of all of the partition function roots for hard squares lie along the negative real axis in the range $-1 \leq z \leq z_d$, which allows for a detailed study of their density in that range. As was the case for hard hexagons, our examination of the divergence of the density of zeros near z_d, which diverges in the thermodynamic limit with a $-1/6$ critical exponent, showed a very slow convergence to this exponent for finite lattices. Oscillations in the density were seen around z_d and the $-1/6$ power law divergence was only discernable in an interval very close to z_d, while the density in the rest of the line segment obeyed a different overall power law exponent.

As opposed to hard hexagons, the resultant of the transfer matrix characteristic polynomials have only single roots, so that along the equimodular curves there are finite sized gaps. Along the line of zeros on the negative real axis, in particular, the number of gaps increases with increasing lattice size so that a countable infinity will exist in the thermodynamic limit.

However, as the size of the transfer row L_h increases, the size of the gaps appears to decrease exponentially. From the Beraha, Kahane, Weiss theorem, the zeros of the partition function for finite L_h as $L_v \to \infty$ will converge to the equimodular curves. We prove a relation between the density of roots $D(z)$ in the limit $L_v \to \infty$ and the phase difference $\theta(z)$ of two equimodular dominant eigenvalues on equimodular curves,

$$2\pi D(z) = \frac{d\theta}{dz} \tag{2.30}$$

We define the density of roots on the square lattice as

$$D(z) = \lim_{L_v \to \infty} \frac{1}{L_v[z_{i+1} - z_i]} \tag{2.31}$$

where z_i is the i-th root from z_d, and likewise for z_{i+1}, and the z in $D(z)$ is the limit of z_i as $L_v \to \infty$.[1] Both $D(z)$ and $\theta(z)$ depend linearly on L_h. The $\theta(z)$ depends on the boundary conditions of the transfer matrix $T_C(L_h)$ or $T_F(L_h)$, and hence also the density of roots. We have noticed, however, that the two $\theta(z)$ appear to be converging to each other for increasing L_h, and the convergence is fastest closest to z_d.

The presence of gaps in the equimodular curve on the negative real axis causes singularities in the derivative of the phase difference. Therefore, according to Equation 2.30, this causes a divergence in the density of roots at the endpoints of the gap in the limit $L_v \to \infty$. However, the thermodynamic limit is the limit where both $L_v, L_h \to \infty$, and so both the gaps and the root densities need to be studied in this limit. As L_h increases, the gap lengths become exponential smaller while for a fixed value of L_v, the distances between consecutive roots of an $L_v \times L_h$ partition function only decrease linearly with L_h. While this would suggest that the gaps will not affect the root density in the thermodynamic limit, nevertheless, the zero densities for $L \times L$ partition functions exhibit what we call "glitches" along intervals centered around the locations of the gaps. For these $L \times L$ lattices, the distance between consecutive roots is orders of magnitude larger than the length of the gaps. It appears that the amplitude of the glitches may be decreasing for increasing $L \times L$ lattice sizes, but it remains unclear how or whether these singularities caused by exponentially smaller gap intervals will affect the density of roots in the thermodynamic limit or the analytic continuation of thermodynamic functions across the line segment. Importantly, for the L_h we have analyzed and for all boundary conditions, any gaps and glitches are superimposed onto a density/phase derivative which appears to be finite as $z \to -1$.

We have also seen a second source of singularities in the $L_v \to \infty$ limit of the density of partition function roots very close to the special point $z = -1$. The gaps mentioned earlier occur when two equimodular dominant eigenvalues become equal and real-valued at the endpoints of the gap. However, a complex conjugate pair of eigenvalues can be overtaken in modulus by another complex conjugate pair, causing a discontinuity in the phase derivative at that point, and therefore also a singularity in the density of roots. We've noticed these

[1]Equation 2.30 was stated without proof in [173] in a different context and proven independently in [38].

level crossing singularities only very near $z = -1$, $-1 + 10^{-5} < z < -1 + 10^{-2}$ and for $L_h > 12$. For a given L_h, there can be multiple such level crossings near $z = -1$. We do not have enough data for a conjecture but it appears that the number of such crossings may be increasing with L_h. The trend of the locations of the level crossings for increasing L_h was inconclusive. The level crossings for $T_C(L_h)$ occurred at locations different fro mthose of $T_F(L_h)$, though the $T_C(L_h)$ crossings farthest from $z = -1$ for a given L_h always occurred at a greater distance than the farthest $T_C(L_h)$ level crossings for the same L_h, and L_h which had level crossings for T_C may not have a level crossing T_F and vice-versa.

We also explore the partition function value at the special point $z = -1$ in considerable detail for lattices oriented parallel to their boundaries. It had already been discovered by Fendley et al [90] and proven for all L_h in [130] that all of the eigenvalues of the cylindrical transfer matrix $T_C(L_h)$ at $z = -1$ are of unit modulus. Its characteristic polynomial, then, factorizes into products of different roots of unity. Jonsson [130] gave a table for $L_h \leq 50$ of the factored characteristic polynomials for the full $T_C(L_h)$, and we have provided a similar table for the 0^+ sector of $T_C(L_h)$ for $L_h \leq 29$. We have looked for the first time at free transfer matrix $T_F(L_h)$ for $L_h \leq 20$ and have found the same phenomena of all eigenvalues being of unit modulus. We also tabulate the partition function values at $z = -1$ of $L_v \times L_h$ lattices for $L_v \leq 20$ and $L_v \leq 16$ on the torus, cylinder, plane, Möbius band, and Klein bottles (both with twists in the L_v direction). Since the transfer matrices satisfy linear recursion relations given by their characteristic polynomials, tabulations of values up to L_v equal to the order of the transfer matrix for a given L_h will yield a generating function for a given L_h for the partition function values at $z = -1$ as a function of L_v; we have determined generating functions for $L_h \leq 16$. We find, surprisingly, that in all cases for the torus and the cylinder, the generating functions for their sequences as a function of L_v are given by the negative of the logarithmic derivative of the characteristic polynomial of the corresponding transfer matrix. We further conjecture that along a periodic direction (including twists), all generating functions are repeating, and we give a conjectured form to the generating functions. We further find that even though twisted boundary conditions satisfy the same linear recursion relation as periodic boundary conditions in L_v, the generating functions in the twisted case are repeating with much smaller period due to extra cancellations that do not occur for the periodic cases. We have also seen cases of $Z(-1) = 0$, but only for free-free boundary conditions, and only for the one-dimensional cases of either $L_v, L_h = 1$ and for either $L_v, L_h = 1 \mod 3$. For two dimensional lattices, the partition function has only been found to equal zero at $z = -1$ for the cylindrical lattice rotated at $45°$ for $L_h = 1 \mod 3$, seen by Baxter for $L_h \leq 12$ [25].

The nature of the special point $z = -1$ continues to remain unknown and very intriguing. The free energy at $z = -1$ may depend on boundary conditions if the lattice is rotated with respect to the boundaries, the segment $-1 < z < z_d$ appears to have a countable number of singularities in the thermodynamic limit due to exponentially decreasing gaps, and level crossing singularities appear to be accumulating near $z = -1$. And yet, the limit $z \to -1$ of the density of roots appears to be finite as $L_h \to \infty$. Clearly much remains to be understood concerning this special point.

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Chapter 3

Paper 1

Factorization of the Ising model form factors

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Abstract

We present a general method for analytically factorizing the n-fold form factor integrals $f^{(n)}_{N,N}(t)$ for the correlation functions of the Ising model on the diagonal in terms of the hypergeometric functions ${}_2F_1([1/2, N+1/2]; [N+1]; t)$ which appear in the form factor $f^{(1)}_{N,N}(t)$. New quadratic recursion and quartic identities are obtained for the form factors for $n = 2, 3$. For $n = 2, 3, 4$ explicit results are given for the form factors. These factorizations are proved for all N for $n = 2, 3$. These results yield the emergence of palindromic polynomials canonically associated with elliptic curves. As a consequence, understanding the form factors amounts to describing and understanding an infinite set of palindromic polynomials, canonically associated with elliptic curves. From an analytical viewpoint the relation of these palindromic polynomials with hypergeometric functions associated with elliptic curves is made very explicitly, and from a differential algebra viewpoint this corresponds to the emergence of direct sums of differential operators homomorphic to symmetric powers of a second order operator associated with elliptic curve.

3.1 Introduction

The form factor expansion of Ising model correlation functions is essential for the study of the long distance behavior and the scaling limit of the model. This study was initiated in 1966 when Wu [253] computed the first term in the expansion of the row correlations both for $T > T_c$, where the result is a one dimensional integral, and for $T < T_c$, where the result is a 2 dimensional integral. By at least 1973 it was recognized [162] that the diagonal correlations and form factors are a specialization of the results for the row correlations. The extension to form factors for correlations in a general position and from the leading term to all terms was first made in 1976 [254]. This leads to the general result that for the two dimensional Ising model with interaction energy $\mathcal{E} = -\sum_{j,k}\{E^v\,\sigma_{j,k}\sigma_{j+1,k} + E^h\,\sigma_{j,k}\sigma_{j,k+1}\}$, with $\sigma_{j,k} = \pm 1$, the form factor expansion for $T < T_c$ is

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \;=\; (1-t)^{1/4}\cdot\{1 + \sum_{n=1}^{\infty} f_{M,N}^{(2n)}\}, \tag{3.1}$$

where $t = (\sinh 2E^v/k_BT\,\sinh 2E^h/k_BT)^{-2}$, and for $T > T_c$

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \;=\; (1-t)^{1/4}\cdot\sum_{n=0}^{\infty} f_{M,N}^{(2n+1)}, \tag{3.2}$$

where $t = (\sinh 2E^v/k_BT\,\sinh 2E^h/k_BT)^{2}$, and where $f_{M,N}^{(n)}$ are n-fold integrals.

The form factor expansions (3.1) and (3.2) are of great importance for the study of the magnetic susceptibility of the Ising model

$$\chi(T) \;=\; \frac{1}{k_BT}\cdot\sum_{M,N}\{\langle\sigma_{0,0}\sigma_{M,N}\rangle - \mathcal{M}^2\}, \tag{3.3}$$

where $\mathcal{M} = (1-t)^{1/8}$ for $T < T_c$ and equals zero for $T > T_c$ is the spontaneous magnetization. The study of this susceptibility has been the outstanding problem in the field for almost 60 years. The susceptibility is expressed in terms of the form factor expansion as

$$k_BT\cdot\chi(T) \;=\; (1-t)^{1/4}\cdot\sum_{m}\chi^{(m)}(T), \tag{3.4}$$

where

$$\chi^{(m)}(T) \;=\; \sum_{M,N} f_{M,N}^{(m)}, \tag{3.5}$$

with $m = 2n$, for $T < T_c$, and $m = 2n+1$, for $T > T_c$. In the last twelve years a large number of remarkable properties have been obtained for both $\chi^{(n)}(T)$ [171, 172, 177, 263, 266, 264, 50, 45, 51, 69] and the specialization to the diagonal [57]

$$\chi_d^{(n)}(t) \;=\; \sum_{N,N} f_{N,N}^{(m)}. \tag{3.6}$$

These remarkable properties of $\chi^{(n)}$ and $\chi_d^{(n)}(t)$ must originate in properties of the $f_{M,N}^{(n)}$ themselves.

For 40 years after the first computations of Wu, the form factor integrals for $n \geq 2$ appeared to be intractable in the sense that they could not be expressed in terms of previously known special functions. However, in 2007 this intractability was shown to be false when Boukraa et al [54] discovered by means of differential algebra computations on Maple, using the form for the form factors proven in [156], many examples for n as large as nine that the form factors in the isotropic case $E^h = E^v$ can be written as sums of products of the complete elliptic integrals $K(t^{1/2})$ and $E(t^{1/2})$ with polynomial coefficients, where for the diagonal case ($M = N$) we may allow $E^v \neq E^h$.

These computer derived examples lead to the obvious

Conjecture 1

All n-fold form factor integrals for Ising correlations may be expressed in terms of sums of products of one dimensional integrals with polynomial coefficients.

The first discovery that the n-fold multiple integrals which arise in the study of integrable models can be decomposed into sums of products of one dimensional integrals (or sums) was made for the correlation functions of the XXZ spin chain

$$H_{XXZ} \;=\; -\sum_{j=-\infty}^{\infty} \{\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\sigma_j^z\sigma_{j+1}^z\}. \tag{3.7}$$

These correlations were expressed as multiple integrals for the massive regime ($\Delta < -1$) in 1992 [128] and in the massless regime ($-1 \leq \Delta \leq 1$) in 1996 [129]. In 2001 Boos and Korepin [40] discovered that for the case $\Delta = -1$, the special correlation function (called the emptiness probability)

$$P(n) \;=\; \langle \prod_{j=1}^{n} \left(\frac{1+\sigma_j^z}{2}\right)\rangle, \tag{3.8}$$

for $n = 4$ could be expressed in terms of $\zeta(3)$, $\zeta(5)$, $\zeta^2(3)$ and $\ln 2$, and this decomposition in terms of sums of products of zeta functions of odd argument was extended to $P(5)$ in [41] and $P(6)$ in [213]. Similar decompositions of the correlation function $\langle\sigma_0^z\sigma_n^z\rangle$ were obtained for $n = 3$ in [209], for $n = 4$ in [43] and for $n = 5$ in [212]. The extension to the XXZ model chain (3.7) with $\Delta \neq -1$ of the decomposition of the integrals for the third neighbor correlation $\langle\sigma_0^i\sigma_3^i\rangle$ for $i = x, z$ was made in [137].

The discovery in [54] that a similar reduction takes place for Ising correlations thus leads to the more far reaching

Conjecture 2
All multiple integral representations of correlations and form factors in all integrable models can be reduced to sums of products of one dimensional integrals.

If correct this conjecture must rest upon a very deep and universal property of integrable models.

In [54] the form factors were reduced to sums of products of the complete elliptic integrals $K(t^{1/2})$ and $E(t^{1/2})$. However, the results become much more simple and elegant when expressed in terms of the hypergeometric functions F_N and F_{N+1} where

$$F_N \;=\; {}_2F_1([1/2,\, N+1/2];\, [N+1];\, t) \tag{3.9}$$

appears in the form factor for $n = 1$

$$f^{(1)}_{N,N}(t) \;=\; \frac{t^{N/2}}{\pi} \cdot \int_0^1 x^{N-1/2}(1-x)^{-1/2}(1-tx)^{-1/2} \cdot dx \;=\; \lambda_N \cdot t^{N/2} \cdot F_N, \tag{3.10}$$

where

$$\lambda_N \;=\; \frac{(1/2)_N}{N!}, \tag{3.11}$$

and $(a)_0 = 1$ and for $n \geq 1$ $(a)_n = a(a+1)\cdots(a+n-1)$ is Pochhammer's symbol. Note that $F_0 = \frac{2}{\pi}K(t^{1/2}) = f^{(1)}_{0,0}(t)$.

The expressions for $f^{(n)}_{N,N}(t)$ in terms of F_N and F_{N+1} are obtained from [54], rewritten by use of the contiguous relations for hypergeometric functions, and we give some of these expressions in 3.A. In all cases studied the form factors have the form

$$f^{(2n)}_{N,N}(t) \;=\; \sum_{m=0}^{n-1} K^{(2n)}_m \cdot f^{(2m)}_{N,N}(t) + \sum_{m=0}^{2n} C^{(2n)}_m(N;t) \cdot F_N^{2n-m} \cdot F^m_{N+1}, \tag{3.12}$$

$$\frac{f^{(2n+1)}_{N,N}(t)}{t^{N/2}} \;=\; \sum_{m=0}^{n-1} K^{(2n+1)}_m \cdot \frac{f^{(2m+1)}_{N,N}(t)}{t^{N/2}} + \sum_{m=0}^{2n+1} C^{(2n+1)}_m(N;t) \cdot F_N^{2n+1-m} \cdot F^m_{N+1}, \tag{3.13}$$

where $f^{(0)}_{N,N} \;=\; 1$. The degrees of the polynomials $C^{(j)}_m(N;t)$ are for $N \geq 1$

$$\deg\, C^{(2n)}_m(N;t) \;=\; \deg\, C^{(2n+1)}_m(N;t) \;=\; n \cdot (2N+1), \tag{3.14}$$

with $C^{(n)}_m(N;t) \;\sim\; t^m$ as $t \sim 0$.

These polynomials are different from the corresponding polynomials in the K, E basis in that they have the palindromic property

$$C^{(2n)}_m(N;t) \;=\; t^{n(2N+1)+m} \cdot C^{(2n)}_m(N;1/t), \tag{3.15}$$

$$C^{(2n+1)}_m(N;t) \;=\; t^{n(2N+1)+m} \cdot C^{(2n+1)}_m(N;1/t). \tag{3.16}$$

We conjecture that these results are true generally.

In this paper we begin the analytic proof of Conjecture 1 and the derivation and generalization of the results of [54] for the diagonal correlation $M = N$ by studying the three lowest order integrals $f^{(n)}_{N,N}(t)$ for $n = 2, 3, 4$. The results are summarized in Sec. 2.

In Sec. 3 we derive the results for $f^{(2)}_{N,N}(t)$. We proceed by first differentiating the integral $f^{(2)}_{N,N}(t)$ with respect to t, which removes the term proportional to $f^{(0)}_{N,N}(t)$ from the general form (3.12). The resulting two dimensional integral is then seen to factorize into a sum of products of one dimensional integrals. This factorized result is then compared with the derivative of (3.12) to give three coupled first order inhomogeneous equations for the three polynomials $C^{(2)}_m(N;t)$. These equations are decoupled to give inhomogeneous equations of degree three which are explicitly solved to find the unique polynomial solutions $C^{(2)}_m(N;t)$.

In Sec. 4 we extend this method to $f^{(3)}_{N,N}(t)$. The first step is to apply to $f^{(3)}_{N,N}(t)$ the second order operator which annihilates $f^{(1)}_{N,N}(t)$. However, in this case we have not found the mechanism which factorizes the resulting three dimensional integral. Instead we use the property discovered in [54] that the resulting integral satisfies a fourth order homogeneous equation which is homomorphic to the symmetric cube of a second order operator and thus a factorized form is obtained. This form is then compared with the form obtained by applying the second order operator to the form (3.13), and from this comparison we obtain 4 coupled inhomogeneous equations for the 4 polynomials $C^{(3)}_m(t)$. These equations are then decoupled to give inhomogeneous equations of degree 5 for $C^{(3)}_3(N;t)$ and of degree 8 for the three remaining polynomials. We then solve these equations under the assumption that a polynomial solution exists.

The results for $f^{(n)}_{N,N}(t)$ with $n = 1, 2, 3$ have a great deal of structure which can be generalized to arbitrary arbitrary n. Of particular interest is the fact that $f^{(2n)}_{N,N}(t)$ vanishes as $t^{n(N+n)}$ and $f^{(2n+1)}_{N,N}(t)/t^{N/2}$ vanishes as $t^{n(N+n+1)}$ at $t \to 0$ while each individual term in the expansions (3.12) and (3.13) vanishes with a power (which may be zero) which is independent of N. This cancellation for $f^{(2)}_{N,N}(t)$ and $f^{(3)}_{N,N}(t)$ is demonstrated in Sec. 5 and gives an interpretation of several features of the results obtained in Secs. 3 and 4. It also provides an alternative form (3.138) for $f^{(3)}_{N,N}(t)$ compared to the form (3.13). In Sec. 6, in a differential algebra viewpoint, the canonical link between the 20-th order ODEs associated with the $C^{(4)}_m(N;t)$ of $f^{(4)}_{N,N}(t)$ and the theory of elliptic curves is made very explicit with the emergence of direct sums of differential operators homomorphic to symmetric powers of a second order operator associated with elliptic curves, and in an analytical viewpoint, is made very explicit with exact expressions (given in Appendix G), for the polynomials $C^{(4))}_m(N;t)$, *valid for any* N. We conclude in Sec. 7 with a discussion of possible generalizations of our results.

3.2 Summary of formalism and results

The form factor integrals for the diagonal correlations are [54, 156] for $T < T_c$

$$f_{N,N}^{(2n)}(t) = \frac{t^{n(N+n)}}{(n!)^2\,\pi^{2n}} \int_0^1 \prod_{k=1}^{2n} dx_k\; x_k^N \prod_{j=1}^{n} \left(\frac{(1-tx_{2j})(x_{2j}^{-1}-1)}{(1-tx_{2j-1})(x_{2j-1}^{-1}-1)} \right)^{1/2}$$
$$\prod_{1\le j\le n}\prod_{1\le k\le n} \left(\frac{1}{1-tx_{2k-1}x_{2j}} \right)^2 \prod_{1\le j<k\le n} (x_{2j-1}-x_{2k-1})^2\,(x_{2j}-x_{2k})^2, \qquad (3.17)$$

and for $T > T_c$

$$f_{N,N}^{(2n+1)}(t) =$$
$$\frac{t^{(n+1/2)N+n(n+1)}}{n!(n+1)!\pi^{2n+1}} \int_0^1 \prod_{k=1}^{2n+1} dx_k\; x_k^N \prod_{j=1}^{n+1} x_{2j-1}^{-1}[(1-tx_{2j-1})(x_{2j-1}^{-1}-1)]^{-1/2}$$
$$\prod_{j=1}^{n} x_{2j}[(1-tx_{2j})\,(x_{2j}^{-1}-1)]^{1/2} \prod_{1\le j\le n+1}\prod_{1\le k\le n} \left(\frac{1}{1-tx_{2j-1}x_{2k}} \right)^2$$
$$\prod_{1\le j<k\le n+1} (x_{2j-1}-x_{2k-1})^2 \prod_{1\le j<k\le n} (x_{2j}-x_{2k})^2. \qquad (3.18)$$

When $t = 0$ the integrals in (3.17) and (3.18) reduce to a special case of the Selberg integral [215, 245]

$$f_{N,N}^{(2n)}(t) \sim \frac{t^{n(N+n)}}{(n!)^2\pi^{2n}} \frac{\Gamma(N+n+1/2)\Gamma(n+1/2)}{\Gamma(N+1/2)\Gamma(1/2)} \times \prod_{j=0}^{n-1} \left[\frac{\Gamma(N+j+1/2)\Gamma(j+1/2)\Gamma(j+2)}{\Gamma(N+n+j+1)} \right]^2 \qquad (3.19)$$

and

$$f_{N,N}^{(2n+1)}(t) \sim \frac{t^{N(n+1/2)+n(n+1)}}{n!\pi^{2n+1}} \frac{\Gamma(N+1/2)\Gamma(1/2)}{\Gamma(N+n+1)} \times \prod_{j=0}^{n-1} \left[\frac{\Gamma(N+j+3/2)\Gamma(j+3/2)\Gamma(j+2)}{\Gamma(N+n+j+2)} \right]^2 \qquad (3.20)$$

In particular

$$f^{(2)}_{N,N}(t) \;=\; t^{N+1} \cdot \frac{\lambda^2_{N+1}}{(2N+1)} \;+ O(t^{N+2}), \qquad (3.21)$$

$$f^{(3)}_{N,N}(t) \;=\; t^{3N/2+2} \cdot \frac{\lambda^3_{N+1}}{2(2N+1)(N+2)^2} \;+ O(t^{3N/2+3}). \qquad (3.22)$$

3.2.1 General Formalism

For the special case $f^{(2)}_{N,N}(t)$ we will analytically derive the form (3.12) without making any assumptions. However, for the general case we will proceed by assuming the forms (3.12) and (3.13) as an ansatz and with this as a conjecture, we will derive inhomogeneous Fuchsian equations for the polynomials $C^{(n)}_m(N;t)$

$$\Omega^{(n)}_m(N;t) \cdot C^{(n)}_m(N;t) \;=\; I^{(n)}_m(N;t), \qquad (3.23)$$

where $\Omega^{(n)}_m(N;t)$ is a linear differential operator and $I^{(n)}_m(N;t)$ a polynomial.

In all cases which have been studied, the operator $\Omega^{(n)}_m(N;t)$, corresponding to the lhs of (3.23), has a *direct sum decomposition* where each term in the direct sum is *homomorphic to a either a symmetric power or a symmetric product for different values of* N*, of the second order operator*

$$O_2(N;t) \;=\; D_t^2 \;-\frac{1+N-Nt}{t(1-t)} \cdot D_t \;+\frac{4+4N\;-t\;-2Nt}{4\,t^2\,(1-t)}, \qquad (3.24)$$

where $D_t \;=\; d/dt$. The operator $O_2(N;t)$ is equivalent to the operator $L_2(N;t)$ which annihilates $f^{(1)}_{N,N}(t)$ [54], as can be seen in the operator isomorphism

$$O_2(N;t) \cdot t^{N/2\,+1} \;=\; t^{N/2\,+1} \cdot L_2(N;t). \qquad (3.25)$$

The solutions of $O_2(N;t)$ are expressed in terms of hypergeometric functions by noting that

$$t^2 \cdot (1-t) \cdot O_2(N) \;=\; t \cdot (t\,D_t\,+a)(t\,D_t\,+b)\;-(t\,D_t\,-a')(t\,D_t\,-b'),$$

with

$$a \;=\; -N-1/2, \qquad b \;=\; -1/2, \qquad a' \;=\; N+1, \qquad b' \;=\; 1, \qquad (3.26)$$

which for $|t| < 1$ [2] has the two fundamental solutions [244, p. 283]

$$t^{a'} \cdot \ {}_2F_1([a+a', b+a'];\ [a'-b'+1];\ t),\ \ t^{b'} \cdot {}_2F_1([a+b', b+b'];\ [b'-a'+1];\ t). \qquad (3.27)$$

Using (3.26) we have the two solutions of $O_2(N)$

$$u_1(N;t) \ = \ t^{N+1} \cdot \ {}_2F_1([1/2, 1/2+N];\ [N+1];\ t) \ = \ t^{N+1} \cdot \ F_N, \qquad (3.28)$$

$$\text{and:} \qquad t \cdot \ {}_2F_1([1/2,\ 1/2-N];\ [1-N];\ t). \qquad (3.29)$$

The solution $u_1(N;t)$ in (3.28) is regular at $t = 0$ and has the expansion

$$u_1(N;t) \ = \ t^{N+1} \cdot \sum_{n=0}^{\infty} b_n(N) \cdot t^n, \qquad (3.30)$$

with

$$b_n(N) \ = \ \frac{(1/2)_n\,(1/2+N)_n}{(N+1)_n\, n!}. \qquad (3.31)$$

Since we will in this paper work with positive integer values of N, it is better to introduce as the second solution

$$t^{N+1} \cdot \ {}_2F_1([1/2,\ 1/2+N];\ [1];\ 1 \ - \ t). \qquad (3.32)$$

When N is *not an integer* the hypergeometric function (3.32) can be written as the following linear combination of the two previous solutions (3.28) and (3.29)

$$\frac{\Gamma(-N)}{\Gamma(1/2)\,\Gamma(1/2-N)} \cdot t^{N+1} \cdot \ {}_2F_1([1/2, 1/2+N];\ [N+1];\ t)$$

$$+ \ \ \frac{\Gamma(N)}{\Gamma(1/2)\,\Gamma(1/2+N)} \cdot t \cdot \ {}_2F_1([1/2,\ 1/2-N];\ [1-N];\ t). \qquad (3.33)$$

The hypergeometric function (3.32) is not analytic at $t = 0$ but, instead, has a *logarithmic singularity.*

From [21, (2) on p.74 and (7) on p.75] we may choose to normalize the analytical part of the second solution to t as $t \rightarrow 0$. Denoting such a solution $u_2(N;t)$, it reads

$$u_2(N;t) \ = \ t \cdot \sum_{n=0}^{N-1} a_n(N) \cdot t^n + t^{N+1} \cdot N \cdot \lambda_N^2 \cdot \sum_{n=0}^{\infty} b_n(N)\,[k_n - \ln(t)] \cdot t^n, \qquad (3.34)$$

[2] For $|t| > 1$, we write $z = 1/t$ and the identical procedure is found to interchange a with a' and b with b'. Thus the two fundamental solutions valid near $t = \infty$ are $\tilde{u}_1(N;z) \ = \ z^{-1/2} \cdot {}_2F_1([1/2, 1/2+N]; [1+N]; z) = z^{-1/2} \cdot F_N,\ \ \tilde{u}_2(N;z) \ = \ z^{-N-1/2} \cdot \ {}_2F_1([1/2, 1/2-N]; [1-N]; z)$. The identification of the hypergeometric functions of (3.28) and (3.29) with these two solutions is a consequence of the palindromic property of the operator $O_2(N;t)$. However, we note that $\tilde{u}_j(N;z)$ is not the analytic continuation of $u_j(N;t)$.

with $a_0(N) \; = \; 1$ and for $n \ge 1$

$$a_n(N) \;=\; \frac{(1/2)_n \, (1/2-N)_n}{(1-N)_n \, n!} \;=\; \lambda_N \cdot \frac{(1/2)_n \, (N-n)!}{(1/2)_{N-n} \, n!} \tag{3.35}$$

and $k_n \;=\; H_n(1) + H_{n+N}(1) - H_n(1/2) - H_{n+N}(1/2)$, where

$$H_n(z) \;=\; \sum_{k=0}^{n-1} \frac{1}{z+k} \tag{3.36}$$

are the partial sums of the harmonic series. The series expansion (3.34) corresponds to the maximal unipotent monodromy structure of $O_2(N;t)$ which amounts to writing the second solution as:

$$u_2(N;t) \;=\; w_2(N;t) \;-\; N \cdot \lambda_N^2 \cdot u_1(N;t) \cdot \ln(t) \tag{3.37}$$

where $w_2(N;t) \;=\; t \;+\; \cdots$ is analytical at $t \;=\; 0$. This function $w_2(N;t)$ is the solution analytic at $t = 0$, different from $u_1(N;t)$, of an order-four operator which factorizes as the product $\tilde{O}_2(N;t) \cdot O_2(N;t)$, where $\tilde{O}_2(N;t)$ and $O_2(N;t)$ are two order-two homomorphic operators

$$\tilde{O}_2(N;t) \cdot I_1 \;=\; J_1 \cdot O_2(N;t), \tag{3.38}$$

where one of the two order-one intertwinners I_1 and J_1 is quite simple, namely

$$I_1 \;=\; \frac{1}{t} \cdot D_t \;-\; \frac{t\,-2}{2\,t^2 \cdot (t\,-1)} \;-\; \frac{N}{2\,t^2}. \tag{3.39}$$

Finally, we note the relation which follows from the Wronskian of $O_2(N;t)$,

$$u_1(N) \cdot u_2(N+1) \,-\, \beta_N \cdot u_2(N) \cdot u_1(N+1) \;=\; t^{N+2}, \tag{3.40}$$

with

$$\beta_N \;=\; \frac{(2N+1)^2}{4N(N+1)}. \tag{3.41}$$

3.2.2 Explicit results for $f_{N,N}^{(2)}(t)$

For $f_{N,N}^{(2)}(t)$ the parameter $K_0^{(2)}$ and the polynomials $C_m^{(2)}(N;t)$ of the form (3.12) are explicitly computed in Section 3.3 as

$$K_0^{(2)} \;=\; N/2, \tag{3.42}$$

and

$$C_m^{(2)}(N;t) \;=\; A_m^{(2)} \cdot t^m \cdot \sum_{n=0}^{2N+1-m} c_{m;n}^{(2)}(N) \cdot t^n, \tag{3.43}$$

with

$$A_n^{(2)} \;=\; (-1)^{n+1} \cdot \frac{N}{2} \cdot \binom{n}{2} \cdot \beta_N^n. \tag{3.44}$$

Using the notation that

$$[f]_n == \text{ the coefficient of } t^n \text{ in the expansion of } f \text{ at } t=0 \tag{3.45}$$

we have for $0 \le n \le N-1$

$$c_{2;n}^{(2)}(N) \;=\; c_{2;\,2N-1-n}^{(2)}(N) = [t^{-2}u_2(N)^2]_n \;=\; \sum_{k=0}^{n} a_k(N) \cdot a_{n-k}(N), \tag{3.46}$$

$$c_{1;n}^{(2)}(N) \;=\; c_{1;\,2N-n}^{(2)}(N) = [t^{-2}u_2(N)u_2(N+1)]_n \;=\; \sum_{k=0}^{n} a_k(N) \cdot a_{n-k}(N+1), \tag{3.47}$$

and

$$c_{1;N}^{(2)}(N) \;=\; \lambda_N^2 \;+ c_{2,N-1}^{(2)}(N), \tag{3.48}$$

and where for $0 \le n \le N$

$$c_{0;\,n}^{(2)}(N) \;=\; c_{0;\,2N+1-n}^{(2)}(N) \;=\; [t^{-2}u_2^2(N+1)]_n \;=\; c_{2;\,n}^{(2)}(N+1), \tag{3.49}$$

where $a_n(N)$ is given by (3.35). We note that the sum (3.46) for $c_{2,N-1}^{(2)}$ may be written by use of the second form of $a_n(N)$ in (3.35) in the alternative form

$$c_{2;N-1}^{(2)} \;=\; \lambda_N^2 \cdot 2N \cdot H_N(1/2), \tag{3.50}$$

where $H_N(z)$ is given by (3.36).

We also derive the recursion relation for $N \ge 1$

$$f_{N,N}^{(2)}(t) \;=\; N\, f_{1,1}^{(2)}(t) \;-\; \frac{N}{2}\, t^{1/2} \cdot \sum_{j=1}^{N-1} \frac{f_{j,j}^{(1)}(t) \cdot f_{j+1,j+1}^{(1)}(t)}{j(j+1)}. \tag{3.51}$$

3.2.3 Explicit results for $f^{(3)}_{N,N}(t)$

For $f^{(3)}_{N,N}(t)$ the parameter $K^{(3)}_0$ and the polynomials $C^{(3)}_m(N;t)$ of the form (3.13) are explicitly computed in Section 3.4 as

$$K^{(3)}_0 \;=\; \frac{3\,N+1}{6}, \tag{3.52}$$

and

$$C^{(3)}_m(N;t) \;=\; A^{(3)}_m \cdot t^m \cdot \sum_{n=0}^{2N+1-m} c^{(3)}_{m,n}(N) \cdot t^n \;+ \frac{N-1}{N}\lambda_N \cdot C^{(2)}_m(N,t), \tag{3.53}$$

where we make the definition $C^{(2)}_3(N,t) = 0$ and

$$A^{(3)}_n \;=\; (-1)^{n+1} \cdot \frac{2}{3} \cdot \binom{n}{3} \cdot \lambda_N \cdot \beta^n_N. \tag{3.54}$$

The coefficients $c^{(3)}_{m;n}(N)$'s are given by a simple *quartic expression* of the a_n's and b_n's. For $0 \le n \le N-1$ they read

$$\begin{aligned} c^{(3)}_{3;n}(N) \;&=\; c^{(3)}_{3;\,2N-2-n}(N) \;=\; [t^{-N-4}u^3_2(N)u_1(N)]_n \;= \\ &=\; \sum_{m=0}^{n}\sum_{l=0}^{m}\sum_{k=0}^{l} a_k(N)\cdot a_{l-k}(N)\cdot a_{m-l}(N)\cdot b_{n-m}(N), \end{aligned} \tag{3.55}$$

and

$$\begin{aligned} c^{(3)}_{2;n}(N) \;&=\; c^{(3)}_{2;\,2N-n-1}(N) \;=\; [t^{-N-4}u^2_2(N)u_2(N+1)u_1(N)]_n \;= \\ &=\; \sum_{m=0}^{n}\sum_{l=0}^{m}\sum_{k=0}^{l} a_k(N)\cdot a_{l-k}(N)\cdot a_{m-l}(N+1)\cdot b_{n-m}(N), \end{aligned} \tag{3.56}$$

for $0 \le n \le N$

$$\begin{aligned} c^{(3)}_{0;n}(N) \;&=\; c^{(3)}_{0;\,2N-n+1}(N) \;=\; [t^{-N-4}u^3_2(N+1)u_1(N)]_n \\ &=\; \sum_{m=0}^{n}\sum_{l=0}^{m}\sum_{k=0}^{l} a_k(N+1)\cdot a_{l-k}(N+1)\cdot a_{m-l}(N+1)\cdot b_{n-m}(N), \end{aligned} \tag{3.57}$$

and for $0 \le n \le N-1$

$$c_{1;n}^{(3)}(N) \;=\; c_{1;\,2N-n}^{(3)}(N) \;=\; [t^{-N-4} u_2(N) u_2^2(N+1) u_1(N)]_n$$
$$= \sum_{m=0}^{n} \sum_{l=0}^{m} \sum_{k=0}^{l} a_k(N) \cdot a_{l-k}(N+1) \cdot a_{k-m}(N+1) \cdot b_{n-m}(N), \qquad (3.58)$$

with the middle term of $C_1^{(3)}(N;t)$ of order $N+1$

$$c_{1;\,N}^{(3)} \;=\; \frac{\beta_N \cdot \lambda_N^2}{N} \;+ \beta_N \cdot \lambda_N \cdot \Big[(N-1) \cdot c_{2;\,N-1}^{(3)} \;+ 4\, c_{2;\,N-1}^{(2)}\Big]$$
$$- \frac{2}{3} \cdot \frac{\beta_N \cdot \lambda_N}{N^2} \cdot \Big[2N^2 \cdot c_{3;\,N-2}^{(3)} \;+ (N^2 - 1/4) \cdot c_{3;\,N-1}^{(3)}\Big], \qquad (3.59)$$

where $a_n(N)$ and $b_n(N)$ are given by (3.35) and (3.31).

3.3 The derivation of the results for $f_{N,N}^{(2)}(t)$

We begin our derivation of the results for $f_{N,N}^{(2)}$ of Sec. 3.2.2 by integrating (3.17) (with $2n = 2$) by parts using

$$u \;=\; y^{N-1/2} \cdot (1-y)^{1/2} \cdot (1-ty)^{1/2}, \qquad (3.60)$$

$$du \;=\; y^{N-3/2} \frac{[N \cdot (1-y) \cdot (1-ty) \;- 1/2\,(1 \;- t\,y^2)]}{(1-y)^{1/2} \cdot (1 \;- t\,y)^{1/2}} \cdot dy, \qquad (3.61)$$

$$dv \;=\; \frac{dy}{(1 \;- t\,xy)^2}, \qquad v \;=\; \frac{y}{1-txy}, \qquad (3.62)$$

to find

$$f_{N,N}^{(2)}(t) \;=$$
$$\int_0^1 dx \int_0^1 dy \; \frac{t^{N+1}}{2\pi^2} \frac{x^{N+1/2}\, y^{N-1/2}\, (1-ty^2)}{(1-x)^{1/2}\, (1 \;- t\,x)^{1/2}\, (1-y)^{1/2}\, (1 \;- t\,y)^{1/2}\, (1-txy)}$$
$$- N \int_0^1 dx \int_0^1 dy \; \frac{t^{N+1}}{\pi^2} \; \frac{x^{N+1/2}\, y^{N-1/2}\, (1-y)^{1/2}\, (1-ty)^{1/2}}{(1-x)^{1/2}\, (1-tx)^{1/2}\, (1-txy)}. \qquad (3.63)$$

The first term in (3.63) is separated into two parts as

$$\int_0^1 dx \int_0^1 dy \; \frac{t \cdot x^N\, y^N}{2\pi^2} \, \frac{x^{1/2}}{y^{1/2}} \frac{1}{(1-x)^{1/2}\, (1-tx)^{1/2}\, (1-y)^{1/2}\, (1-ty)^{1/2}\, (1-txy)}$$
$$- \int_0^1 dx \int_0^1 dy \; \frac{t \cdot x^N\, y^N}{2\pi^2} \frac{t\, x^{1/2} y^{3/2}}{(1-x)^{1/2}\, (1-tx)^{1/2}\, (1-y)^{1/2}\, (1-ty)^{1/2} (1-txy)}, \qquad (3.64)$$

and in this second term we interchange $x \leftrightarrow y$. Then, recombining these two terms, we see that the factor $1 - txy$ cancels between the numerator and denominator in (3.64). Thus the first term in (3.63) factorizes and we find

$$\begin{aligned} f^{(2)}_{N,N}(t) &= \int_0^1 dx \int_0^1 dy \; \frac{t^{N+1}}{2\pi^2} \frac{x^{N+1/2} y^{N-1/2}}{(1-x)^{1/2}\,(1-tx)^{1/2}\,(1-y)^{1/2}\,(1-ty)^{1/2}} \\ &\quad - N \int_0^1 dx \int_0^1 dy \; \frac{t^{N+1}}{\pi^2} \; \frac{x^{N+1/2}\,y^{N-1/2}\,(1-y)^{1/2}\,(1-ty)^{1/2}}{(1-x)^{1/2}\,(1-tx)^{1/2}\,(1-txy)} \\ &= \frac{t^{1/2}}{2} \cdot f^{(1)}_{N,N} \cdot f^{(1)}_{N+1,N+1} \\ &\quad - N \int_0^1 dx \int_0^1 dy \; \frac{t^{N+1}}{\pi^2} \; \frac{x^{N+1/2}\,y^{N-1/2}\,(1-y)^{1/2}\,(1-ty)^{1/2}}{(1-x)^{1/2}\,(1-tx)^{1/2}\,(1-txy)}. \end{aligned} \tag{3.65}$$

From (3.17) we find for $N \geq 1$ that the integral in the second term of (3.65) is $f^{(2)}_{N,N}(t) - f^{(2)}_{N+1,N+1}(t)$ and thus we have

$$f^{(2)}_{N,N}(t) \;=\; \frac{t^{1/2}}{2} \cdot f^{(1)}_{N,N}(t) \cdot f^{(1)}_{N+1,N+1}(t) \; - N \cdot [f^{(2)}_{N,N}(t) \; - f^{(2)}_{N+1,N+1}(t)]. \tag{3.66}$$

From (3.66) we obtain the recursion relation

$$f^{(2)}_{N+1,N+1}(t) \;=\; \frac{N+1}{N} \cdot f^{(2)}_{N,N}(t) \; - \frac{t^{1/2}}{2\,N} \cdot f^{(1)}_{N.N}(t) \cdot f^{(1)}_{N+1,N+1}(t), \tag{3.67}$$

and thus for $N \geq 1$

$$f^{(2)}_{N,N}(t) \;=\; N\, f^{(2)}_{1,1}(t) \; - \frac{N}{2}\, t^{1/2} \cdot \sum_{j=1}^{N-1} \frac{f^{(1)}_{j,j}(t) \cdot f^{(1)}_{j+1,j+1}(t)}{j(j+1)}. \tag{3.68}$$

To proceed further we return to (3.65) which we write in terms of F_N as

$$\begin{aligned} f^{(2)}_{N,N}(t) &= \frac{\lambda_N\, \lambda_{N+1}}{2} \cdot t^{N+1} \cdot F_N \cdot F_{N+1} \\ &\quad - N \int_0^1 dx \int_0^1 dy \; \frac{t^{N+1}}{\pi^2} \; \frac{x^{N+1/2}\,y^{N-1/2}\,(1-y)^{1/2}\,(1-ty)^{1/2}}{(1-x)^{1/2}\,(1-tx)^{1/2}\,(1-txy)}. \end{aligned} \tag{3.69}$$

The integral in (3.69) does not have a manifest factorization. However, if we compute

$df^{(2)}_{N,N}(t)/dt$ in the contour integral form of (3.17), and note that

$$\begin{aligned}&\frac{d}{dt}\left[\frac{(y-t^{1/2})\,(1-t^{1/2}y)}{(x-t^{1/2})\,(1-t^{1/2}x)}\right]^{1/2}\\ &= \ \frac{1}{t^{1/2}}\left[\frac{(y-t^{1/2})(1-t^{1/2}y)}{(x-t^{1/2})(1-t^{1/2}x)}\right]^{1/2}\frac{(xy-1)(x-y)(t-1)}{(y-t^{1/2})(1-t^{1/2}y)(x-t^{1/2})(1-t^{1/2}x)}, \end{aligned} \tag{3.70}$$

the resulting integral does factorize and, introducing G_N, some well-suited linear combination of F_N and F_{N+1},

$$\begin{aligned} G_N &= {}_2F_1([3/2, N+3/2];\ [N+1];\ t) \\ &= \frac{1+t}{(1-t)^2}\cdot F_N \ - \ \frac{t}{(1-t)^2}\cdot\frac{2\,N\,+1}{N\,+1}\cdot F_{N+1}, \end{aligned} \tag{3.71}$$

we find

$$\begin{aligned}\frac{df^{(2)}_{N,N}(t)}{dt} \ &= \ (1-t)\cdot t^N\cdot\frac{(2N+1)\lambda_N^2}{16\,(N+1)}\cdot\big[(2N+1)^2\cdot F_{N+1}\cdot G_N \\ &\qquad -(2N-1)(2N+3)\cdot F_N\cdot G_{N+1}\big]. \end{aligned} \tag{3.72}$$

It remains to integrate (3.72). However, in general, integrals of products of two hypergeometric functions with respect to the argument will not have the form of the product of two hypergeometric functions. We will thus proceed in the opposite direction by differentiating (3.12) for $2n = 2$ with respect to t and equating the result to (3.72) to obtain differential equations for the $C^{(2)}_m(N;t)$ which we will then solve to obtain the final results (3.42)–(3.44).

From a straightforward use of the contiguous relations of hypergeometric functions [21], we introduce the following well-suited linear combination of F_N and F_{N+1}

$$\begin{aligned}\bar{F}_N \ &= \ {}_2F_1([3/2, N+3/2];\ [N+2];\ t) \ = \ \frac{4\,(N+1)}{2N+1}\cdot\frac{dF_N}{dt} \\ &= \ \frac{1}{1-t}\cdot\Big(2\cdot(N+1)\cdot F_N \ -(2\,N+1)\cdot F_{N+1}\Big). \end{aligned} \tag{3.73}$$

The derivative of (3.12) with $2n = 2$ may be written in the quadratic form[3]

$$B_1\cdot F_N^2 \ + \ B_2\cdot F_N\cdot\bar{F}_N \ + \ B_3\cdot\bar{F}_N^2, \tag{3.74}$$

[3]For convenience the dependence of the $C^{(2)}_m$ on N and t is suppressed here and below (see (3.78)).

with

$$B_1 \;=\; \frac{dC_0^{(2)}}{dt} \;-\; \frac{(N{+}1)}{2(N{+}1/2)t}\cdot C_1^{(2)} + \frac{(N{+}1)}{(N{+}1/2)}\cdot\frac{dC_1^{(2)}}{dt}$$
$$- \frac{(N{+}1)^2}{(N{+}1/2)^2\, t}\cdot C_2^{(2)} \;+\; \frac{(N{+}1)^2}{(N{+}1/2)^2}\cdot\frac{dC_2^{(2)}}{dt}, \tag{3.75}$$

$$B_2 \;=\; \frac{(N{+}1/2)}{(N{+}1)}\cdot C_0^{(2)}$$
$$+\left[1+\frac{1}{2(N{+}1/2)} + \frac{1-2t+N(1-t)}{2(N{+}1/2)t}\right]\cdot C_1^{(2)} \;-\; \frac{(1-t)}{2(N{+}1/2)}\cdot\frac{dC_1^{(2)}}{dt}$$
$$+\frac{(N{+}1)(3{+}2N{-}2t)}{2(N{+}1/2)^2 t}\cdot C_2^{(2)} \;-\; \frac{(N{+}1)(1{-}t)}{(N{+}1/2)^2}\cdot\frac{dC_2^{(2)}}{dt}, \tag{3.76}$$

$$B_3 \;=\; -\frac{(1-t)}{4(N+1)}\cdot C_2^{(2)} \;-\; \frac{(2{+}2N{-}t)(1{-}t)}{4(N{+}1/2)^2 t}\cdot C_2^{(2)} \;+\; \frac{(1{-}t)^2}{4(N{+}1/2)^2}\cdot\frac{dC_2^{(2)}}{dt}. \tag{3.77}$$

The derivative of $f^{(2)}_{N,N}(t)$ in (3.72) by use of contiguous relations [21] is expressed in terms of F_N and $\bar{F}_N$ as

$$\frac{df^{(2)}_{N,N}(t)}{dt} \;=\; B_4\cdot F_N^2 \;+ B_5\cdot F_N\cdot\bar{F}_N \;+ B_6\cdot\bar{F}_N^2, \tag{3.78}$$

where,

$$B_4 \;=\; \frac{2N+1}{4}\cdot\lambda_N^2 t^N,$$
$$B_5 \;=\; \frac{[t\,-N(1-t)](2N+1)}{4(N+1)}\cdot\lambda_N^2 t^N,$$
$$B_6 \;=\; -\frac{N\beta_N\lambda_N^2}{4\;(N+1)}\cdot(1-t)\cdot t^{N+1} \tag{3.79}$$

3.3.1 Linear differential equations for $C_m^{(2)}(N;t)$

To obtain the $C_m^{(2)}(N;t)$ we equate (3.74) with (3.78) and find the following first order system of equations for $C_m^{(2)}(N;t)$

$$\frac{(2N+1)}{4}\cdot\lambda_N^2\cdot t^N \;=\; \frac{dC_0^{(2)}}{dt} - \frac{(N+1)}{2(N+1/2)t}\cdot C_1^{(2)} + \frac{(N+1)}{(N+1/2)}\cdot\frac{dC_1^{(2)}}{dt} - \frac{(N+1)^2}{(N+1/2)^2 t}\cdot C_2^{(2)} + \frac{(N+1)^2}{(N+1/2)^2}\cdot\frac{dC_2^{(2)}}{dt}, \tag{3.80}$$

$$\frac{(2N+1)\cdot[t-N(1-t)]}{4\,(N+1)}\cdot\lambda_N^2\cdot t^N \;=\; \frac{(N+1/2)}{(N+1)}\cdot C_0^{(2)} + \left[1+\frac{1}{2(N+1/2)}+\frac{1-2t+N\,(1-t)}{2(N+1/2)t}\right]\cdot C_1^{(2)} - \frac{(1-t)}{2\,(N+1/2)}\frac{dC_2^{(2)}}{dt} + \frac{(N+1)(3+2N-2t)}{2\,(N+1/2)^2 t}\cdot C_2^{(2)} - \frac{(N+1)(1-t)}{(N+1/2)^2}\cdot\frac{dC_2^{(2)}}{dt}, \tag{3.81}$$

$$-\frac{(2N+1)^2}{16\,(N+1)^2}\cdot\lambda_N^2\cdot(1-t)\cdot t^{N+1} \;=\; -\frac{(1-t)}{4\,(N+1)}\cdot C_1^{(2)} - \frac{(2+2N-t)(1-t)}{4\,(N+1/2)^2 t}\cdot C_2^{(2)} + \frac{(1-t)^2}{4\,(N+1/2)^2}\cdot\frac{dC_2^{(2)}}{dt}. \tag{3.82}$$

From this first order coupled system we obtain third order uncoupled equations for the $C_m^{(2)}(N;t)$

$$2\,(1-t)^2\cdot t^2\cdot\frac{d^3C_0^{(2)}}{dt^3} - 6\,(N-(N-1)\,t)\,(1-t)\,t\cdot\frac{d^2C_0^{(2)}}{dt^2} + 2\,[N+2N^2+(1+4N-4N^2)\,t-(5N-2N^2)\,t^2]\cdot\frac{dC_0^{(2)}}{dt} + (2N+1)(2Nt-2N-1)\cdot C_0^{(2)} \;=\; \frac{N\,(N+1)\,(2N+1)^2}{2}\cdot\lambda_N^2\cdot(1-t)\cdot t^N, \tag{3.83}$$

$$2\,(1-t)^2\,(1+t)\cdot t^3\cdot \frac{d^3C_1^{(2)}}{dt^3}\;\; -2\,(1-t)\,[1+3N+4t+(1-3N)t^2]\cdot t^2\cdot \frac{d^2C_1^{(2)}}{dt^2}$$
$$+\,2[2+4N+2N^2+(3+4N-2N^2)\cdot t-(3+8N+2N^2)\cdot t^2\;+2\,N^2\cdot t^3]\cdot t\cdot \frac{dC_1^{(2)}}{dt}$$
$$-\,[4+8N+4N^2\;+(5+6N)\cdot t-(5+10N+4N^2)\cdot t^2]\cdot C_1^{(2)}$$
$$=\quad \frac{(2N+1)^2\cdot[-2N^2\,(N+1)\cdot(t+1)^2\;+(4N+1)\cdot t]}{(N+1)}\cdot \lambda_N^2\cdot(1-t)\cdot t^{N+1}, \qquad (3.84)$$

and

$$2\,(1-t)^2\cdot t^3\cdot \frac{d^3C_2^{(2)}}{dt^3}\;\; -6\,(1+N-Nt)\cdot(1-t)\cdot t^2\cdot \frac{d^2C_2^{(2)}}{dt^2}$$
$$+\;\;2\,[7+9N+2N^2\;-(7+12N+4N^2)\cdot t\;+(1+3N+2N^2)\cdot t^2]\cdot t\cdot \frac{dC_2^{(2)}}{dt}$$
$$-\;\;[16+24N+8N^2\;-(15+28N+12N^2)\cdot t\;+(2+6N+4N^2)\cdot t^2]\cdot C_2^{(2)}$$
$$=\quad \frac{N^2\,(2N+1)^4\cdot\;(1-t)}{8(N+1)^2}\;\cdot\lambda_N^2\cdot t^{N+2}. \qquad (3.85)$$

From (3.83)–(3.85) it follows that $C_m^{(2)}(N;t)$ and $t^{2N+m+1}\cdot C_m^{(2)}(N;1/t)$ satisfy the same equation and thus, if $C_m^{(2)}(N;t)$ are polynomials they will satisfy the palindromic property (3.15). From (3.83) and (3.85) it follows that the polynomials $C_0^{(2)}(N;t)$ and $C_2^{(2)}(N;t)$ satisfy

$$C_0^{(2)}(N;t)\;\;=\;\;\frac{N}{(N+1)\cdot\beta_{N+1}^2\cdot t^2}\;\cdot\; C_2^{(2)}(N+1;t). \qquad (3.86)$$

We therefore may restrict our considerations to $C_1^{(2)}(N;t)$ and $C_2^{(2)}(N;t)$.

We will obtain the polynomial solutions for the differential equations (3.83)–(3.85) by demonstrating that the homogeneous parts of the equations are homomorphic to symmetric products or symmetric powers of the second order operator $O_2(N)$.

3.3.2 Polynomial solution for $C_2^{(2)}(N;t)$

Denote $\Omega_2^{(2)}(N,t)$ the order-three linear differential operator acting on $C_2^{(2)}(N,t)$ on the left hand side of (3.85). Then it is easy to discover that the operator $\Omega_2^{(2)}(N,t)$ is *exactly* the symmetric square of the second-order operator $O_2(N;t)$

$$\Omega_2^{(2)}(N,t)\;\;=\;\;\mathrm{Sym}^2\Big(O_2(N;t)\Big), \qquad (3.87)$$

which has the three linearly independent solutions

$$u_1(N;t)^2, \qquad u_1(N;t)\cdot u_2(N;t), \qquad u_2^2(N;t) \qquad (3.88)$$

where the functions $u_j(N;t)$ for $j = 1, 2$ are defined by (3.30)-(3.36). The indicial exponents of (3.85) at $t = 0$ are

$$2N+2, \qquad N+2, \qquad 2, \qquad (3.89)$$

which are the exponents respectively of the three solutions (3.88). Therefore, because the inhomogeneous term in (3.85) starts at t^{N+1} the coefficients $c^{(2)}_{2,n}$ in (3.43) for $0 \le n \le N-1$ will be proportional to the first N coefficients in the expansion of $u_2^2(N;t)$ about $t = 0$.

Equation (3.85) is invariant under the substitution

$$C_2^{(2)}(N;t) \quad \longrightarrow \quad t^{2N+3} \cdot C_2^{(2)}(N;1/t), \qquad (3.90)$$

which maps one solution into another. Therefore if it is known that the solution $C_2^{(2)}(N;t)$ is a polynomial the palindromic property

$$c^{(2)}_{2;n} \; = \; c^{(2)}_{2;2N-1-n} \qquad (3.91)$$

must hold and thus $C_2^{(2)}(N;t)$ is given by (3.46) where the normalizing constant $A_2^{(2)}$ remains to be determined.

However, the invariance (3.90) is by itself is not sufficient to guarantee the existence of a polynomial solution with the palindromic property (3.15). To demonstrate that there is a polynomial solution we examine the recursion relation which follows from (3.85)

$$\begin{aligned} A_2^{(2)} \cdot \{ & 2n\,(2N-n)\,(N-n) \cdot c^{(2)}_{2;n}(N) \\ & + (4N\,n \,-2N \,-2n^2+2n-1)\,(2n-1-2N))) \cdot c^{(2)}_{2;n-1}(N) \\ & + 2\,(n-1)\,(2N-n+1)(N-n+1)) \cdot c^{(2)}_{2;n-2}(N) \} \\ & = \, (\delta_{n,N} - \delta_{n,N+1}) \cdot \frac{N^2\,(2N+1)^4}{8\,(N+1)^2} \cdot \lambda_N^2. \end{aligned} \qquad (3.92)$$

where $c^{(2)}_{2;n}(N) \, = \, 0$ for $n \, \le \, -1$ and we may set $c^{(2)}_{2;0} \, = \, 1$ by convention . By sending $n \, \to \, 2N-n+1$ in (3.92) we see that $c^{(2)}_{2;n}(N)$ and $c^{(2)}_{2;2N-n-1}(N)$ do satisfy the same equation as required by (3.91).

To prove that the solution $C_2^{(2)}(N;t)$ is indeed a polynomial we examine the recursion relation (3.92) for $n = N$. If there were no inhomogeneous term then, because of the factor $N-n$ in front of $c^{(2)}_{2;n}$, the recursion relation (3.92) for $n = N$ would give a constraint on $c^{(2)}_{2;N-1}$ and $c^{(2)}_{2;N-2}$. This constraint does in fact not hold, which is the reason that the solution $u_2^2(N;t)$ is not analytic at $t = 0$ but instead has a term $t^{N+2} \ln t$. However, when there is a nonzero inhomogeneous term at order t^{N+2} the recursion equation (3.92) is satisfied with a nonzero $A_2^{(2)}$. The remaining coefficients $c^{(2)}_{2,n}$ for $N \le 2N-1$ are determined by the palindromy constraint (3.91).

For $C_2^{(2)}(N;t)$ to be a polynomial we must have $c^{(2)}_{2;n}(N) \, = \, 0$ for $n \, \ge \, 2N$. From the recursion relation (3.92) we see that because of the coefficient $2N-n$ in front of $c^{(2)}_{2;n}(N)$

the coefficient $c_{2;2N}^{(2)}(N)$ may be freely chosen. The choice of $c_{2;2N}^{(2)}(N) \neq 0$ corresponds to the solution of $\Omega_2^{(2)}(N;t)$ which has the indicial exponent $N+2$ and clearly does not give a polynomial solution. However by setting $n = 2N+1$ in (3.92) we obtain

$$2\,(N+1)\,(2\,N+1) \cdot c_{2;2N+1}^{(2)}(N) \;\; - \;\; (2\,N+1)^2 \cdot c_{2;2N}^{(2)}(N) \;\; = \;\; 0. \qquad (3.93)$$

and if we choose $c_{2;2N}^{(2)}(N) = 0$ we obtain $c_{2;2N+1}^{(2)}(N) = 0$ also. Therefore because (3.92) is a three term relation, it follows that $c_{2;n}^{(2)}(N) = 0$ for $n \geq 2N$ as required for a polynomial solution.

It remains to explicitly evaluate the normalization constant $A_2^{(2)}$ which satisfies (3.92) with $n = N$. A more efficient derivation is obtained if we return to the original inhomogeneous equation (3.85). Then we note that if we include the term with $n = 0$ in the second terms on the right-hand side of (3.34) in the computation of the term of order t^{N+2} in the left hand side of (3.85) we must get zero because u_2^2 is a solution of the homogeneous part of (3.85). Therefore when we use the extra term in u_2^2 of

$$-\,2\,t^{N+2} \cdot N \cdot \lambda_N^2 \cdot \ln t, \qquad (3.94)$$

in the lhs of (3.85), and keep the terms which do not involve $\ln t$, we find

$$2\,(N^2-1) \cdot c_{2;N-2}^{(2)}(N) \;\; -\,(2N^2-1) \cdot c_{2;N-1}^{(2)}(N) \;\; = \;\; -4\,N^3 \cdot \lambda_N^2. \qquad (3.95)$$

Thus, using (3.95) we evaluate (3.92) with $n = N$ as

$$-\,4\,A_2^{(2)} N^3\,\lambda_N^2 \;\; = \;\; \frac{N^2\,(2N+1)^4}{8\,(N+1)^2} \cdot \lambda_N^2, \qquad (3.96)$$

and thus

$$A_2^{(2)} \;\; = \;\; -\frac{N}{2} \cdot \beta_N^2. \qquad (3.97)$$

3.3.3 Polynomial solution for $C_1^{(2)}(N;t)$

The computation of $C_1^{(2)}(N;t)$ has features which are characteristic of $C_m^{(n)}(N;t)$ which are not seen in $C_2^{(2)}(N;t)$. Similarly to what has been done in the previous subsection we introduce $\Omega_1^{(2)}(N;t)$, the order-three linear differential operator acting on $C_1^{(2)}(N;t)$ in the lhs of (3.84).

The indicial exponents at $t = 0$ of the operator $\Omega_1^{(2)}(N;t)$ are

$$1, \qquad N+1, \qquad 2N+2 \qquad (3.98)$$

This order-three operator $\Omega_1^{(2)}(N;t)$ is found to be related to the *symmetric product* of $O_2(N)$

and $O_2(N+1)$ by the direct sum decomposition

$$\mathrm{Sym}\Big(O_2(N),\, O_2(N+1)\Big)\cdot t \;\; = \;\; \Omega_1^{(2)} \oplus \Big(D_t \;\; - \frac{N+1}{t}\Big). \qquad (3.99)$$

The three linearly independent solutions of $\Omega_1^{(2)}(N;t)$ are to be found in the set of four functions

$$\begin{array}{ll} t^{-1}\cdot u_1(N;t)\cdot u_1(N+1;t), & t^{-1}\cdot u_2(N,t)\cdot u_1(N+1;t), \\ t^{-1}\cdot u_1(N;t)\cdot u_2(N+1;t), & t^{-1}\cdot u_2(N;t)\cdot u_2(N+1;t), \end{array} \qquad (3.100)$$

where from the definitions of $u_1(N;t)$ in (3.30) and $u_2(N;t)$ in (3.34) the behaviors of these four solutions as $t \to 0$ are t^{2N+2}, t^{N+2}, t^{N+1}, t respectively.

Following the argument given above for $C_2^{(2)}(N;t)$ we conclude that because the inhomogeneous term in (3.83) is of order t^{N+1} that the terms up through order t^N must be proportional to the solution of the homogeneous equation

$$t^{-1}\cdot u_2(N;t)\cdot u_2(N+1;t), \qquad (3.101)$$

which begins at order t. This observation determines the form (3.43) and the coefficients (3.47) $c_{1;n}^{(2)}(N)$ for $0 \le n \le N-1$. The normalizing constant $A_1^{(2)}$ and the remaining coefficient $c_{1;N}^{(2)}(N)$ (3.48) are then obtained from the inhomogeneous equation (3.83). Finally, to prove that $C_1^{(2)}(N;t)$ is actually a palindromic polynomial the recursion relation for the coefficients $c_{1;n}^{(2)}(N)$ must be used. Details of these computations are given in 3.B.

3.3.4 The constant $K_0^{(2)}$

Finally, we need to evaluate the constant of integration $K_0^{(2)}$ in (3.12). This is easily done by noting that from the original integral expression (3.17) that $f_{N,N}^{(2)}(0) = 0$ for all N. From (3.43)–(3.44) we see that

$$C_0^{(2)}(N;0) \;=\; -\frac{N}{2}, \qquad C_1^{(2)}(N;0) \;=\; C_2^{(2)}(N;0) \;=\; 0, \qquad (3.102)$$

and using this in (3.12) we obtain $K_0^{(2)} \;=\; N/2$ as desired.

3.4 The derivation of the results for $f_{N,N}^{(3)}(t)$

The form factor $f_{N,N}^{(3)}(t)$ is defined by the integral (3.18) with $2n+1 \;=\; 3$, and if we are to follow the method of evaluation developed for $f_{N,N}^{(2)}(t)$, we need to demonstrate analytically that there is an operator which, when acting on the integral, will split it into three factors. Unfortunately we have not analytically obtained such a result.

However, we are able to proceed by using the methods of differential algebra and from [54] it is known computationally for integer N that $f^{(3)}_{N,N}$ is annihilated by the operator $L_4(N) \cdot L_2(N)$ where

$$L_2(N) \;=\; D_t^2 \;+\frac{2t-1}{(t-1)t} \cdot D_t \;-\frac{1}{4t} \;+\frac{1}{4(t-1)} \;-\frac{N^2}{4t^2}, \qquad (3.103)$$

and $L_2(N)$ annihilates $f^{(1)}_{N,N}(t)$, and where,

$$\begin{aligned} L_4(N) \;=\; & D_t^4 \;+10\frac{(2t-1)}{(t-1)\,t} \cdot D_t^3 \;+\frac{(241t^2-241t+46)}{2\,(t-1)^2\,t^2} \cdot D_t^2 \\ & + \frac{(2t-1)(122t^2-122t+9)}{(t-1)^3\,t^3} \cdot D_t \;+\frac{81}{16}\frac{(5t-1)(5t-4)}{t^3\,(t-1)^3} \;-\frac{5}{2}\frac{N^2}{t^2} \cdot D_t^2 \\ & + \frac{(23-32t)N^2}{2\,(t-1)\,t^3} \cdot D_t \;+\frac{9}{8}\,\frac{(8-17t)\,N^2}{(t-1)\,t^4} \;+\frac{9}{16}\,\frac{N^4}{t^4}. \end{aligned} \qquad (3.104)$$

Furthermore the operator $L_4(N)$ is homomorphic to the symmetric cube of $L_2(N)$ by the following relation,

$$L_4(N) \cdot Q(N) \;=\; R(N) \cdot \mathrm{Sym}^3(L_2(N)), \qquad (3.105)$$

where,

$$\begin{aligned} Q(N) \;=\; & (t-1) \cdot t \cdot D_t^3 \;+\frac{7}{2}(2t-1) \cdot D_t^2 \;+\frac{(41t^2-41t+6)}{4\,(t-1)\,t} \cdot D_t \\ & +\frac{9}{8}\frac{(2t-1)}{(t-1)\,t} \;-\frac{9}{4}\frac{(t-1)N^2}{t} \cdot D_t \;-\frac{9}{8}\frac{(2t-1)}{t^2}\,N^2, \end{aligned} \qquad (3.106)$$

and

$$\begin{aligned} R(N) \;=\; & (t-1) \cdot t \cdot D_t^3 \;+\frac{23}{2}\,(2t-1) \cdot D_t^2 \;+\frac{21}{4}\,\frac{6-29t+29t^2}{(t-1)\,t} \cdot D_t \\ & +\frac{9}{8}\frac{(2t-1)\,(125t^2-125t+16)}{(t-1)^2\,t^2} \;-\frac{9\,N^2}{4} \cdot \left(\frac{(t-1)}{t} \cdot D_t \;+\;\frac{(10t-9)}{2\,t^2}\right). \end{aligned} \qquad (3.107)$$

We therefore conclude that since $f^{(3)}_{N,N}(t)$ is regular at $t = 0$ and the solution of $L_2(N)$ which is regular at $t = 0$ is F_N, that

$$Q(N) \cdot B_0 \cdot t^{3N/2} \cdot F_N^3 \;=\; L_2(N) \cdot f^{(3)}_{N,N}, \qquad (3.108)$$

where B_0 is a normalizing constant which is determined from the behavior at $t = 0$. From the integral (3.18) we find

$$f^{(3)}_{N,N} \;=\; \frac{N+2}{4\,(N+1/2)} \left(\frac{(1/2)_{N+1}}{(N+2)!^3}\right)^3 \cdot t^{3N/2+2} \;+O(t^{3N/2+3}), \qquad (3.109)$$

and from the expansion of F_N we have

$$Q(N) \cdot t^{3N/2} \cdot F_N^3 \;=\; \frac{3(2N+1)^3}{8\,(N+1)^2\,(N+2)} \cdot t^{3N/2} \;+\; O(t^{3N/2+1}), \tag{3.110}$$

and thus

$$B_0 \;=\; \frac{1}{3} \cdot \lambda_N^3. \tag{3.111}$$

Operating $Q(N)$ on $t^{3N/2} F_N^3$, one can write the result in the basis F_N and $\bar{F}_N$. Similarly, one can operate on the form $f_{N,N}^{(3)}$ in (3.13) with $L_2(N)$ and write the result in the same basis F_N and $\bar{F}_N$. Then, matching powers of the hypergeometric functions on both sides of the relation (3.108) will yield four coupled inhomogeneous ODEs to be solved. The four coupled ODEs are given in 3.C.

For $C_m^{(3)}(N;t)$ with $m = 0, 1, 2$, the reduction of the four coupled second order equations leads to inhomogeneous 8-th order uncoupled ODEs for each $C_m^{(3)}(N;t)$ separately, of the form

$$\sum_{j=0}^{8} P_{m,j}\,(t) \cdot t^j \cdot \frac{d^j}{dt^j} C_m^{(3)}(N;t) \;=\; I_m(t), \tag{3.112}$$

where

$$I_0 \;=\; t^{N+1} \cdot \sum_{j=0}^{14} I_0(j) \cdot t^j, \qquad I_1 \;=\; t^{N+1} \cdot \sum_{j=0}^{17} I_1(j) \cdot t^j,$$

$$I_2 \;=\; t^{N+2} \cdot \sum_{j=0}^{14} I_2(j) \cdot t^j, \tag{3.113}$$

where the $I_m(t)$ are antipalinromic and $P_{m,n}(t)$ are polynomials. In particular

$$P_{m,8}(t) \;=\; (1-t)^9 \cdot P_m(t), \tag{3.114}$$

where $P_0(t)$ and $P_2(t)$ are order six and $P_1(t)$ is order eight.

However, for $C_3^{(3)}(N;t)$ a step-by-step elimination process in the coupled system terminates in a fifth order equation instead. We derive and present this 5th order equation in 3.D, but the eighth order equations given by Maple are too long to present.

3.4.1 Polynomial solution for $C_3^{(3)}(N;t)$

The homogeneous operator on the LHS of the ODE (3.176) for $C_3^{(3)}(N,t)$ is found on Maple to be isomorphic to $\mathrm{Sym}^4(O_2(N)) \cdot t^{(N+1)}$, the symmetric fourth power of $O_2(N)$ multiplied by $t^{(N+1)}$. Therefore all five solutions of the homogeneous equation are given as $t^{-(N+1)}$ times products of the solutions $u_1(N;t)$ and $u_2(N;t)$. The fifth order ODE has at

$t\ =\ 0$ the indicial exponents

$$-N+3, \quad 3, \quad N+3, \quad 2N+3, \quad 3N+3. \tag{3.115}$$

Therefore because the polynomial solution must by definition be regular at $t\ =\ 0$ the first $N+1$ terms (from t^3 through t^{N+3}) in the solution

$$t^{-(N+1)} \cdot u_2^3(N) \cdot u_1(N), \tag{3.116}$$

which vanishes as t^3, will solve the inhomogeneous equation (3.176), so that

$$C_3^{(3)}(N;t) \ = \ A_3^{(3)} \cdot t^3 \cdot \sum_{n=0}^{2N-2} c_{3;n}^{(3)} \cdot t^n, \tag{3.117}$$

where for $0\ \le\ n\ \le\ N-1$

$$c_{3;n}^{(3)} \ = \ \sum_{m=0}^{n}\sum_{l=0}^{m}\sum_{k=0}^{l} a_k(N) \cdot a_{l-k}(N) \cdot a_{m-l}(N) \cdot b_{n-m}(N). \tag{3.118}$$

The lowest order inhomogeneous term is t^{N+3} which is the next indicial exponent in (3.115) and therefore the normalizing constant $A_3^{(3)}$ is found from the first logarithmic term in the solution of the homogeneous equation by exactly the same argument used for $C_2^{(2)}(N;t)$. Thus we find

$$A_3^{(3)} \ = \ \frac{2}{3} \cdot \beta_N^3 \cdot \lambda_N. \tag{3.119}$$

The remaining demonstration that $C_3^{(3)}(N;t)$ is a palindromic polynomial follows from the recursion relation for the coefficients, as was done for $C_2^{(2)}(N;t)$, with the exception that because the inhomogeneous term in (3.176) is proportional to $t^{N+1}(t^2-1)$ instead of $t^{N+1}(t-1)$, there is an identity which must be verified. Details are given in 3.D.

3.4.2 Polynomial solutions for $C_2^{(3)}(N;t)$ and $C_0^{(3)}(N;t)$.

A new feature appears in the computation of $C_2^{(3)}(N;t)$ and $C_0^{(3)}(N;t)$.
The indicial exponents at $t=0$ of the 8-th order operator $\Omega_2^{(3)}(N;t)$

$$-N+2, \ 2, \ 3, \ N+2, \ N+3, \ 2N+2, \ 2N+3, \ 3N+3, \tag{3.120}$$

and for $\Omega_0^{(3)}(N;t)$ are

$$-N, \quad 0, \quad 1, \quad N+1, \quad N+2, \quad 2N+2, \quad 2N+3, \quad 3N+3, \tag{3.121}$$

and from these exponents it might be expected that the solution of $\Omega_2^{(3)}(N;t)$ $(\Omega_0^{(3)}(N;t))$ which is of order t^2 (t^0) could have a logarithmic term $t^3\ln t$ $(t\ln t)$ which would preclude the existence of a polynomial solution of the corresponding inhomogeneous equation. However, this does, in fact, not happen because there is a decomposition of the 8-th order operators into a direct sum of the third order operators $\Omega_2^{(2)}(N;t)$ $(\Omega_0^{(2)}(N;t))$ with exponents $2,\ N+2,\ 2N+2$ $(0, N+1, 2N+2)$ and new fifth order operators $M_m^{(3)}(N;t)$

$$\Omega_m^{(3)}(N;t) \;=\; M_m^{(3)}(N;t) \oplus \Omega_m^{(2)}(N;t) \tag{3.122}$$

with exponents $-N+2,\ 2,\ N+2,\ 2N+2,\ 3N+2$ for $M_2^{(3)}(N;t)$ and $-N,\ 0,\ N+1,\ 2N+2,\ 3N+3)$ for $M_0^{(3)}(N;t)$. Furthermore $M_2^{(3)}(N;t)$ is homomorphic to the symmetric fourth power of $O_2(N)$ and $M_0^{(3)}(N;t)$ is homomorphic to the symmetric fourth power of $O_2(N+1)$ (see 3.E for details). The inhomogeneous equation is solved in terms of a linear combination of the solutions of the third order and fifth order homogeneous equations.

However, a simpler form of the answer results if we notice the isomorphisms

$$\Omega_2^{(3)}(N;t) \;=\; \mathrm{Sym}\,(O_2(N), O_2(N), O_2(N), O_2(N+1)) \cdot t^{N+2}, \tag{3.123}$$

$$\Omega_0^{(3)}(N;t) \;=\; \mathrm{Sym}\,(O_2(N), O_2(N+1), O_2(N+1), O_2(N+1)) \cdot t^{N+4}, \tag{3.124}$$

The desired solutions for $\Omega_2^{(3)}(N;t)$ are constructed from the two solutions which have the exponents 2 and 3,

$$t^{-N-2} \cdot u_2^2(N) \cdot u_1(N) \cdot u_2(N+1), \qquad t^{-N-2} \cdot u_2^3(N) \cdot u_1(N+1), \tag{3.125}$$

which by use of the Wronskian condition (3.40) may be rewritten as a linear combination of two solutions each with the exponent of 2 as

$$A_2^{(3)} \cdot t^{-N-2} \cdot u_2^2(N) \cdot u_1(N) \cdot u_2(N+1) \quad + B_2^{(3)} \cdot u_2^2(N), \tag{3.126}$$

and similarly for $C_0^{(3)}(N;t)$, we choose as the solution of the homogeneous equation the two solutions with exponent 0

$$A_0^{(3)} \cdot t^{-N-4} \cdot u_2^3(N+1) \cdot u_1(N) \quad + B_0^{(3)} t^{-2} \cdot u_2^2(N+1). \tag{3.127}$$

This procedure determines the constants $c_{2;n}^{(3)}$ for $0 \leq n \leq N-1$ and and $c_{0;n}^{(3)}$ for $0 \leq n \leq N$, with palindromy determining the remaining $c_{2;n}^{(3)}$ for $N \leq n \leq 2N-1$ (3.56) and and $c_{0;n}^{(3)}$ for $N+1 \leq n \leq 2N+1$ (3.57).

The constants $A_2^{(3)}$ and $B_2^{(3)}$ in (3.53) are found by using (3.53) with (3.56) in the inhomogeneous equation for $C_2^{(3)}(N;t)$ and matching the first two terms in the inhomogeneous terms of orders t^{N+2} and t^{N+3} (which are the same orders as the corresponding indicial exponents (3.120)). This generalizes the determination of $A_m^{(2)}$ for $C_m^{(2)}$ above. Similarly the constants $A_0^{(3)}$ and $B_0^{(3)}$ are found using (3.53) with (3.57) in the inhomogeneous equation for $C_0^{(3)}$ and matching to the inhomogeneous terms t^{N+1} and t^{N+2}. Thus we obtain the results (3.53)-(3.54) summarized in section 3.2.3.

3.4.3 Polynomial solution for $C_1^{(3)}(N;t)$

The computation of $C_1^{(3)}(N;t)$ has further new features.

The 8-th order homogeneous operator $\Omega_1^{(3)}(N;t)$ of the inhomogeneous equation for $C_1^{(3)}(N;t)$ has the eight indicial exponents at $t=0$

$$-N+1,\ \ 1,\ \ 2,\ \ N+1,\ \ N+2,\ \ 2N+2,\ \ 2N+3,\ \ 3N+3, \qquad (3.128)$$

and, as in the case of $\Omega_0^{(3)}(N;t)$ and $\Omega_2^{(3)}(N;t)$ has a decomposition into a direct sum of $\Omega_1^{(2)}(N;t)$ and a fifth order operator. However, simpler results are obtained by observing that $\Omega_1^{(3)}(N;t)$ is homomorphic to the symmetric product

$$\begin{aligned}&\mathrm{Sym}\Big(O_2(N),\, O_2(N),\, O_2(N+1), O_2(N+1)\Big)\cdot t^{N+3}\\ &\quad = \ \Omega_1^{(3)}(N;t)\oplus\Big(D_t-\frac{(N+1)}{t}\Big),\end{aligned} \qquad (3.129)$$

which satisfies a 9-th order ODE with indicial exponents at $t=0$

$$-N+1,\ \ 1,\ \ 2,\ \ N+1,\ \ N+2,\ \ N+3,\ \ 2N+2,\ \ 2N+3,\ \ 3N+3. \qquad (3.130)$$

The solutions with exponents of 1 and 2 are respectively

$$t^{-N-3}\cdot u_2(N)\cdot u_1(N)\cdot u_2^2(N+1), \qquad t^{-N-3}\cdot u_2^2(N)\cdot u_2(N+1)\cdot u_1(N+1), \qquad (3.131)$$

and again, recalling the Wronskian relation (3.40), we may construct the polynomial $C_1^{(3)}(N;t)$, similar to the construction of $C_2^{(3)}(N;t)$, from the linear combination

$$A_1^{(3)}\cdot t^{-N-3}\cdot u_2(N)\cdot u_1(N)\cdot u_2^2(N+1)\ +\ B_1^{(3)}\cdot t^{-1}\cdot u_2(N)\cdot u_2(N+1), \qquad (3.132)$$

which determines the coefficients $c_{1;n}^{(3)}$ for $0\le n\le N-1$, with palindromy determining the remaining $c_{1;n}^{(3)}$ for $N+1\le n\le 2N$ (3.58). The coefficients $A_1^{(3)}$ and $B_1^{(3)}$ (3.132) are determined in a manner similar to the determination of $A_2^{(3)}$ and $B_2^{(3)}$, by matching to the terms of order t^{N+1} and t^{N+2}.

Finally the term $c_{1;\,N}^{(3)}$ is computed by using the previously determined results for $C_2^{(3)}(N;t)$ and $C_3^{(3)}(N;t)$ in the coupled differential equation (3.174), giving the result (3.59).

3.4.4 Determination of $K_0^{(3)}$

It remains to determine the constant $K_0^{(3)}$ (3.52), which is easily done by setting $t=0$ in (3.13) to obtain

$$0\ =\ K_0^{(3)}\cdot\lambda_N\ +A_0^{(3)}\ +\frac{N-1}{N}\cdot\lambda_N\cdot A_0^{(2)}, \qquad (3.133)$$

and using (3.44) and (3.54).

3.5 The Wronskian cancellation for $f^{(2)}_{N,N}(t)$ and $f^{(3)}_{N,N}(t)$

The polynomials $C^{(n)}_m(N;t)$ are of order t^m as $t \to 0$. However, from (3.21) and (3.22) we see that $f^{(2)}_{N,N}(t)$ vanishes as t^{N+1} and $f^{(3)}_{N,N}(t)$ vanishes as t^{N+2}. Therefore for $t \to 0$, a great deal of cancellation must occur in (3.12) and (3.13). This cancellation is an important feature of the structure of the results of sec. 2.2 and 2.3.

To prove the cancellations we note that the n-th power of the Wronskian relation (3.40) is

$$t^{-n(N+2)} \cdot \sum_{j=0}^{n} (-1)^j \cdot \binom{n}{j} \cdot \beta_N^j \cdot [u_2(N+1)u_1(N)]^{n-j} \cdot [u_2(N)u_1(N+1)]^j \; = \; 1, \qquad (3.134)$$

or alternatively,

$$\sum_{j=0}^{n} (-1)^j \cdot \binom{n}{j} \cdot \beta_N^j \cdot \left[\frac{u_2(N+1)}{t}\right]^{n-j} \cdot u_2(N)^j \cdot F_N^{n-j}\, F_{N+1}^j \; = \; 1. \qquad (3.135)$$

Thus, by defining $\stackrel{N}{=}$ to mean equality up though and including terms of order t^N we see immediately from the form (3.12) with (3.42) for $K_0^{(2)}$ and (3.46), (3.47) and (3.49) for the $c^{(2)}_{m,n}$ with $0 \le n \le N$ that the terms though order t^N in $f^{(2)}_{N.N}(t)$ are

$$f^{(2)}_{N,N} \; \stackrel{N}{=} \; \frac{N}{2} \cdot \left\{ 1 - \sum_{j=0}^{2} (-1)^j \binom{2}{j} \cdot \beta_N^j \cdot \left[\frac{u_2(N+1)}{t}\right]^{2-j} \cdot u_2(N)^j \; F_N^{2-j} F_{N+1}^j \right\}, \qquad (3.136)$$

which vanishes by use of (3.135). This derivation has made no use of $c^{(2)}_{1;N}$. This term contributes only to order t^{N+1} and may be determined from the normalization amplitude (3.21). This provides an alternative to the derivation of (3.48) of Appendix B.

To prove the cancellation for $f^{(3)}_{N,N}(t)$ we note that because of the term $C^{(2)}_m(N;t)$ in $C^{(3)}_m(N;t)$ for $m = 0, 1, 2$ in (3.53) we may use the expression (3.12) and (3.42)-(3.49) for $f^{(2)}_{N,N}(t)$ in the form

$$\sum_{m=0}^{2} C^{(2)}_m(N;t) \cdot F_N^{2-m}\, F_{N+1}^m \; = \; f^{(2)}_{N,N}(t) \; - \frac{N}{2}. \qquad (3.137)$$

Thus from (3.13), (3.10) and (3.137) we obtain an alternative form for $f^{(3)}_{N,N}(t)$ of

$$f^{(3)}_{N,N}(t) \; = \; \Bigl\{ \frac{2}{3} \; + \frac{N-1}{N} f^{(2)}_{N,N}(t) \Bigr\} \cdot f^{(1)}_{N,N}(t) \; + t^{N/2} \cdot \sum_{m=0}^{3} \bar{C}^{(3)}_m(N;t) \cdot F_N^{3-m} \, F_{N+1}^m, \quad (3.138)$$

where

$$\bar{C}^3_m(N;t) \; = \; (-1)^{n+1} \cdot \frac{2}{3} \cdot \binom{n}{3} \cdot \beta_N^n \cdot \lambda_N \cdot \sum_{n=0}^{2N+1-m} c^{(3)}_{m;n} t^n. \quad (3.139)$$

We have already demonstrated by use of (3.136) that $f^{(2)}_{N,N}(t)$ vanishes though order t^N. Therefore using the expressions (3.55)-(3.58) for $c^{(3)}_{m;n}$ which are all valid through (at least) order t^N and the definition (3.10) of $f^{(1)}_{N,N}(t)$ we find

$$\frac{f^{(3)}_{N,N}(t)}{t^{N/2}} \; \stackrel{N}{=} \; \frac{2}{3}\lambda_N F_N \cdot \Bigl\{ 1 \; - \sum_{j=0}^{3} (-1)^j \cdot \binom{3}{j} \cdot \beta_N^j \cdot \Bigl[\frac{u_2(N+1)}{t} \Bigr]^{3-j} \cdot u_2(N)^j \cdot F_N^{3-j} \, F_{N+1}^j \Bigr\}, \quad (3.140)$$

which vanishes by use of the Wronskian relation (3.135) with $n = 3$.

We have thus demonstrated that $f^{(3)}_{N,N}(t)/t^{N/2}$ vanishes to order t^N as $t \to 0$. However we see, from the original integral (3.18), that in fact $f^{(3)}_{N,N}(t)/t^{N/2}$ is of order t^{N+2}. Therefore the coefficient of t^{N+1} must also vanish. This is not proven by (3.140). However the coefficient $c^{(3)}_{1,N}$ has not been used in the derivation of (3.140) and the choice of $c^{(3)}_{1,N}$ to make the coefficient of t^{N+1} vanish provides an alternative derivation of (3.59).

3.6 Factorization for $f^{(n)}_{N,N}$ with $n \geq 4$

In principle the methods of differential algebra of the previous sections can be extended to form factors $f^{(n)}_{N,N}(t)$ with $n \geq 4$. However, the complexity of the calculations rapidly increases.

For $f^{(2n)}_{N,N}(t)$ there are $2n+1$ polynomials $C^{(2n)}_m(N;t)$ and since from [54] we find that for $N \geq 1$

$$L_{2n+1} \cdots L_3 \cdot L_1 \cdot f^{(2n)}_{N,N}(t) \quad = \quad 0, \quad (3.141)$$

where L_k is a linear differential operator of order k, the polynomials $C^{(2n)}_m(N;t)$ will satisfy a system of $2n+1$ coupled differential equations where the maximum derivative order is n^2. These equations can be decoupled into $2n+1$ Fuchsian ODEs which generically have order $n^2\,(2n+1)$.

Similarly for $f^{(2n+1)}_{N,N}(t)$ we found in [54] that

$$L_{2n+2} \cdots L_4 \cdot L_2 \cdot f^{(2n+1)}_{N,N}(t) \quad = \quad 0, \quad (3.142)$$

and thus the $2n+2$ polynomials $C_m^{(2n+1)}(N;t)$ satisfy inhomogeneous coupled equations of maximum differential order $n(n+1)$ which for $N \geq 1$ are generically decoupled into Fuchsian equations of order $2n(n+1)^2$.

We have obtained for $f_{N,N}^{(4)}(t)$ the 20-th order ODEs for $C_m^{(4)}(N;t)$ in the cases $N = 1, \cdots, 10$ and will illustrate the new features which arise by considering the case $m=4$.

We find by use of Maple that (at least for low values of N) the operator $\Omega_4^{(4)}(N;t)$ has a direct sum decomposition

$$\Omega_4^{(4)}(N;t) \quad = \quad M_7^{(4)}(N) \oplus M_{5;1}^{(4)}(N) \oplus M_{5;2}^{(4)}(N) \oplus M_3^{(4)}(N), \qquad (3.143)$$

where $M_{k;n}^{(4)}(N)$ is order k and is homomorphic to the symmetric $k-1$ power of $O_2(N)$

$$M_7^{(4)}(N) \cdot J_2^{(4)}(N;t) \; = \; G_2^{(4)}(N;t) \cdot \mathrm{Sym}^6(O_2(N)), \qquad (3.144)$$

$$M_{5;1}^{(4)}(N) \cdot J_1^{(4)}(N;t) \; = \; G_1^{(4)}(N;t) \cdot \mathrm{Sym}^4(O_2(N)), \qquad (3.145)$$

$$M_{5;2}^{(4)}(N) \; = \; \mathrm{Sym}^4(O_2(N)), \qquad (3.146)$$

$$M_3^{(4)}(N) \cdot J_0(N;t) \; = \; G_0^{(4)}(N;t) \cdot \mathrm{Sym}^2(O_2(N)), \qquad (3.147)$$

where the intertwinners $J_m^{(4)}(2;t)$ and $G_m^{(4)}(2;t)$ are linear differential operator of order m. The intertwinners $J_m^{(4)}(2;t)$ in (3.144)-(3.147), are explicitly given in 3.F. Further examples of intertwinners are given in 3.F. These differential algebra exact results (in particular (3.144)-(3.147)) are the illustration of the *canonical link between the palindromic polynomials and the theory of elliptic curves*.

Direct sum decompositions[1] have been obtained for $\Omega_m^{(2)}(N;t)$, $\Omega_m^{(3)}(N;t)$ and $\Omega_m^{(4)}(N;t)$ and *we conjecture that this occurs generically for all* $\Omega_m^{(n)}(N;t)$. Taking into account the homomorphism of $O_2(N;t)$ and $O_2(N+1;t)$, and recalling, for instance, subsections 3.4.2) and 3.4.3, it may be easier to write direct sum decomposition formulae in terms of sum of symmetric products of $O_2(N;t)$ and $O_2(N+1;t)$. In order to extend these results, beyond these few special cases of $\Omega_m^{(4)}(N;t)$, a deeper and systematic study of the homomorphisms is still required.

From an analytical viewpoint, a complication which needs to be understood is how to use the solutions of the homogeneous operators $\Omega_m^{(n)}(N;t)$ to obtain the polynomial solution of the inhomogeneous equations. The first difficulty here is that for $C_m^{(4)}(N;t)$ the inhomogeneous terms are large polynomials, of order 100 and higher. Moreover, the orders of palindromy point of the $C_4^{(4)}(N;t)$ with $N = 1, \cdots, 10$ are all larger than the order t^{N+4} where the solutions of the homogeneous operators $M_{k;n}^{(4)}(N;t)$ have their first logarithmic singularity. Consequently linear combinations of solutions must be made which cancel these logarithmic singularities at t^{N+4} to give sets of solutions to $\Omega_4^{(4)}(N;t)$ which are analytic up

[1]Note that in direct sum decomposition like (3.143), some ambiguity may occur with terms like $M_{5;1}^{(4)}(N) \oplus M_{5;2}^{(4)}(N)$ where $M_{5,1}^{(4)}(N)$ and $M_{5,2}^{(4)}(N)$ are both homomorphic to a same operator (here $\mathrm{Sym}^4(O_2(N))$).

to the order of the first inhomogeneous terms. Thus the determination of the correct linear combination of solutions of the operators $M^{(4)}_{k;n}(N;t)$ is significantly more complex than was the case for $C^{(3)}_m(N;t)$. Exact results for the $C^{(4)}_j$'s, based on the Wronskian cancellation method of Sec. 3.5, and *valid for any value of* N are displayed in 3.G. These are exact results for the palindromic polynomials in terms of F_N and $u_2(N)$, namely two *hypergeometric functions associated with elliptic curves*. Thus, these analytical results can also be seen as an illustration of the canonical link between our palindromic polynomials and the theory of elliptic curves. They confirm the deep relation we find, algebraically and analytically, on these structures with the theory of elliptic curves. In a forthcoming publication we will show that the relation is in fact, more specifically, a close relation with *modular forms*.

3.7 Conclusions

In this paper we have proven the factorization, *for all* N, of the diagonal form factor $f^{(n)}_{N,N}(t)$ for $n = 2$, 3 previously seen in [54] for $N \leq 4$ and provided a conjecture for $n = 4$. Besides new results like the quadratic recursion (3.51), or non trivial quartic identities (like (3.55)– (3.58)), one of the main result of the paper is the fact that, introducing the selected hypergeometric functions F_N, which are also elliptic functions, and are simply related to the (simplest) form factor $f^{(1)}_{N,N}$, the form factors actually become polynomials of these F_N's with palindromic polynomial coefficients. The complexity of the form factors, is, thus, reduced to some encoding in terms of palindromic polynomials. As a consequence, understanding the form factors amounts to describing and understanding an infinite set of palindromic polynomials, canonically associated with elliptic curves.

We also observe that all of these palindromic polynomials are built from the solutions of the operator $O_2(N)$, and, therefore, are all properties of the basic elliptic curve which underlies all computations of the Ising model. There is a deep structure here which needs to be greatly developed. The differential algebra approach of the linear differential operators associated with these palindromic polynomials is found to be a surprisingly rich structure canonically associated with elliptic curves. In a forthcoming publication, we will show that such rich structures are *closely related to modular forms*.

Analytically, the conjecture and the Wronskian method of logarithm cancellation can be extended to large values of n, but the method of proof by differential equations becomes prohibitively cumbersome for $n \geq 4$. This is very similar to the situation which occurred for the factorization of correlations in the XXZ model where the factorizations of [40, 41, 213, 209, 43, 212, 137] done for small values of the separation of the spins by means of explicit computations on integrals was proven for all separations in [42] by means of the qKZ equation satisfied by the correlations and not by the explicit integrals which are the solution of this equation. This suggests that our palindromic polynomials may profitably be considered as a specialization of polynomials of n variables. Moreover, if the two conjectures presented in the introduction are indeed correct, then such kind of structures could also have relevance to the 8 vertex model and to the higher genus curves which arise in the chiral Potts model. Consequently the computations presented here could be a special case of a much larger modularity phenomenon. This could presumably generalize the relations which the Ising model has with modular forms and Calabi-Yau structures [46].

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Appendix

3.A Form factors in the basis F_N and F_{N+1}

By use of the contiguous relations for hypergeometric functions the examples given in [54] of $f_{N,N}^{(n)}(t)$ expressed in terms of the elliptic integrals $K(t^{1/2})$ and $E(t^{1/2})$ may be re-expressed in terms of the functions F_N and F_{N+1}. Several examples are as follows

$$f_{0,0}^{(2)} = \frac{t}{4} \cdot F_0 \cdot F_1, \qquad (3.148)$$

$$f_{1,1}^{(2)} = \frac{1}{2} - \frac{1}{4}(t+1)\left(2t^2+t+2\right) \cdot F_1^2 + \frac{3^2}{2^5} \cdot t \cdot (4t^2+5t+4) \cdot F_1 \cdot F_2 - \frac{3^4}{2^7} t^2 (t+1) \cdot F_2^2, \qquad (3.149)$$

$$f_{2,2}^{(2)} = 1 - \frac{1}{2^6}(t+1)(64t^4+16t^3+99t^2+16t+64) \cdot F_2^2 + \frac{5^2}{2^8 \cdot 3} \cdot t \cdot (64t^4+88t^3+105t^2+88t+64) \cdot F_2 \cdot F_3 - \frac{5^4}{2^7 \cdot 3^2} \cdot t^2 \cdot (t+1)(2t^2+t+2) \cdot F_3^2, \qquad (3.150)$$

$$f_{3,3}^{(2)} = \frac{3}{2} - \frac{1}{2^7 \cdot 3} \cdot (t+1)\left(576t^6+96t^5+730t^4+425t^3+730t^2+96t+576\right) \cdot F_3^2 + \frac{7^2}{2^{12} \cdot 3} \cdot t\,(768t^6+928t^5+1240t^4+1455t^3+1240t^2+928t+768) \cdot F_3 F_4 - \frac{7^4}{2^{15} \cdot 3} \cdot t^2 (t+1)(64t^4+16t^3+99t^2+16t+64) \cdot F_4^2. \qquad (3.151)$$

For $f^{(3)}_{N,N}$ with $N = 0, \cdots, 4$

$$f^{(3)}_{0,0} = \frac{1}{2\cdot 3}\cdot f^{(1)}_{0,0} - \frac{1}{2\cdot 3}(1+t)\cdot {F_0}^3 + \frac{1}{2^2}t\cdot {F_0}^2\cdot F_1, \tag{3.152}$$

$$\frac{f^{(3)}_{1,1}}{t^{1/2}} = \frac{2}{3}\cdot\frac{f^{(1)}_{1,1}}{t^{1/2}} - \frac{1}{2^3\cdot 3}(1+t)\left(2^3t^2+13\,t+2^3\right)\cdot {F_1}^3$$
$$+\frac{3^2}{2^6}t\left(8t^2+15\,t+8\right)\cdot {F_1}^2\cdot F_2 - \frac{3^4}{2^6}t^2(t+1)F_1F_2^2 + \frac{3^5}{2^9}t^3\cdot {F_2}^3, \tag{3.153}$$

$$\frac{f^{(3)}_{2,2}}{t} = \frac{7}{2\cdot 3}\cdot\frac{f^{(1)}_{2,2}}{t}$$
$$-\frac{1}{2^{10}\cdot 3}(1+t)\left(2^6\cdot 3\cdot 7\,t^4+1136\,t^3+3229\,t^2+1136\,t+1344\right)\cdot {F_2}^3$$
$$+\frac{5^2}{2^{11}\cdot 3}\,t\left(2^5\cdot 3^2t^4+596\,t^3+859\,t^2+596\,t+2^5\cdot 3^2\right)\cdot {F_2}^2\cdot F_3$$
$$-\frac{5^5}{2^{10}\cdot 3^2}(t+1)(3t^2+4t+3)\,t^2\cdot F_2\cdot F_3^2 + \frac{5^6}{2^{11}\cdot 3^4}t^3\left(3t^2+8\,t+3\right)\cdot {F_3}^3, \tag{3.154}$$

$$\frac{f_{3,3}^{(3)}}{t^{3/2}} = \frac{5}{3} \cdot \frac{f_{3,3}^{(1)}}{t^{3/2}}$$
$$- \frac{1}{2^{11} \cdot 3^4}(t+1)(2^7 \cdot 3^3 \cdot 5^2 t^6 + 49680\, t^5 + 153306\, t^4 + 160427\, t^3$$
$$+ 153306\, t^2 + 49680\, t + 2^7 \cdot 3^3 \cdot 5^2) \cdot F_3^3$$
$$+ \frac{7^2}{2^{16} \cdot 3^3} t(2^{10} \cdot 3^2 \cdot 5 t^6 + 79200\, t^5 + 128104\, t^4 + 168593\, t^3$$
$$+ 128104\, t^2 + 79200\, t + 2^{10} \cdot 3^2 \cdot 5) \cdot F_3^2 \cdot F_4$$
$$- \frac{7^4}{2^{16} \cdot 3^3}(t+1)t^2(2^4 \cdot 3^2 \cdot 5 t^4 + 670\, t^3 + 1763\, t^2 + 670\, t + 2^4 \cdot 3^2 \cdot 5) \cdot F_3 \cdot F_4^2$$
$$+ \frac{7^6}{2^{21} \cdot 3^4} t^3(2^6 \cdot 5 t^4 + 740\, t^3 + 1407\, t^2 + 740\, t + 2^6 \cdot 5) \cdot F_4^3, \tag{3.155}$$
$$\frac{f_{4,4}^{(3)}}{t^2} = \frac{13}{6} \cdot \frac{f_{4,4}^{(1)}}{t^2}$$
$$- \frac{1}{2^{22} \cdot 3}(t+1)(2^{14} \cdot 5 \cdot 7 \cdot 13 t^8 + 3254272\, t^7 + 11474624\, t^6 + 8672032\, t^5$$
$$+ 20423231\, t^4 + 8672032\, t^3 + 11474624\, t^2 + 3254272\, t + 2^{14} \cdot 5 \cdot 7 \cdot 13) \cdot F_4^3$$
$$+ \frac{3^3}{2^{23} \cdot 5} t(2^{12} \cdot 3 \cdot 5^2 \cdot 7 t^8 + 3334912\, t^7 + 4845120\, t^6 + 7068720\, t^5$$
$$+ 8865649\, t^4 + 7068720\, t^3 + 4845120\, t^2 + 3334912\, t + 2^{12} \cdot 3 \cdot 5^2 \cdot 7) \cdot F_4^2 \cdot F_5$$
$$- \frac{3^6}{2^{20} \cdot 5^3} t^2(t+1)(2^4 \cdot 3^2 \cdot 5 \cdot 7^2 t^6 + 26292\, t^5 + 69377\, t^4 + 78580\, t^3$$
$$+ 69377\, t^2 + 26292\, t + 2^4 \cdot 3^2 \cdot 5 \cdot 7^2) \cdot F_4 \cdot F_5^2$$
$$+ \frac{3^8}{2^{20} \cdot 5^3} t^3(2^3 \cdot 3^3 \cdot 5 \cdot 7\, t^6 + 2^3 \cdot 3^3 \cdot 7 \cdot 11 t^5 + 28413\, t^4 + 46432\, t^3$$
$$+ 28413\, t^2 + 2^3 \cdot 3^3 \cdot 7 \cdot 11\, t + 2^3 \cdot 3^3 \cdot 5 \cdot 7) \cdot F_5^3. \tag{3.156}$$

The coefficients which are not given in factored form all contain large prime factors.

For $f_{N,N}^{(4)}$ with $N = 0, 1, 2, 3$

$$f_{0,0}^{(4)} = \frac{1}{3} \cdot f_{0,0}^{(2)} - \frac{1}{2^2 \cdot 3} \cdot t \cdot F_0^4 + \frac{1}{2^5} \cdot t \cdot F_0^2 \cdot F_1^2, \tag{3.157}$$
$$f_{1,1}^{(4)} = -\frac{1}{2^3 \cdot 3} + \frac{5}{2 \cdot 3} \cdot f_{1,1}^{(2)} + \frac{1}{2^5 \cdot 3}(4t^4 + 4t^3 + 15t^2 + 4t + 4)(t+1)^2 \cdot F_1^4$$
$$- \frac{3}{2^7} t(t+1)(8t^4 + 18t^3 + 35t^2 + 18t + 8) \cdot F_1^3 \cdot F_2$$
$$+ \frac{3^4}{2^{11}} \cdot t^2 (8t^4 + 28t^3 + 45t^2 + 28t + 8) \cdot F_1^2 \cdot F_2^2$$
$$- \frac{3^5}{2^{12}} \cdot t^3 \cdot (t+1) \cdot (4t^2 + 11t + 4) \cdot F_1 \cdot F_2^3 + \frac{3^7}{2^{15}} t^4(t^2 + 4t + 1) \cdot F_2^4, \tag{3.158}$$

$$
\begin{aligned}
f_{2,2}^{(4)} \; = \;\; & -\frac{1}{3} \; + \frac{2^2}{3} \cdot f_{2,2}^{(2)} \\
& + \frac{1}{2^{14} \cdot 3} \; \big(2^{14}\, t^{10} + 40960\, t^9 + 84480\, t^8 + 136640\, t^7 + 176180\, t^6 \\
& + 201075\, t^5 + 176180\, t^4 + 136640\, t^3 + 84480\, t^2 + 40960\, t + 2^{14} \big) \cdot F_2^4 \\
& - \frac{5^2}{2^{14} \cdot 3^2}\, t\,(t+1)\, \big(2^{13}\, t^8 + 13312\, t^7 + 29504\, t^6 + 36320\, t^5 + 45337\, t^4 \\
& + 36320\, t^3 + 29504\, t^2 + 13312\, t + 2^{13} \big) \cdot F_2^3 \cdot F_3 \\
& + \frac{5^4}{2^{17} \cdot 3^2}\, t^2\, \big(2^{12}\, t^8 + 11264\, t^7 + 21760\, t^6 + 31576\, t^5 + 36209\, t^4 \\
& + 31576\, t^3 + 21760\, t^2 + 11264\, t + 2^{12} \big) \cdot F_2^2 \cdot F_3^2 \\
& - \frac{5^6}{2^{15} \cdot 3^4} \cdot t^3\, (t+1)\, \big(2^8\, t^6 + 480\, t^5 + 906\, t^4 + 979\, t^3 + 906\, t^2 \\
& + 480\, t + 2^8 \big) \cdot F_2 \cdot F_3^3 \\
& + \frac{5^8}{2^{15} \cdot 3^4}\, t^4\, \big(2^5\, t^6 + 96\, t^5 + 177\, t^4 + 224\, t^3 + 177\, t^2 + 96\, t + 2^5 \big) \cdot F_3^4, \qquad (3.159)
\end{aligned}
$$

$$
\begin{aligned}
f_{3,3}^{(4)} \;=\;& -\frac{7}{2^3} + \frac{11}{2\cdot 3}\cdot f_{3,3}^{(2)} \\
&+ \frac{1}{2^{16}\cdot 3^4}\,\big(2^{13}\cdot 3^4\cdot 7t^{14} + 10838016\,t^{13} + 19643904\,t^{12} + 34169856\,t^{11} \\
&+50403584\,t^{10} + 62791680\,t^9 + 73309425\,t^8 + 79935700\,t^7 + 73309425\,t^6 \\
&+62791680\,t^5 + 50403584\,t^4 + 34169856\,t^3 + 19643904\,t^2 + 10838016\,t \\
&+2^{13}\cdot 3^4\cdot 7\big)\cdot F_3^4 \\
&- \frac{7^2}{2^{19}\cdot 3^4}\,t\,(t+1)\,\big(2^{14}\cdot 3^3\cdot 7t^{12} + 4257792\,t^{11} + 9547776\,t^{10} + 13813120\,t^9 \\
&+19341120\,t^8 + 21399090\,t^7 + 24976435\,t^6 + 21399090\,t^5 + 19341120\,t^4 \\
&+13813120\,t^3 + 9547776\,t^2 + 4257792\,t + 2^{14}\cdot 3^3\cdot 7\big)\cdot F_3^3\cdot F_4 \\
&+ \frac{7^4}{2^{25}\cdot 3^5}\,t^2\cdot\big(2^{15}\cdot 3^2\cdot 7\;t^{12} + 4988928\,t^{11} + 9680384\,t^{10} + 15992320\,t^9 \\
&+21863120\,t^8 + 26325960\,t^7 + 28527015\,t^6 + 26325960\,t^5 + 21863120\,t^4 \\
&+15992320\,t^3 + 9680384\,t^2 + 4988928\,t + 2^{15}\cdot 3^2\cdot 7\big)\cdot F_3^2\cdot F_4^2 \\
&- \frac{7^6}{2^{27}\cdot 3^4}\,t^3\cdot(t+1)\,\big(2^{14}\cdot 3\cdot 7t^{10} + 501760\,t^9 + 1191680\,t^8 + 1548640\,t^7 \\
&+2065400\,t^6 + 2169745\,t^5 + 2065400\,t^4 + 1548640\,t^3 \\
&+1191680\,t^2 + 501760\,t + 2^{14}\cdot 3\cdot 7\big)\cdot F_3\cdot F_4^3 \\
&+ \frac{7^8}{2^{31}\cdot 3^4}\,t^4\cdot\big(2^{12}\cdot 7t^{10} + 71680\,t^9 + 147840\,t^8 + 235040\,t^7 + 299555\,t^6 \\
&+339180\,t^5 + 299555\,t^4 + 235040\,t^3 + 147840\,t^2 + 71680\,t + 2^{12}\cdot 7\big)\cdot F_4^4. \qquad (3.160)
\end{aligned}
$$

For $f_{N,N}^{(5)}$ with $N \;=\; 1,2,3$

$$
\begin{aligned}
\frac{f_{1,1}^{(5)}}{t^{1/2}} \;=\;& -\frac{2^2}{5}\cdot\frac{f_{1,1}^{(1)}}{t^{1/2}} + \frac{f_{1,1}^{(3)}}{t^{1/2}} \\
&+ \frac{1}{2^6\cdot 3\cdot 5}(t+1)^2(2^6 + 136t^3 + 159t^2 + 136t + 2^6)\cdot F_1^5 \\
&- \frac{3}{2^8}t(t+1)(2^5t^4 + 80t^3 + 99t^2 + 80t + 2^5)\cdot F_1^4\cdot F_2 \\
&+ \frac{3^3}{2^{12}}t^2(2^7t^4 + 368t^3 + 483t^2 + 368t + 2^7)\cdot F_1^3\cdot F_2^2 \\
&- \frac{3^5}{2^{10}}t^3(t+1)(4t^2 + 5t + 4)\cdot F_1^2\cdot F_2^3 \\
&+ \frac{3^7}{2^{15}}t^4(8t^2 + 13t + 8)\cdot F_1\cdot F_2^4 \;-\frac{3^9}{2^{15}\cdot 5}(t+1)\cdot t^5\cdot F_2^5, \qquad (3.161)
\end{aligned}
$$

$$
\begin{aligned}
\frac{f_{2,2}^{(5)}}{t} \;=\;& -\frac{137}{2^3\cdot 5}\cdot\frac{f_{2,2}^{(1)}}{t}+\frac{3}{2}\cdot\frac{f_{2,2}^{(3)}}{t} \\
&+\frac{1}{2^{18}\cdot 3\cdot 5}\,\left(8\,t^2+7\,t+8\right)\left(2^9\cdot 3\cdot 61\,t^8+241856\,t^7+508200\,t^6+708609\,t^5\right. \\
&\left.+780244\,t^4+708609\,t^3+508200\,t^2+241856\,t+2^9\cdot 3\cdot 61\right)\cdot F_2^5 \\
&-\frac{5^2}{2^{18}\cdot 3^2}\,t\,\left(t+1\right)\left(92160\,t^8+239360\,t^7+540576\,t^6+723924\,t^5\right. \\
&\left.+868861\,t^4+723924\,t^3+540576\,t^2+239360\,t+92160\right)\cdot F_2^4\cdot F_3 \\
&+\frac{5^4}{2^{20}\cdot 3^3}\,t^2\left(90624\,t^8+338816\,t^7+743304\,t^6+1122432\,t^5+1278697\,t^4\right. \\
&\left.+1122432\,t^3+743304\,t^2+338816\,t+90624\right)\cdot {F_2}^3\,{F_3}^2 \\
&-\frac{5^6}{2^{17}\cdot 3^4}\,t^3\left(t+1\right)\left(1392\,t^6+4010\,t^5+6983\,t^4+8136\,t^3\right. \\
&\left.+6983\,t^2+4010\,t+1392\right)\cdot F_2^2\cdot F_3^3 \\
&+\frac{5^8}{2^{20}\cdot 3^5}\,t^4\left(684\,t^6+2752\,t^5+5161\,t^4+6240\,t^3+5161\,t^2+2752\,t\right. \\
&\left.+684\right)\cdot F_2\cdot F_3^4 \\
&-\frac{5^9}{2^{19}\cdot 3^6}\,t^5\left(t+1\right)\left(42\,t^4+133\,t^3+167\,t^2+133\,t+42\right)\cdot F_3^5, \qquad (3.162)
\end{aligned}
$$

$$
\begin{aligned}
\frac{f_{3,3}^{(5)}}{t^{3/2}} \;=\;& -\frac{127}{3\cdot 5}\cdot\frac{f_{3,3}^{(1)}}{t^{3/2}} + 2\cdot\frac{f_{3,3}^{(3)}}{t^{3/2}} \\
&+\frac{1}{2^{20}\cdot 3^5\cdot 5}\big(2^{16}\cdot 3^4\cdot 5\cdot 17\,t^{14} + 1377976320\,t^{13} + 3016452096\,t^{12} \\
&+5930641920\,t^{11} + 9308313280\,t^{10} + 12328157240\,t^{9} + 14834544515\,t^{8} \\
&+15849843292\,t^{7} + 14834544515\,t^{6} + 12328157240\,t^{5} + 9308313280\,t^{4} \\
&+5930641920\,t^{3} + 3016452096\,t^{2} + 1377976320\,t + 2^{16}\cdot 3^4\cdot 5\cdot 17\big)\cdot F_3^5 \\
&-\frac{7^2}{2^{22}\cdot 3^5}\,t\,(t+1)\,\big(2^{19}\cdot 3^3\cdot 5\,t^{12} + 151511040\,t^{11} + 351000576\,t^{10} \\
&+605214208\,t^{9} + 835692208\,t^{8} + 1025976166\,t^{7} + 1112168875\,t^{6} \\
&+1025976166\,t^{5} + 835692208\,t^{4} + 605214208\,t^{3} + 351000576\;t^{2} \\
&+151511040\,t + 2^{19}\cdot 3^3\cdot 5\big)\cdot F_3^4\cdot F_4 \\
&+\frac{7^4}{2^{29}\cdot 3^5}\,t^2\,\big(2^{18}\cdot 3^3\cdot 5^2\,t^{12} + 572129280\,t^{11} + 1334317056\,t^{10} \\
&+2446757888\,t^{9} + 3545541888\,t^{8} + 4425343776\,t^{7} + 4784608975\,t^{6} \\
&+4425343776\,t^{5} + 3545541888\,t^{4} + 2446757888\,t^{3} + 1334317056\,t^{2} \\
&+572129280\,t + 2^{18}\cdot 3^3\cdot 5^2\big)\cdot F_3^3\cdot F_4^2 \\
&-\frac{7^6}{2^{27}\cdot 3^5}\,t^3\,(t+1)\,\big(2^{13}\cdot 3\cdot 5\cdot 7\,t^{10} + 2007040\,t^{9} + 4885888\,t^{8} + 7228048\,t^{7} \\
&+9666130\,t^{6} + 10423545\,t^{5} + 9666130\,t^{4} + 7228048\,t^{3} + 4885888\,t^{2} \\
&+2007040\,t + 2^{13}\cdot 3\cdot 5\cdot 7\big)\cdot F_3^2\cdot F_4^3 \\
&+\frac{7^8}{2^{34}\cdot 3^5}\,t^4\,\big(2^{14}\cdot 5\cdot 13\,t^{10} + 3665920\,t^{9} + 9078784\,t^{8} + 15185664\,t^{7} \\
&+20375540\,t^{6} + 22605185\,t^{5} + 20375540\,t^{4} + 15185664\,t^{3} + 9078784\,t^{2} \\
&+3665920\,t + 2^{14}\cdot 5\cdot 13\big)\cdot F_3\cdot F_4^4 \\
&-\frac{7^{10}}{2^{35}\cdot 3^5\cdot 5}\,t^5\,(t+1)\,\big(2^{13}\cdot 5\,t^{8} + 104960\,t^{7} + 267136\,t^{6} + 319904\,t^{5} \\
&+436441\,t^{4} + 319904\,t^{3} + 267136\,t^{2} + 104960\,t + 2^{13}\cdot 5\big)\cdot F_4^5.
\end{aligned}
\tag{3.163}
$$

3.B Polynomial solution calculations for $C_1^{(2)}(N;t)$

We here give explicitly the calculational details for $C_1^{(2)}(N;t)$.
Using the form (3.43) in the inhomogeneous equation (3.83) we find the recursion relation

for the coefficients $c^{(2)}_{1;n}$ for $n \neq N,\ N+1,\ N+2,\ N+3$

$$
\begin{aligned}
&2n\cdot(n-N)\,(n-2N-1)\cdot c^{(2)}_{1;n}\\
&\quad -\{2n^3-6Nn^2-2(4+N-2N^2)n+5+6N\}\cdot c^{(2)}_{1;n-1}\\
&\quad -\{2n^3-6(3+N)n^2+(46+34N+4N^2)n\,-35-38N-8N^2\}\cdot c^{(2)}_{1;n-2}\\
&\quad +2\,(n-2)(n-2N-3)(n-N-3)\cdot c^{(2)}_{1;n-3} \;=\; 0. \qquad (3.164)
\end{aligned}
$$

where by definition $c^{(2)}_{1;n} = 0$ for $n \leq -1$. This recursion relation has four terms instead of the three terms in the corresponding relation (3.92) for $c^{(2)}_{2;n}$. We note that, if we send $n \to 2N-n+3$ in (3.164), we see that $c^{(2)}_{1;n}$ and $c^{(2)}_{2N-n}$ satisfy the same equation. Since the coefficient of $c^{(2)}_{1;n}$ vanishes for $n = 0$, the term $c^{(2)}_{1;0}$ is not determined from (3.164) and by convention we set $c^{(2)}_{1;0} = 1$

Following the procedure used for $C^{(2)}_2(N;t)$ we note that equation (3.84) will be satisfied to order t^N if we choose the $c^{(2)}_{1;n}$ for $0 \leq n \leq N-1$ to be the corresponding coefficients in $t^{-1}\cdot u_2(N;t)\cdot u_2(N+1;t)$ and hence (3.47) follows.

The inhomogeneous recursion relations for $n = N,\ N+1$ are

$$
\begin{aligned}
A^{(2)}_1\{&-(2N^2+2N-5)\cdot c^{(2)}_{1;N-1} \;+(8N^2+8N-35)\cdot c^{(2)}_{1;N-2}\\
&-6(N-2)(N+3)\cdot c^{(2)}_{1;N-3}\} \;=\; -2N^2(2N+1)^2\,\lambda_N^2, \qquad (3.165)
\end{aligned}
$$

$$
\begin{aligned}
A^{(2)}_1\{&-2\,N\,(N+1)\cdot c^{(2)}_{1;N+1} \;-(2N+1)^2\cdot c^{(2)}_{1;N}\\
&+(6N^2+6N-5)\cdot c^{(2)}_{1;N-1} \;+4\,(N+2)(N-1)\cdot c^{(2)}_{1;N-2}\}\\
&= -\frac{(2N+1)^2\,(4N^3+4N^2-4N-1)\,\lambda_N^2}{4\,(N+1)}, \qquad (3.166)
\end{aligned}
$$

and the relations for $N+2,\ N+3$ are identical with $N,\ N+1$, respectively, with the (palindromic) replacement

$$
c^{(2)}_{1;N-m} \;\longrightarrow\; c^{(2)}_{1;N+m}. \qquad (3.167)
$$

If there were no inhomogeneous term (3.165) would be a new constraint in the coefficients $c^{(2)}_{1;n}$ for $n = N-1,\ N-2,\ N-3$. However this constraint does not hold (because the solution to the homogeneous equation has a term $t^{N+1}\ln t$).

The normalizing constant $A^{(2)}_1$ can be evaluated from (3.165) and the sum on the LHS of (3.165) is evaluated the same way the corresponding sum was for $C^{(2)}_2(N;t)$, by comparing with the full solution $t^{-1}\, u_2(N;t)\, u_2(N+1;t)$ of the homogeneous equation. Thus we find

$$- \, (2N^2+2N-5) \cdot \, c^{(2)}_{1;N-1}(N) \; + (8N^2+8N-35) \cdot \, c^{(2)}_{1;N-2}(N)$$
$$- \, 6\,(N+3)\,(N-2) \cdot \, c^{(2)}_{1;N-3}(N) \;\; = \;\; -2\,N^2\,(N+1)\,\lambda_N^2, \quad (3.168)$$

and, hence, we find from (3.165)

$$A_1^{(2)} \;\; = \;\; N\beta_N. \quad (3.169)$$

It remains to compute $c^{(2)}_{1;N}$ from (3.166). We obtain the palindromic solution by requiring that $c^{(2)}_{1,N+1} \; = \; c^{(2)}_{1;N-1}$ and thus (3.166) reduces to

$$(2N+1)^2 \cdot c^{(2)}_{1;N} \; + (4N^2+4N-5) \cdot c^{(2)}_{1;N-1} \; + 4(N+2)(N-1) \cdot c^{(2)}_{1;N-2}$$
$$= \;\; -\frac{(2N+1)^2\,(4N^3+4N^2-4N-1)\,\lambda_N^2}{4(N+1)}. \quad (3.170)$$

An equivalent and more efficient method for evaluating $c^{(2)}_{1;N}$, which avoids the need to evaluate the sums on the LHS of (3.170), is to directly evaluate $C_1^{(2)}(N;t)$ in terms of $C_2^{(2)}(N;t)$ by use of the coupled equation (3.82). From this we find

$$c^{(2)}_{1;N}(N) \;\; = \;\; \lambda_N^2 \;\; + \sum_{k=0}^{N-1} \, a_k(N) \cdot a_{N-1-k}(N), \quad (3.171)$$

and, by explicitly evaluating the sum in (3.171), we obtain the result (3.48). Finally, the $c^{(2)}_{1;\,n}$ for $N+1 \le n \le 2N$ are determined from the palindromy of (3.164).

3.C Coupled differential equations for $C_m^{(3)}(N;t)$

The four coupled differential equations for $C_m^{(3)}(N;t)$ are

$$
\begin{aligned}
&- \frac{2\,N+1}{2\cdot(t-1)\,t}\cdot C_0^{(3)}(t) \;\; - \frac{(N+1)\,(2\,tN+1+t)}{t^2\cdot(2\,N+1)\,(t-1)}\cdot C_1^{(3)}(t)\\
&- 2\,\frac{(N+1)^2\,(2\,tN+3)}{t^2\,(2\,N+1)^2\,(t-1)}\cdot C_2^{(3)}(t) \;\; - 8\,\frac{(N+1)^3\,(tN-t+3)}{(t-1)\,(2\,N+1)^3\,t^2}\cdot C_3^{(3)}(t)\\
&+ \frac{tN+2\,t-N-1}{(t-1)t}\cdot\frac{d}{dt}C_0^{(3)}(t) \; + 2\,\frac{(N+1)\,(tN-N+t)}{t\,(t-1)\,(2\,N+1)}\cdot\frac{d}{dt}C_1^{(3)}(t)\\
&+ 4\,\frac{(N+1)^2\,(tN-N+1)}{t\,(t-1)\,(2\,N+1)^2}\cdot\frac{d}{dt}C_2^{(3)}(t) + 8\,\frac{(N+1)^3\,(tN-N+2-t)}{t\,(2\,N+1)^3\,(t-1)}\cdot\frac{d}{dt}C_3^{(3)}(t)\\
&+ \frac{d^2}{dt^2}C_0^{(3)}(t) \; + 2\,\frac{N+1}{2\,N+1}\cdot\frac{d^2}{dt^2}C_1^{(3)}(t) + 4\,\frac{(N+1)^2}{(2\,N+1)^2}\cdot\frac{d^2}{dt^2}C_2^{(3)}(t)\\
&+ 8\,\frac{(N+1)^3}{(2\,N+1)^3}\cdot\frac{d^2}{dt^2}C_3^{(3)}(t) \;\; = \;\; \frac{3}{4}\,t^{N-1}\cdot(2\,N+1)\cdot B_0(N),
\end{aligned}
\tag{3.172}
$$

$$
\begin{aligned}
&- 2\,\frac{(N+1)\,(2\,N+6\,tN+3\,t+2)}{t^2\,(2\,N+1)^2}\cdot C_1^{(3)}(t)\\
&- 8\,\frac{(N+1)^2\,(4\,tN+4\,N+5+t)}{t^2\,(2\,N+1)^3}\cdot C_2^{(3)}(t)\\
&- 24\,\frac{(N+1)^3\,(6\,N+2\,tN+9-2\,t)}{(2\,N+1)^4\,t^2}\cdot C_3^{(3)}(t) \;\; + 6\,\frac{d}{dt}C_0^{(3)}(t)\\
&+ 4\,\frac{(N+1)\,(5\,tN+N+3\,t+1)}{t\,(2\,N+1)^2}\cdot\frac{d}{dt}C_1^{(3)}(t)\\
&+ 8\,\frac{(N+1)^2\,(2\,N+4\,tN+t+4)}{t\,(2\,N+1)^3}\cdot\frac{d}{dt}C_2^{(3)}(t)\\
&+ 48\,\frac{(N+1)^3\,(tN+N+3-t)}{t\,(2\,N+1)^4}\cdot\frac{d}{dt}C_3^{(3)}(t) \; + 4\,\frac{(t-1)\,(N+1)}{(2\,N+1)^2}\cdot\frac{d^2}{dt^2}C_1^{(3)}(t)\\
&+ 16\,\frac{(N+1)^2\,(t-1)}{(2\,N+1)^3}\cdot\frac{d^2}{dt^2}C_2^{(3)}(t) \; + 48\,\frac{(N+1)^3\,(t-1)}{(2\,N+1)^4}\cdot\frac{d^2}{dt^2}C_3^{(3)}(t)\\
&= \;\; \frac{3}{2}\,t^{N-1}\cdot(2\,N^2t+t+4\,tN-2\,N-2\,N^2)\cdot B_0(N),
\end{aligned}
\tag{3.173}
$$

$$
\begin{aligned}
&C_1^{(3)}(t) \;\; + 4\, \frac{(N+1)\,(2\,N+2-t)}{t\,(2\,N+1)^2} \cdot C_2^{(3)}(t) \;\; + 4\, \frac{(t-1)\,(N+1)}{(2\,N+1)^2} \cdot \frac{d}{dt} C_2^{(3)}(t) \\
&+ 4\, \frac{(N+1)^2\,(12\,N^2 - 16\,tN - 2\,t^2 N + 30\,N + 2\,t^2 + 18 - 17\,t)}{(2\,N+1)^4\,t^2} \cdot C_3^{(3)}(t) \\
&+ 8\, \frac{(t-1)\,(N+1)^2\,(tN + 5\,N - t + 5)}{t\,(2\,N+1)^4} \cdot \frac{d}{dt} C_3^{(3)}(t) \\
&+ 8\, \frac{(t-1)^2\,(N+1)^2}{(2\,N+1)^4} \cdot \frac{d^2}{dt^2} C_3^{(3)}(t) \quad = \quad \frac{3}{4}\, \frac{(2N+1)^2}{(N+1)} \cdot t^{N+1} \cdot B_0(N),
\end{aligned}
\tag{3.174}
$$

$$
\begin{aligned}
&6 \cdot C_0^{(3)}(t) \;\; + 4\, \frac{(N+1)\,(4\,N + 2\,tN + 4 - t)}{t\,(2\,N+1)^2} \cdot C_1^{(3)}(t) \\
&+ 8\, \frac{(N+1)^2\,(4\,N^2 + 8\,N^2 t - 10\,t^2 N + 10\,tN + 12\,N - t - 4\,t^2 + 8)}{(2\,N+1)^4 t^2} \cdot C_2^{(3)}(t) \\
&+ 48\, \frac{(N+1)^3\,(4\,N^2 - 2\,t^2 N - 10\,tN + 16\,N + 2\,t^2 + 13 - 14\,t)}{(2\,N+1)^5\,t^2} \cdot C_3^{(3)}(t) \\
&+ 16\, \frac{(t-1)\,(N+1)}{(2\,N+1)^2} \cdot \frac{d}{dt} C_1^{(3)}(t) \\
&+ 16\, \frac{(t-1)\,(N+1)^2\,(5\,tN + 3\,N + 2\,t + 3)}{t\,(2\,N+1)^4} \cdot \frac{d}{dt} C_2^{(3)}(t) \\
&+ 96\, \frac{(N+1)^3\,(t-1)\,(tN + 3\,N + 4 - t)}{t\,(2\,N+1)^5} \cdot \frac{d}{dt} C_3^{(3)}(t) \\
&+ 16\, \frac{(t-1)^2\,(N+1)^2}{(2\,N+1)^4} \cdot \frac{d^2}{dt^2} C_2^{(3)}(t) \;\; + 96\, \frac{(t-1)^2 (N+1)^3}{(2\,N+1)^5} \cdot \frac{d^2}{dt^2} C_3^{(3)}(t) \\
&= \quad 3\; t^N \cdot (3\,N\,(t-1) \;\; + 2\,t - 1) \cdot B_0(N),
\end{aligned}
\tag{3.175}
$$

where $B_0(N)$ is given by (3.111).

3.D The ODE and recursion relation for $C_3^{(3)}(N;t)$

The ODE for $C_3^{(3)}(N;t)$ can be found by carefully using the four coupled ODEs (3.172)–(3.175). First use (3.174) to solve for $C_1^{(3)}(N;t)$ and then use this is in Equation (3.175) in order to solve for $C_0^{(3)}(N;t)$. Next, use both $C_0^{(3)}(N;t)$ and $C_1^{(3)}(n;t)$ in (3.172) and (3.173) to produce ODEs of orders four in $C_2^{(3)}(N,t)$ and five in $C_3^{(3)}(N;t)$ in (3.172) and orders three in $C_2^{(3)}(N;t)$ and four in $C_3^{(3)}(N;t)$ in (3.173).

In the new (3.172), the fourth derivative of $C_2^{(3)}(N;t)$ can be solved in terms of the other derivatives, and likewise in the new (3.173), the third derivative of $C_2^{(3)}(N;t)$ can be solved in terms of the other derivatives. Taking the derivative of the expression for the third derivative of $C_2^{(3)}(N;t)$ and equating it to the expression for the fourth derivative of $C_2^{(3)}(N;t)$ we find an alternate expression for the third derivative of $C_2^{(3)}(N;t)$. Finally, equating the two expressions for the third derivative of $C_2^{(3)}(N;t)$, a full cancellation of all of the derivatives of $C_2^{(3)}(N;t)$ takes place, leaving a fifth order ODE in terms of only $C_3^{(3)}(t)$

$$
\begin{aligned}
&4\,\Big[2\,(N-1)\,(2\,N+1)\,(3\,N+1)\,(N+1)\,t^4\\
&\qquad -(2\,N+3)\,(36\,N^3-7\,N^2-69\,N-32)\,t^3\\
&\qquad +4\,(N+2)\,(36\,N^3-10\,N^2-116\,N-69)\,t^2\\
&\qquad -(2\,N+5)\,(60\,N^3-23\,N^2-275\,N-188)t\\
&\qquad +18\,(2\,N+3)\,(N+3)\,(N-3)\,(N+1)]\cdot C_3^{(3)}(t)\\
&-8\,\big[(N-1)\,(2\,N+1)\,(3\,N+1)\,(N+1)\,t^4\\
&\qquad -(-130\,N+40\,N^3-47+24\,N^4-73\,N^2)\,t^3\\
&\qquad +2\,\Big(18\,N^4-129+45\,N^3-113\,N^2-270\,N\Big)\,t^2\\
&\qquad -(-253\,N^2-422+24\,N^4-740\,N+80\,N^3)\,t\\
&\qquad +(N+1)\,\Big(6\,N^3+19\,N^2-114\,N-211\Big)\Big]\cdot t\cdot\frac{d}{dt}C_3^{(3)}(t)\\
&+20\,(t-1)\,\big[2\,N\,(N-1)\,(N+1)\cdot t^3\\
&\qquad\qquad -3\,(2\,N^3-4\,N^2-8\,N-3)\cdot t^2+3\,(-13+2\,N^3-8\,N^2-24\,N)\,t\big]\\
&\qquad\qquad -2\,(N-9)\,(N+2)\,(N+1)]\cdot t^2\cdot\frac{d^2}{dt^2}C_3^{(3)}(t)\\
&+40\,(t-1)^2\,\big[(N-1)^2\,t^2\;-\;(4\,N+1+2\,N^2)t+(N+5)\,(N+1)\big]\cdot t^3\cdot\frac{d^3}{dt^3}C_3^{(3)}(t)\\
&-40\,(t-1)^3\,\left[(N-1)t-N-1\right]\,t^4\cdot\frac{d^4}{dt^4}C_3^{(3)}(t)+8\,(t-1)^4\cdot t^5\cdot\frac{d^5}{dt^5}C_3^{(3)}(t)\\
&=\quad -\frac{3\,(t^2-1)\cdot N^2\,(2N+1)^6}{(N+1)^3}\cdot t^{N+3}\cdot B_0(N).
\end{aligned}
\tag{3.176}
$$

From this differential equation we obtain the recursion relation for the coefficients $c_{3;n}^{(3)}$ and the normalization constant $A_3^{(3)}$ defined by the form (3.53), where by definition $c_{3;n}^{(3)}=0$

for $n \leq -1$

$$
\begin{aligned}
& A_3^{(3)} \cdot \{8\,n\,(2\,N-n)\,(N-n)\,(N+n)\,(3\,N-n) \cdot c_{3;n}^{(3)} \\
& +4\,(2\,N+1-2\,n)\big(2-7\,n+7\,N-N^2+4\,n^4-12\,N^3-8\,n^3+24\,N^3n \\
& -4\,N^2n+11\,n^2+4\,N^2n^2-16\,Nn^3+24\,Nn^2-22\,Nn\big) \cdot c_{3;n-1}^{(3)} \\
& -16\,(N+1-n)\big(9-22\,n+22\,N+N^2+3\,n^4-18\,N^3-12\,n^3+18\,N^3n \\
& -6\,N^2n+23\,n^2+3\,N^2n^2-12\,Nn^3+36\,Nn^2-46\,Nn\big) \cdot c_{3;n-2}^{(3)} \\
& +4\,(2\,N+3-2\,n)\big(32-69\,n+69\,N+7\,N^2+4\,n^4-36\,N^3-24\,n^3+24\,N^3n \\
& -12\,N^2\,n+59\,n^2+4\,N^2n^2-16\,N\,n^3+72\,Nn^2-118\,N\,n\big) \cdot c_{3;n-3}^{(3)} \\
& -8\,(n-2)\,(2\,N+2-n)\,(N+2-n)\,(N-2+n)\,(3\,N+2-n) \cdot c_{3;n-4}^{(3)}\} \\
& = \ (\delta_{n,N}-\delta_{n,N+2}) \cdot \frac{3(2N+1)^6}{(N+1)^3} \cdot B_0. \qquad (3.177)
\end{aligned}
$$

We note by sending $n \to 2N-n+2$ that $c_{3;n}^{(3)}$ and $c_{3;2N-2-n}^{(3)}$ satisfy the same equation.

For $n=0$ (3.177) is identically zero for any $c_{3;0}^{(3)}$ which we set equal to unity by convention. For $0 \leq n \leq N-1$ the rhs of (3.177) vanishes and hence the $c_{3;n}^{(3)}$ are identical with the coefficients (3.118) of the solution (3.116) ot the homogeneous equation.

For $n=N$ the coefficient of $c_{3;N}^{(3)}$ vanishes, and thus if there were no inhomogeneous term, the coefficients $c_{3;n}^{(3)}$ for $n = N-4,\ N-3\ , N-2\ N-1$ would have to satisfy a non trivial constraint. This constraint does not, in fact, hold and is the reason that the homogeneous equation has a term $t^{N+3}\ln t$. However, with a nonvanishing inhomogeneous term, the equation for $n=N$ determines the normalization constant.

For $n=N+1$ the equation (3.177) reduces to

$$
\begin{aligned}
& 8\,(N+1)\,(N-1)\,(2\,N+1)\,(2\,N-1) \cdot (c_{3;N+1}^{(3)}-c_{3,N-4}^{(3)}) \\
& -8\,(2\,N+1)\,(2\,N-1)\big(2\,N^2-1\big) \cdot (c_{3;N}^{(3)}-c_{3;N-2}^{(3)}) \ = \ 0 \qquad (3.178)
\end{aligned}
$$

which will be satisfied by the palindromic property

$$
c_{3;n}^{(3)} \ = \ c_{3;2N-2-n}^{(3)} \qquad (3.179)
$$

with $n = N+1$ and $n=N$. Finally, the $c_{3;n}^{(3)}$ for $N \leq n \leq 2N-2$ are determined from the palindromy of (3.177).

3.E Homomorphisms for $C_0^{(3)}(N;t)$ and $C_2^{(3)}(N;t)$

The fifth order operator $M_0^{(3)}(N;t)$ in the direct sum decomposition (3.122) of $\Omega_0^{(3)}(N;t)$ has the homomorphism (in terms of the operator $L_2(N)$)

$$M_0^{(3)}(N) \cdot J_0^{(3)}(N;t) \;=\; G_0^{(3)}(N;t) \cdot \mathrm{Sym}^4(L_2(N+1)), \qquad (3.180)$$

where the intertwinners $J_0^{(3)}(N;t)$ and $G_0^{(3)}(N;t)$ are:

$$\begin{aligned} J_0^{(3)}(N;t) \;&=\; t^{N+1} \cdot (t-1) \cdot t \cdot \Bigl(D_t \,-\, \tfrac{d\ln(R_N^A)}{dt}\Bigr) \\ &=\; t^{N+1} \cdot \Bigl((t-1) \cdot t \cdot D_t \,-(2\,N \,+\, 2\,(N+1))\Bigr), \qquad (3.181) \\ G_0^{(3)}(N;t) \;&=\; t^{N+1} \cdot (t-1) \cdot t \cdot \Bigl(D_t \,-\, \tfrac{d\ln(R_N^B)}{dt}\Bigr), \qquad (3.182) \end{aligned}$$

where

$$\begin{aligned} R_N^A \;&=\; (t-1)^{2\,(2\,N+1)} \cdot t^{-2\,(N+1)}, \qquad (3.183) \\ R_N^B \;&=\; \tfrac{(t+1)\,(t-1)^{4\,N-3}}{t^{2\,N+6}} \cdot P_N, \qquad (3.184) \\ P_N \;&=\; (4\,N+3) \cdot (3\,N+2) \cdot (t^2+1) \,+2\,(20\,N^2 \,+15\,N \,+2) \cdot t \\ &=\; (4\,N+3) \cdot (3\,N+2) \cdot (t+1)^2 \qquad (3.185) \\ &\quad +4\,\,(2\,(2\,N+1)\,(N-1) \,+N) \cdot t. \end{aligned}$$

The homomorphism for $M_2^{(3)}(N;t)$ is

$$M_2^{(3)}(N;t) \cdot J_2^{(3)}(N;t) \;=\; G_2^{(3)}(N;t) \cdot \mathrm{Sym}^4(L_2(N+1)), \qquad (3.186)$$

where the intertwinners $J_2^{(3)}(N;t)$ and $G_2^{(3)}(N;t)$ are

$$J_2^{(3)}(N;t) \;=\; t^{N+2} \cdot \Bigl((t-1) \cdot t \cdot D_t \,+\, 2\,\,(N+1) \cdot t \,+2\,N\Bigr), \qquad (3.187)$$

$$G_2^{(3)}(N;t) \;=\; t^{N+2} \cdot (t-1) \cdot t \cdot \Biggl(D_t \,-\, \frac{d\ln\Bigl(R_N^B\Bigl(-(N+1)\Bigr)\Bigr)}{dt}\Biggr), \qquad (3.188)$$

where R_N^B is *exactly* the R_N^B in (3.184).

3.F Homomorphisms for $\Omega_4^{(4)}(N;t)$

Many exact results have been obtained on the intertwinners occurring in (3.144), (3.145), (3.146), (3.147) . Let us display the simplest ones.

For $J_0^{(4)}(N;t)$ we have

$$J_0^{(4)}(2;t) = t^2 \cdot (t+1) \cdot (2t^2+t+2),$$
$$J_0^{(4)}(3;t) = t^2 \cdot (t+1) \cdot \left(64\,t^4 + 16\,t^3 + 99\,t^2 + 16\,t + 64\right),$$
$$J_0^{(4)}(4;t) = t^2 \cdot (t+1) \cdot \left(576\,t^6 + 96\,t^5 + 730\,t^4 + 425\,t^3 + 730\,t^2 + 96\,t + 576\right),$$
$$J_0^{(4)}(5;t) = t^2 \cdot (t+1) \cdot \big(16384\,t^8 + 2048\,t^7 + 19264\,t^6$$
$$+6608\,t^5 + 28861\,t^4 + 6608\,t^3 + 19264\,t^2 + 2048\,t + 16384\big). \quad (3.189)$$

For $J_1^{(4)}(N;t)$ we have

$$2\,t^3 \cdot J_1^{(4)}(2;t) = (t-1) \cdot J_0^{(4)}(2;t) \cdot D_t - 2\,t \cdot (10t^4 + 2t^3 - 5t - 4),$$
$$64\,t^4 \cdot J_1^{(4)}(3;t) = (t-1) \cdot J_0^{(4)}(3;t) \cdot D_t$$
$$-\ 2\,t \cdot (448\,t^6 + 32\,t^5 + 95\,t^4 - 220\,t^2 - 112\,t - 128),$$
$$576 \cdot t^5 \cdot J_1^{(4)}(4;t) = (t-1) \cdot J_0^{(4)}(4;t) \cdot D_t$$
$$-\ 2\,t \cdot (5184\,t^8 + 192\,t^7 + 406\,t^6 + 1148\,t^5 - 2471\,t^3 - 1288\,t^2 - 864\,t - 1152),$$
$$16384 \cdot t^6 \cdot J_1^{(4)}(5;t) = (t-1) \cdot J_0^{(4)}(5;t) \cdot D_t$$
$$-\ 2\,t \cdot (180224\,t^{10} + 4096\,t^9 + 7488\,t^8 + 15168\,t^7 + 41307\,t^6$$
$$-\,83454\,t^4 - 44112\,t^3 - 29952\,t^2 - 22528\,t - 32768). \quad (3.190)$$

Finally, the simplest $J_2^{(4)}(N;t)$, namely $J_2^{(4)}(2;t)$ reads:

$$16\,t^6 \cdot J_2^{(4)}(2;t) = 8\,(t-1)^2 \cdot J_0^{(4)}(2;t) \cdot D_t^2$$
$$-\ t \cdot (t-1) \cdot (432t^4 + 80t^3 - 99t^2 - 240t - 208) \cdot D_t$$
$$+\ 3\,(1040t^5 - 1176t^4 - 233t^3 - 100t^2 + 168t + 256). \quad (3.191)$$

3.G Exact results for the $C_m^{(4)}$'s

The $f_{N,N}^{(4)}(t)$'s have a new feature not previously seen. The inhomogeneous terms on the ODE's for $C_m^{(2)}(N;t)$ and $C_m^{(3)}(N;t)$ begin at t^{N+a} where a is 0,1 or 2 depending on the values of m. Therefore to the order needed for the polynomial solution the logarithms in the solution $u_2(N)$ never can contribute. However, for $f_{N,N}^{(4)}(N;t)$ the order of the inhomogeneous terms grows as t^{2N} instead of t^N. Therefore, since logarithms occur in $u_2(N)$ at order t^{N+1} in order to find the polynomial solution to the 20-th order inhomogeneous equation in terms of the solutions of $u_2(N)$ and $u_1(N)$ we need to find linear combinations of solutions of the terms in the direct sum decomposition which cancel these logarithms.

This procedure for solving the inhomogeneous equations is too cumbersome by itself to obtain explicit results as was done for $f^{(2)}_{N,N}(t)$ and $f^{(3)}_{N,N}(t)$. However, when the cancellation of logarithms is combined with the Wronskian cancellation method of section 5 it is possible to conjecture results for $C^{(4)}_m(N;t)$ which have been verified to satisfy the 20th order inhomogeneous equations through $N = 10$:

$$\begin{aligned} C_0^{(4)} \overset{2N+1}{=} & -\bar{K}_0^{(4)} \cdot \frac{u_2^4(N+1)}{t^4} - \bar{K}_0^{(4)} \cdot \frac{4}{N} \cdot C_0^{(2)} \cdot \frac{u^2(N+1)}{t^2} \\ & + \frac{2}{3} \cdot \Big[C_0^{(2)} \cdot \frac{u_2^2(N+1)}{t^2} - 2\beta_N \cdot C_0^{(2)} \cdot \frac{u_2^2(N+1) \cdot u_2(N)}{t^2} \cdot F_{N+1} - C_1^{(2)} \cdot \frac{u_2^3(N+1)}{t^3} \cdot F_{N+1} \Big] \\ & + \frac{N\lambda^2}{3} \cdot \beta_N \cdot \frac{u_2^3(N+1)}{t^4} \cdot t^{N+2} \cdot F_{N+1}, \end{aligned} \tag{3.192}$$

$$\begin{aligned} C_1^{(4)} \overset{2N+1}{=} & \; 4 \cdot \bar{K}_0^{(4)} \cdot \beta_N \frac{u_2^3(N+1) u_2(N)}{t^3} \\ & + \bar{K}_0^{(4)} \cdot \frac{4}{N} \cdot \Big[2\,\beta_N \cdot C_0^{(2)} \cdot \frac{u_2(N+1) \cdot u_2(N)}{t} - C_1^{(2)} \cdot \frac{u_2^2(N+1)}{t^2} \Big] \\ & + \frac{2}{3} \cdot \Big[6\,\beta_N^2 \cdot C_0^{(2)} \cdot \frac{u_2(N+1) \cdot u_2^2(N)}{t} \cdot F_{N+1} + 2\,C_1^{(2)} \cdot \frac{u_2^3(N+1)}{t^3} \cdot F_N - 2\,C_2^{(2)} \cdot \frac{u_2^3(N+1)}{t^3} \cdot F_{N+1} \Big] \\ & - \frac{N\lambda^2}{3} \Big[\beta_N \cdot \frac{u_2^3(N+1)}{t^3} \cdot t^{N+1} \cdot F_N + 3\beta_N^2 \cdot \frac{u_2^2(N+1) \cdot u_2(N)}{t^3} \cdot t^{N+2} \cdot F_{N+1} \Big], \end{aligned} \tag{3.193}$$

$$\begin{aligned} C_2^{(4)} \overset{2N+1}{=} & -6\,\bar{K}_0^{(4)} \cdot \beta_N^2 \cdot \frac{u_2^2(N+1) \cdot u_2^2(N)}{t^2} \\ & - \Big(\frac{4}{N} \cdot \bar{K}_0^{(4)} + 2 \Big) \cdot \Big[\beta_N^2 \cdot C_0^{(2)} \cdot u_2^2(N) - 2\beta_N \cdot C_1^{(2)} \frac{u_2(N+1) \cdot u_2(N)}{t} + C_2^{(2)} \frac{u_2^2(N+1)}{t^2} \Big] \\ & + \frac{2}{3} \cdot \Big[-6\beta_N^3 \cdot C_0^{(2)} \cdot u_2^3(N) \cdot F_{N+1} - 9\,\beta_N \cdot C_1^{(2)} \cdot \frac{u_2(N+1) \cdot u_2(N)}{t} + 6\,C_2^{(2)} \cdot \frac{u_2^3(N+1)}{t^3} \cdot F_N \Big] \\ & + \frac{N\lambda^2}{3} \cdot \Big[3\beta_N^2 \cdot \frac{u_2^2(N+1) \cdot u_2(N)}{t^2} \cdot t^{N+1} \cdot F_N + 3 \cdot \beta_N^3 \cdot \frac{u_2(N+1) \cdot u_2^2(N)}{t^2} \cdot t^{N+2} \cdot F_{N+1} \Big], \end{aligned} \tag{3.194}$$

$$
\begin{aligned}
C_3^{(4)} \overset{2N+2}{=} \;& \bar{K}_0^{(4)} 4 \cdot \beta_N^3 \cdot \frac{u_2(N+1) \cdot u_2^3(N)}{t} \\
&- \bar{K}_0^{(4)} \cdot \frac{4}{N} \cdot \left[\beta_N^2 \cdot C_1^{(2)} \cdot u_2^2(N) \; - 2\, \beta_N \cdot C_2^{(2)} \cdot \frac{u_2(N+1)\, u_2(N)}{t} \right] \\
&+ \frac{2}{3} \cdot \left[2\, \beta_N^3 \cdot C_0^{(2)} \cdot u_2^3(N) \cdot F_N \; - 2\, \beta_N^3 \cdot C_1^{(2)} \cdot u_2^3(N) \cdot F_{N+1} \; - 6\, \beta_N \cdot C_2^{(2)} \cdot \frac{u_2^2(N+1) \cdot u_2(N)}{t^2 \cdot} \cdot F_N \right] \\
&- \frac{N\lambda^2}{3} \cdot \left[3\, \beta_N^3 \cdot \frac{u_2(N+1) \cdot u_2^2(N)}{t} \cdot t^{N+1} \cdot F_N \; + \beta_N^4 \cdot \frac{u_2^3(N)}{t}\, t^{N+2} \cdot F_{N+1} \right],
\end{aligned}
\tag{3.195}
$$

$$
\begin{aligned}
C_4^{(4)} \overset{2N+3}{=} \;& -\bar{K}_0^{(4)} \cdot \beta_N^4 \cdot u_2^4(N) \; - \bar{K}_0^{(4)} \cdot \frac{4}{N} \cdot \beta_N^2 \cdot C_2^{(2)} \cdot u_2^2(N) \\
&+ \frac{2}{3} \cdot \left[\beta_N^3 \cdot C_1^{(2)} \cdot u_2^3(N) \cdot F_N \; + 2\, \beta_N^2 \cdot C_2^{(2)} \cdot \frac{u_2(N+1) \cdot u_2^2(N)}{t} \cdot F_N \; + \beta_N^2 \cdot C_2^{(2)} \cdot u_2^2(N) \right] \\
&+ \frac{N\,\lambda^2}{3} \cdot \beta_N^4 \cdot u_2^3(N) \cdot t^{N+1} \cdot F_N
\end{aligned}
\tag{3.196}
$$

In order to construct the full $C_m^{(4)}$, the expressions above are series expanded up to the order of palindromy, with palindromy determining the rest of the terms. The palindromy points of the $C_m^{(4)}$ are given as follows: $m = 0 : 2N+1$, $m = 1 : 2N+1$, $m = 2 : 2N+2$, $m = 3 : 2N+2$, $m = 4 : 2N+3$. Therefore, the expressions above give all terms to all $C_m^{(4)}$ except for the middle term of $C_2^{(4)}$ at order $2N+2$, which is determined such that all terms in $f_N^{(4)}$ cancel up to and including $2N+3$.

Note that while these $C_m^{(4)}$ guarantee that all terms will vanish up to and including $2N+3$, it is not obvious that the expansion at order $2N+4$ will match the expansion of $f_N^{(4)}$, even though it is the case.

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Chapter 4

Paper 2

Diagonal Ising susceptibility: elliptic integrals, modular forms and Calabi-Yau equations

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Abstract

We give the exact expressions of the partial susceptibilities $\chi_d^{(3)}$ and $\chi_d^{(4)}$ for the diagonal susceptibility of the Ising model in terms of modular forms and Calabi-Yau ODEs, and more specifically, ${}_3F_2([1/3, 2/3, 3/2], [1, 1]; z)$ and ${}_4F_3([1/2, 1/2, 1/2, 1/2], [1, 1, 1]; z)$ hypergeometric functions. By solving the connection problems we analytically compute the behavior at all finite singular points for $\chi_d^{(3)}$ and $\chi_d^{(4)}$. We also give new results for $\chi_d^{(5)}$. We see in particular, the emergence of a remarkable order-six operator, which is such that its symmetric square has a rational solution. These new exact results indicate that the linear differential operators occurring in the n-fold integrals of the Ising model are not only "Derived from Geometry" (globally nilpotent), but actually correspond to "Special Geometry" (homomorphic to their formal adjoint). This raises the question of seeing if these "special geometry" Ising-operators, are "special" ones, reducing, in fact systematically, to (selected, k-balanced, ...) ${}_{q+1}F_q$ hypergeometric functions, or correspond to the more general solutions of Calabi-Yau equations.

4.1 Introduction

The magnetic susceptibility of the Ising model is defined in terms of the two point spin correlation function as

$$k_BT \cdot \chi \;=\; \sum_{M=-\infty}^{\infty} \sum_{N=-\infty}^{\infty} \{\langle \sigma_{0,0}\sigma_{M,N}\rangle \,-\mathcal{M}^2\}, \tag{4.1}$$

where $\mathcal{M}$ is the spontaneous magnetization of the Ising model.

The exact analysis of the Ising model susceptibility is the most challenging and important open question in the study of the Ising model today. This study [20, 254] began in 1973-76 by means of summing the $n^{\rm th}$ particle form factor contribution to the correlation function $\langle \sigma_{0,0}\sigma_{M,N}\rangle$. In these papers it was shown that for $T < T_c$

$$k_BT \cdot \chi(t) \;=\; (1-t)^{1/4} \cdot\, (1+\sum_{n=1}^{\infty} \tilde{\chi}^{(2n)}(t)), \tag{4.2}$$

where[1] $t = (\sinh 2E^v/k_BT \sinh 2E^h/k_BT)^{-2}$ and for $T > T_c$ by

$$k_BT \cdot \chi(t) \;=\; (1-t)^{1/4} \cdot \sum_{n=0}^{\infty} \tilde{\chi}^{(2n+1)}(t), \tag{4.3}$$

where $t = (\sinh 2E^v/k_BT \sinh 2E^h/k_BT)^{2}$.

The $\tilde{\chi}^{(n)}$ are given by n-fold integrals. In [254] the integrals for $\tilde{\chi}^{(1)}$ and $\tilde{\chi}^{(2)}$ were evaluated, and since that time there have been many important studies [234, 177, 69], of the behavior as $t \to 1$, of the singularities in the complex t-plane [177, 171, 172] and the analytic properties of $\tilde{\chi}^{(n)}$ as a function of t for the isotropic case [263, 266, 264, 265, 59, 47, 45, 51, 46, 170, 50] for $n = 3, 4, 5, 6$. These studies are still ongoing.

More recently it was discovered [57] that if in (4.1) the sum is restricted to the spins on the diagonal

$$k_BT \cdot \chi_d(t) \;=\; \sum_{N=-\infty}^{\infty} \{\langle \sigma_{0,0}\sigma_{N,N}\rangle -\mathcal{M}^2\}, \tag{4.4}$$

where

$$k_BT \cdot \chi_d(t) \;=\; (1-t)^{1/4} \cdot \left(1+\sum_{n=1}^{\infty} \tilde{\chi}_d^{(2n)}(t)\right), \tag{4.5}$$

for $T < T_c$ and

$$k_BT \cdot \chi_d(t) \;=\; (1-t)^{1/4} \cdot \sum_{n=0}^{\infty} \tilde{\chi}_d^{(2n+1)}(t), \tag{4.6}$$

[1] The classical interaction energy of the Ising model is $\mathcal{E} = -\sum_{j,k}\left(E^v \sigma_{j,k}\sigma_{j+1,k} + E^h \sigma_{j,k}\sigma_{j.k+1}\right)$ where $j(k)$ specifies the row (column) of a square lattice and the sum is over all sites of the lattice.

for $T > T_c$, **the** $\tilde{\chi}_d^{(n)}(t)$ **are** n**-fold integrals which have a much simpler form than the integrals for** $\tilde{\chi}^{(n)}(t)$ but retain all of the physically interesting properties of these integrals.

For $T < T_c$, the integrals $\tilde{\chi}_d^{(n)}(t)$ read

$$\begin{aligned}
\tilde{\chi}_d^{(2n)}(t) \; = \; & \frac{t^{n^2}}{(n!)^2} \frac{1}{\pi^{2n}} \cdot \int_0^1 \cdots \int_0^1 \prod_{k=1}^{2n} dx_k \cdot \frac{1 + t^n \, x_1 \cdots x_{2n}}{1 - t^n \, x_1 \cdots x_{2n}} \\
& \times \prod_{j=1}^{n} \left(\frac{x_{2j-1}(1-x_{2j})(1-tx_{2j})}{x_{2j}(1-x_{2j-1})(1-t\,x_{2j-1})} \right)^{1/2} \\
& \times \prod_{1 \le j \le n} \prod_{1 \le k \le n} (1 - t\, x_{2j-1}\, x_{2k})^{-2} \\
& \times \prod_{1 \le j < k \le n} (x_{2j-1} - x_{2k-1})^2 \, (x_{2j} - x_{2k})^2, \qquad (4.7)
\end{aligned}$$

where t is given by $t \, = \, (\sinh 2E^v/k_BT \sinh 2E^h/k_BT)^{-2}$.

For $T > T_c$, the integrals $\tilde{\chi}_d^{(n)}(t)$ read

$$\begin{aligned}
\tilde{\chi}_d^{(2n+1)}(t) \; = \; & \frac{t^{n(n+1)}}{\pi^{2n+1} n!(n+1)!} \cdot \int_0^1 \cdots \int_0^1 \prod_{k=1}^{2n+1} dx_k \\
\times & \frac{1 + t^{n+1/2}\, x_1 \cdots x_{2n+1}}{1 - t^{n+1/2}\, x_1 \cdots x_{2n+1}} \cdot \prod_{j=1}^{n} \Big((1-x_{2j})(1-t\,x_{2j}) \cdot x_{2j} \Big)^{1/2} \\
\times & \prod_{j=1}^{n+1} \Big((1-x_{2j-1})(1-t\,x_{2j-1}) \cdot x_{2j-1} \Big)^{-1/2} \\
\times & \prod_{1 \le j \le n+1} \prod_{1 \le k \le n} (1 - t\, x_{2j-1}\, x_{2k})^{-2} \qquad (4.8) \\
\times & \prod_{1 \le j < k \le n+1} (x_{2j-1} - x_{2k-1})^2 \prod_{1 \le j < k \le n} (x_{2j} - x_{2k})^2,
\end{aligned}$$

where $x \, = \, \sinh 2E^v/k_BT \sinh 2E^h/k_BT \, = \, t^{1/2}$.

In [57] we found that

$$\tilde{\chi}_d^{(1)}(t) \; = \; \frac{1}{1 - t^{1/2}}, \qquad \text{and:} \qquad \tilde{\chi}_d^{(2)}(t) \; = \; \frac{1}{4} \cdot \frac{t}{1-t}, \qquad (4.9)$$

and that $\tilde{\chi}_d^{(3)}(t)$ and $\tilde{\chi}_d^{(4)}(t)$ are solutions of differential equations of order 6 and 8. The corresponding linear differential operators of each is a direct sum of three factors. In both cases, there was a differential equation which was not solved in [57].

In this paper we complete this study of $\tilde{\chi}_d^{(3)}(t)$ and $\tilde{\chi}_d^{(4)}(t)$ by solving all of the differential equations involved. We then use the solutions of these equations to analytically compute the singular behavior at all of the finite singular points. In this way we are able to give analytic proofs of the results conjectured in appendix B of [57] by numerical means.

We split the presentation of our results into two parts: the solution of the differential equations and the use of the differential equations to compute the behavior of $\chi_d^{(3)}(t)$ and $\chi_d^{(4)}(t)$ at the singularities. The solution of the differential equations is presented in section 4.2 for $\chi_d^{(3)}(t)$ and in section 4.3 for $\chi_d^{(4)}(t)$. In particular we focus on the difficult problem of solving a particular order-four operator to discover, finally, a surprisingly simple result. The linear differential equation for $\chi_d^{(5)}(t)$ is studied in section 4.4, yielding the emergence of a remarkable order-six operator. The singular behaviors of $\chi_d^{(3)}(t)$ and $\chi_d^{(4)}(t)$ are given in section 4.5 and 4.6, respectively. This analysis requires that the (global) connection problem to be solved. The details of these computations are given in appendices C and D. We conclude in section 4.7 with a discussion of the emergence of ${}_{q+1}F_q$ hypergeometric functions, with all these previous results underlying modularity in the Ising model [262, 153] through elliptic integrals, modular forms and Calabi-Yau ODEs [7, 6].

4.2 Computations for $\tilde{\chi}_d^{(3)}(t)$

It was shown in [57] that $\tilde{\chi}_d^{(3)}(x)$ is annihilated by an order-six linear differential equation. The corresponding linear differential operator $\mathcal{L}_6^{(3)}$ is a direct sum of irreducible linear differential operators (the indices are the orders):

$$\mathcal{L}_6^{(3)} \; = \; L_1^{(3)} \oplus L_2^{(3)} \oplus L_3^{(3)}. \qquad (4.10)$$

The solution of $\mathcal{L}_6^{(3)}$ which is analytic at $x \, = \, 0$ is thus naturally decomposed as a sum:

$$Sol(\mathcal{L}_6^{(3)}) \; = \; a_1 \cdot \tilde{\chi}_{d;1}^{(3)}(x) \, + a_2 \cdot \tilde{\chi}_{d;2}^{(3)}(x) \, + a_3 \cdot \tilde{\chi}_{d;3}^{(3)}(x), \qquad (4.11)$$

where the $\tilde{\chi}_{d;j}^{(3)}$ are analytic at $x \, = \, 0$. The solutions $\tilde{\chi}_{d;1}^{(3)}(x)$ and $\tilde{\chi}_{d;2}^{(3)}(x)$ were explicitly found in [57] to be

$$\tilde{\chi}_{d;1}^{(3)}(x) \; = \; \frac{1}{1-x}, \qquad \text{and:} \qquad (4.12)$$

$$\tilde{\chi}_{d;2}^{(3)} \; = \; \frac{1}{(1-x)^2} \cdot {}_2F_1([1/2, -1/2], [1]; \, x^2) \; - \frac{1}{1-x} \cdot {}_2F_1([1/2, 1/2], [1]; \, x^2) \qquad (4.13)$$

where one notes the occurrence of $\tilde{\chi}_d^{(1)} = \tilde{\chi}_{d;1}^{(3)}$ in $\tilde{\chi}_d^{(3)}(x)$. The last term, $\tilde{\chi}_{d;3}^{(3)}(x)$, is annihilated by the order-three linear differential operator

$$L_3^{(3)} = D_x^3 + \frac{3}{2}\frac{n_2(x)}{d(x)} \cdot D_x^2 + \frac{n_1(x)}{(x+1)(x-1)\cdot x \cdot d(x)} \cdot D_x + \frac{n_0(x)}{(x+1)\,(x-1)^2 \cdot x \cdot d(x)},$$

where:

$$\begin{aligned}
d(x) &= (x+2)\,(1+2\,x)\,(x+1)\,(x-1)\,(1+x+x^2)\cdot x,\\
n_0(x) &= 2\,x^8 + 8\,x^7 - 7\,x^6 - 13\,x^5 - 58\,x^4 - 88\,x^3 - 52\,x^2 - 13\,x + 5,\\
n_1(x) &= 14\,x^8 + 71\,x^7 + 146\,x^6 + 170\,x^5 + 38\,x^4\\
&\quad -112\,x^3 - 94\,x^2 - 19\,x + 2.\\
n_2(x) &= 8\,x^6 + 36\,x^5 + 63\,x^4 + 62\,x^3 + 21\,x^2 - 6\,x - 4.
\end{aligned} \tag{4.14}$$

The linear differential operator $L_3^{(3)}$ has the following regular singular points and exponents:

$$\begin{array}{rccl}
1+x+x^2 = 0, & \rho = 0,\, 1,\, 7/2 & \rightarrow & x^{7/2},\\
x = 0 & \rho = 0,\, 0,\, 0 & \rightarrow & log^2 \;\; terms,\\
x = 1 & \rho = -2,\, -1,\, 1 & \rightarrow & x^{-2},\; x^{-1},\\
x = -1 & \rho = 0,0,0 & \rightarrow & log^2 \;\; terms,\\
x = \infty & \rho = 1,\, 1,\, 1 & \rightarrow & log^2 \;\; terms.
\end{array} \tag{4.15}$$

The singularities at $x = 2,\, -1/2$ are apparent.

By use of the command dsolve in Maple, we found in [47] that the solution to $L_3^{(3)}[\chi_{d;3}^{(3)}] = 0$ which is analytic at $x = 0$ is

$$\chi_{d;3}^{(3)}(x) = \frac{(1+2x)\cdot(x+2)}{(1-x)\cdot(x^2+x+1)} \cdot {}_3F_2([1/3, 2/3, 3/2], [1, 1];\, Q), \tag{4.16}$$

where the pullback Q reads:

$$Q = \frac{27}{4}\frac{(1+x)^2\cdot x^2}{(x^2+x+1)^3}. \tag{4.17}$$

Now the coefficients a_i in the sum decomposition (4.11) of $\tilde{\chi}_d^{(3)}(x)$, can be fixed by expanding and matching the rhs of (4.11) with the expansion of $\tilde{\chi}_d^{(3)}(x)$, and solving for the expressions in front of three x^n, with $n \geq n_0$, n_0 being the highest local exponent of $\mathcal{L}_6^{(3)}$.

This gives

$$\tilde{\chi}_d^{(3)}(x) \;=\; \frac{1}{3}\cdot\tilde{\chi}_{d;1}^{(3)}(x) \;+\frac{1}{2}\cdot\tilde{\chi}_{d;2}^{(3)}(x) \;-\frac{1}{6}\cdot\tilde{\chi}_{d;3}^{(3)}(x). \qquad (4.18)$$

By use of a family of identities on ${}_3F_2$ hypergeometric functions [185] (see eqn. 27 page 499) the expression (4.16) of $\tilde{\chi}_d^{(3)}(x)$ reduces to

$$\chi_{d;3}^{(3)}(x) \;=\; \frac{(1\,+2x)\cdot(x\,+2)}{(1-x)\cdot(x^2+x+1)}\cdot\Big[{}_2F_1([1/6,1/3],\,[1];\,Q)^2 \qquad (4.19)$$
$$+\frac{2Q}{9}\cdot{}_2F_1([1/6,1/3],\,[1];\,Q)\cdot{}_2F_1([7/6,4/3],\,[2];\,Q)\Big].$$

It is instructive, however, to discuss further the reason why $\chi_{d;3}^{(3)}(x)$ has this solution in terms of ${}_2F_1$ functions.

4.2.1 Differential algebra structures and modular forms

From a differential algebra viewpoint, the linear differential operator $L_3^{(3)}$ can be seen to be homomorphic[4] to its formal adjoint:

$$L_3^{(3)}\cdot adjoint(T_2) \quad=\quad T_2\cdot adjoint(L_3^{(3)}), \qquad (4.20)$$

where:

$$T_2 \quad=\quad \frac{(1+x+x^2)}{(1\,-x)^4}\cdot D_x^2 \quad+\frac{m_1(x)}{(x\,+1)\,(x\,-1)^5\,(2\,x+1)\,(x+2)\cdot x}\cdot D_x$$
$$-\frac{1}{4}\cdot\frac{m_0(x)}{(2\,x+1)\,(x+2)\,(x\,+1)\,(1+x+x^2)\,(x\,-1)^6\cdot x}, \qquad (4.21)$$

and where:

$$m_1(x) \;=\; 2\,x^6\,-6\,x^5\,-53\,x^4\,-92\,x^3\,-81\,x^2\,-34\,x\,-6,$$
$$m_0(x) \;=\; 8\,x^8\,-4\,x^7-222\,x^6\,-769\,x^5\,-1153\,x^4$$
$$-1341\,x^3\,-1129\,x^2\,-490\,x\,-84.$$

Related to (4.20) is the property that the symmetric square[2] of $L_3^{(3)}$ has a (very simple) rational solution $R(x)$. It thus factorises into an (involved) order-five linear differential

[4] For the notion of differential operator equivalence see [186] and [113].

[2] In general, for an irreducible operator homomorphic to its adjoint, a rational solution occurs for the symmetric square (resp. exterior square) of that operator when it is of odd (resp. even) order.

operator and an order-one operator having the rational solution:

$$R(x) \;=\; \frac{1\,+x\,+x^2}{(x-1)^4}, \qquad Sym^2(L_3^{(3)}) \;=\; L_5 \cdot \Bigl(D_x \;-\; \frac{d}{dx}\,\ln(R(x))\Bigr). \qquad (4.22)$$

In a forthcoming publication we will show that the homomorphisms of an operator with its adjoint naturally leads to a rational solution for its *symmetric square or exterior square* (according to the order of the operator).

Relation (4.20), or the fact that its symmetric square has a rational solution, means that this operator is not only a globally nilpotent operator [47], but it corresponds to "Special Geometry". In particular it has a "special" differential Galois group [139]. We will come back to this crucial point below, in section 4.3.1 (see (4.43)).

Operator $L_3^{(3)}$ is in fact homomorphic to the symmetric square of a second order linear differential operator[3]

$$X_2 \;=\; D_x^2 \;+\frac{1}{2}\cdot\frac{(2\,x\,+1)\cdot(x^2+x+2)}{(1+x+x^2)\cdot(1+x)\cdot x}\cdot D_x \;-\frac{3}{2}\cdot\frac{1}{(1+x+x^2)^2}, \qquad (4.23)$$

since one has the following simple operator equivalence [186] with two order-one intertwinners:

$$L_3^{(3)} \cdot M_1 \;=\; N_1 \cdot Sym^2(X_2), \qquad \text{with:} \qquad (4.24)$$
$$M_1 \;=\; \frac{(1+x)\cdot x}{(1-x)^2}\cdot D_x \;+\; \frac{1}{2}\cdot\frac{(1\,+2\,x)\cdot(x+2)}{(1+x+x^2)\cdot(1-x)},$$
$$N_1 \;=\; \frac{(1+x)\cdot x}{(1-x)^2}\cdot D_x \;-\; \frac{1}{2}\cdot\frac{24\,x^5+15\,x^4+8\,x^6-10\,x^3-69\,x^2-60\,x-16}{(1-x)^3(1\,+2\,x)\,(x\,+2)\,(1+x+x^2)}.$$

The second order operator X_2 is not homomorphic to the second order operators associated with the complete elliptic integrals of the first or second kind. However, from (4.20) and (4.22), we expect X_2 to be "special". This is confirmed by the fact that the solution $Sol(X_2,\, x)$ of X_2, analytical at $x \;=\; 0$ has the integrality property[1]: if one performs a simple rescaling $x \,\rightarrow\, 4\,x$ the series expansion of this solution has *integer* coefficients:

$$\begin{aligned} Sol(X_2,\,4\,x) \;=\;\; & 1\,+6\,x^2\,-24\,x^3\,+60\,x^4\,-96\,x^5 \\ & +120\,x^6\,-672\,x^7\,+5238\,x^8\,-25440\,x^9\,+\;\cdots \end{aligned} \qquad (4.25)$$

From this *integrality* property [46, 143], we thus expect the solution of X_2 to be associated with a modular form, and thus, we expect this solution to be a ${}_2F_1$ up to not just one, *but two pullbacks*. Finding these pullbacks is a difficult task, except if the pullbacks are rational functions. Fortunately we are in this simpler case of rational pullbacks, and consequently,

[3]Finding X_2 (or an operator equivalent to it) can be done by downloading the implementation [112].

[1]See also the concept of "Globally bounded" solutions of linear differential equations by G. Christol [101].

we have been able to find the solution [47] to deduce that the third order operator $L_3^{(3)}$ is ${}_3F_2$-solvable or ${}_2F_1$-solvable up to a Hauptmodul pullback [110] (see (4.16), (4.19)).

We can make the modular form character of (4.16), (4.19), which is already quite clear from the Hauptmodul form of (4.17), very explicit by introducing another rational expression, similar to (4.17):

$$Q_1(x) \;=\; \frac{27\,x\cdot(1+x)}{(1\,+\,2\,x)^6}. \tag{4.26}$$

The elimination of x between $Q \,=\, Q(x)$ (see (4.17)) and $Q_1 \,=\, Q_1(x)$ gives a polynomial relation with integer coefficients $\Gamma(Q,\, Q_1) \,=\, 0$, where the algebraic curve $\Gamma(u,\, v) \,=\, 0$ (which is, of course, a rational curve) is in fact a *modular curve* already encountered [46] associated with an order-three operator F_3 which emerged in $\tilde{\chi}^{(5)}$ (see [45]):

$$\begin{aligned} -4\,u^3\,v^3\,+12\,u^2\,v^2\cdot(v+u)\,-3\,u\,v\cdot(4\,v^2+4\,u^2\,-127\,u\,v) \\ +4\,(v+u)\cdot(u^2+v^2\,+83\,u\,v)\,-432\,u\,v \;=\; 0. \end{aligned} \tag{4.27}$$

The hypergeometric functions we encounter in (4.19), in the expression of the solution of $L_3^{(3)}$ actually have *two possible pullbacks* as a consequence of the remarkable identity on the *same* hypergeometric function[2]:

$$\begin{aligned} &(1\,+2\,x)\cdot\,{}_2F_1\Big([\frac{1}{6},\,\frac{1}{3}],\,[1];\,Q(x)\Big) \\ &\quad=\;(1+x+x^2)^{1/2}\cdot\,{}_2F_1\Big([\frac{1}{6},\,\frac{1}{3}],\,[1];\,Q_1(x)\Big). \end{aligned} \tag{4.28}$$

Other rational parametrizations and pullbacks can also be introduced, as can be seen in 4.A.

Relation (4.28) on ${}_2F_1$ yields other remarkable relations on the ${}_3F_2$ with the two pullbacks Q and Q_1: their corresponding order-three linear differential operators are homomorphic. Consequently one deduces, for instance, that ${}_3F_2([1/3, 2/3, 3/2], [1, 1];\, Q_1)$ is equal to the

[2] Along this line see for instance [238].

action of the second order operator U_2 on ${}_3F_2([1/3, 2/3, 3/2], [1, 1]; \, Q)$:

$$(x^2 \, + x \, + 1)^3 \cdot (1 \, - 8\, x \, - 8\, x^2) \cdot \, {}_3F_2([1/3, 2/3, 3/2], [1, 1]; \, Q_1)$$
$$= \, - U_2 \Big[{}_3F_2([1/3, 2/3, 3/2], [1, 1]; \, Q) \Big], \qquad \text{where:} \qquad (4.29)$$
$$U_2 \, = \, p(x) \cdot \Big(D_x^2 \, - \, 2 \cdot \frac{d}{dx} \ln \Big(\frac{x^2 \, + x \, + 1}{(x \, - 1)\,(x \, + 2)\,(1 + 2\,x)} \Big) \cdot D_x \Big)$$
$$+ \, \Big(\frac{1 + 2\,x}{x^2 \, + x \, + 1} \Big)^2 \cdot q(x), \qquad \text{with:}$$
$$p(x) \, = \, x^2 \cdot \, (1 + x)^2 \, (1 + 2\,x)^2 \, (1 + 8\,x + 12\,x^2 + 8\,x^3 + 4\,x^4),$$
$$q(x) \, = \, 8\,x^{10} \, + 40\,x^9 \, + 81\,x^8 \, + 84\,x^7 \, + 24\,x^6 \, - 54\,x^5 \, - 63\,x^4$$
$$-18\,x^3 \, - 2\,x \, - 1. \qquad (4.30)$$

thus generalizing the simple automorphic relation (4.28).

The *modularity* of these functions can also be seen from the fact that the series expansions of (4.16), (4.19), or (4.28) have the *integrality property* [46]. Actually, if one performs a simple rescaling $x \, \rightarrow \, 4\,x$, their series expansions actually have *integer coefficients* [46, 143]:

$$\tilde{\chi}^{(3)}_{d;3}(4\,x) \, = \, 2 \, + 20\,x \, + 104\,x^2 \, + 560\,x^3 \, + 2648\,x^4 \, + 12848\,x^5$$
$$+58112\,x^6 \, + 267776\,x^7 \, + 1181432\,x^8 \, + 5281328\,x^9 \, + \, \cdots, \qquad (4.31)$$

or

$${}_2F_1\Big([\frac{1}{6}, \frac{1}{3}], [1]; \, Q(x)\Big)[x \, \rightarrow \, 4 \cdot x] \, = \, 1 \, + 6\,x^2 \, - 24\,x^3 \, + 60\,x^4 \, - 96\,x^5$$
$$+120\,x^6 \, - 672\,x^7 + 5238\,x^8 \, - 25440\,x^9 \, + 81972\,x^{10} + \, \cdots, \qquad (4.32)$$

which can be turned into *positive integers* if we also change x into $-x$.

This provides more examples of the almost quite systematic occurrence [46] in the Ising model of (globally nilpotent [255]) linear differential operators associated with *elliptic curves*, either because one gets straightforward elliptic integrals, or because one gets operators associated with *modular forms*. For the diagonal susceptibility of the Ising model, are we also going to see the emergence of *Calabi-Yau*-like operators [7, 6] as already discovered in $\tilde{\chi}^{(6)}$ (see [46]) ?

4.3 Computations for $\tilde{\chi}^{(4)}_d(t)$

We now turn to the computation of $\tilde{\chi}^{(4)}_d(t)$, whose differential operator $\mathcal{L}^{(4)}_8$ is of order eight and is a direct sum of three irreducible differential operators [57]:

$$\mathcal{L}^{(4)}_8 \, = \, L^{(4)}_1 \oplus L^{(4)}_3 \oplus L^{(4)}_4. \qquad (4.33)$$

The solution of $\mathcal{L}_8^{(4)}$ analytic at $t = 0$, is thus naturally decomposed as a sum:

$$Sol(\mathcal{L}_8^{(4)}) \; = \; a_1 \cdot \tilde{\chi}^{(4)}_{d;1}(t) \, + a_2 \cdot \tilde{\chi}^{(4)}_{d;2}(t) \, + a_3 \cdot \tilde{\chi}^{(4)}_{d;3}(t). \qquad (4.34)$$

The solutions $\tilde{\chi}^{(4)}_{d;1}(t)$ and $\tilde{\chi}^{(4)}_{d;2}(t)$ were explicitly found[1] to be [57]

$$\tilde{\chi}^{(4)}_{d;1}(t) \; = \; \frac{t}{1-t}, \qquad \text{and:} \qquad (4.35)$$

$$\begin{aligned}
\tilde{\chi}^{(4)}_{d;2} \; &= \; \frac{9}{8} \cdot \frac{(1+t)\cdot t^2}{(1-t)^5} \cdot {}_3F_2\Big([\frac{3}{2}, \frac{5}{2}, \frac{5}{2}], [3, 3]; \frac{-4\,t}{(1-t)^2}\Big) \\
&= \frac{1+t}{(1-t)^2} \cdot {}_2F_1([1/2, -1/2], [1]; t)^2 \, - \, {}_2F_1([1/2, 1/2], [1]; t)^2 \\
& \quad - \frac{2t}{1-t} \cdot {}_2F_1([1/2, 1/2], [1]; t) \cdot {}_2F_1([1/2, -1/2], [1]; t). \qquad (4.36)
\end{aligned}$$

Here, again, one notes the occurrence of $\tilde{\chi}^{(2)}_d$ which is $\tilde{\chi}^{(4)}_{d;1}$ up to a normalization factor. One should be careful that the ${}_3F_2$ closed form (4.36) for $\tilde{\chi}^{(4)}_{d;2}$, together with the previous exact result (4.16), may yield to a ${}_{q+1}F_q$ with rational pullback, prejudice which has no justification for the moment.

Similar to $L_3^{(3)}$, the order-three operator for $\tilde{\chi}^{(4)}_{d;2}$, is homomorphic to its adjoint and its symmetric square has a simple rational function solution. The exact expressions (4.36) for $\tilde{\chi}^{(4)}_{d;2}$ are obtained in a similar way to the solution (4.16), (4.19) of $L_3^{(3)}$ in the previous section. We first find [112] that the corresponding linear differential operator is homomorphic to the symmetric square of a second order operator, which turns out to have complete elliptic integral solutions. The emergence in (4.36) of a ${}_3F_2$ hypergeometric function with the selected[2] rational pullback $-4\,t/(1-t)^2$ is totally reminiscent (even if it is not exactly of the same form) of Kummers's quadratic relation [238, 48], and its generalization to ${}_3F_2$ hypergeometric functions (see the relations (4.12), (4.13) in [15, 16], and (7.1) and (7.4) in [243]), for example:

$$\begin{aligned}
&{}_3F_2\Big([1 + \alpha - \beta - \gamma, \, \frac{\alpha}{2}, \frac{\alpha+1}{2}], [1+\alpha-\beta, \; 1+\alpha-\gamma]; \, \frac{-4\,t}{(1-t)^2}\Big) \\
& \quad = \; (1-t)^{\alpha} \cdot \, {}_3F_2([\alpha, \beta, \gamma], [1+\alpha-\beta, \; 1+\alpha-\gamma]; t). \qquad (4.37)
\end{aligned}$$

which relates *different*[8] ${}_3F_2$ hypergeometric functions. In fact, similar to (4.29), we do have

[1]The first line in (4.36) can, for instance, be found by directly using the command dsolve in Maple, and the second line follows by use of identity 520 on page 526 of [185]. This result is also easily obtained by using Maple to directly compute the homomorphisms between the order-three operator and the operator which annihilates ${}_2F_1([1/2, 1/2], [1]; t)$.

[2]The fundamental role played by such specific pullbacks as *isogenies of elliptic curves* has been underlined in [48].

[8]Note that the Saalschützian difference (4.54) (see below) of the ${}_3F_2$ in the lhs of (4.37) is independent

an equality between the ${}_3F_2$ hypergeometric function with the pullback $u \, = \, -4\,t/(1-t)^2$ and the *same* ${}_3F_2$ hypergeometric, where the pullback has been changed[5] into $v \, = \, -4\,(1-t)/t^2$,

$$ {}_3F_2\Big([\frac{3}{2}, \, \frac{5}{2}, \, \frac{5}{2}], \, [3, \, 3]; \, \frac{-4\,(1-t)}{t^2}\Big) \,\, = \,\, V_2\Big[{}_3F_2\Big([\frac{3}{2}, \, \frac{5}{2}, \, \frac{5}{2}], \, [3, \, 3]; \, \frac{-4\,t}{(1-t)^2}\Big)\Big], \qquad (4.38) $$

where V_2 is a second-order operator similar to the one in (4.29). The elimination of t in these two pullbacks, gives the simple genus zero curve

$$ u^2\,v^2 \,\, - 48\,v\,u \,\, + 64 \cdot \, (u+\,v) \,\,\, = \,\,\, 0, \qquad (4.39) $$

reminiscent of the simplest *modular equations* [109, 187, 241]. This genus zero curve can also be simply parametrized with $u \, = \, -4\,t/(1-t)^2$ and[9] $v \, = \, 4\,t\cdot(1-t)$. Again, one gets an identity similar to (4.38), with another order-two intertwinner $\mathcal{V}_2$:

$$ {}_3F_2\Big([\frac{3}{2}, \, \frac{5}{2}, \, \frac{5}{2}], \, [3, \, 3]; \, 4\,t\cdot(1-t)\Big) \,\, = \,\, \mathcal{V}_2\Big[{}_3F_2\Big([\frac{3}{2}, \, \frac{5}{2}, \, \frac{5}{2}], \, [3, \, 3]; \, \frac{-4\,t}{(1-t)^2}\Big)\Big]. \qquad (4.40) $$

4.3.1 Computation of $\tilde{\chi}^{(4)}_{d,3}(t)$

The third term $\tilde{\chi}^{(4)}_{d;3}$ in the sum (4.64) is **the solution analytic at** $x=0$ of the order-four linear differential operator

$$ L_4^{(4)} \,\, = \,\, D_t^4 \,\, + \frac{n_3(t)}{(t+1)\cdot d_4(t)} \cdot D_t^3 \,\, + 2\,\frac{n_2(t)}{(t^2-1)\cdot t\cdot d_4(t)} \cdot D_t^2 $$
$$ +2\,\frac{n_1(t)}{(t^2-1)\cdot t\cdot d_4(t)} \cdot D_t \,\,\, - 3\,\frac{(t+1)^2}{(t-1)\cdot t^2\cdot d_4(t)}, \qquad (4.41) $$

where:

$$ d_4(t) \,\, = \,\, (t^2-10\,t+1)\cdot\,(t-1)\cdot t, \qquad n_1(t) \,\, = \,\, t^4-13\,t^3-129\,t^2+49\,t\,-4, $$
$$ n_2(t) \,\, = \,\, 5\,t^5-55\,t^4-169\,t^3+149\,t^2-28\,t\,+2, $$
$$ n_3(t) \,\, = \,\, 7\,t^4-68\,t^3-114\,t^2+52\,t\,-5. $$

of α, β, γ and equal to $1/2$, in contrast with the rhs.

[5] This amounts to changing t into $1-t$.

[9] This amounts to changing t into $-t/(1-t)$ or $-1/(1-t)$.

The operator $L_4^{(4)}$ has the following regular singular points and exponents

$$\begin{array}{llll} t = \ \ 0, & \rho = 0,0,0,1 & \rightarrow & log^3 \quad terms, \\ t = \ \ 1, & \rho = -2,-1,0,1 & \rightarrow & t^{-2}, \ t^{-1}, \ log \quad term, \\ t = -1, & \rho = 0,1,2,7 & \rightarrow & t^7 \, log \quad term, \\ t = \ \infty, & \rho = 0,0,0,1 & \rightarrow & log^3 \quad terms. \end{array} \tag{4.42}$$

The singularities at the roots of $t^2 - 10t + 1 = 0$ are apparent. This order-four operator (4.41) is actually homomorphic to its formal adjoint:

$$adjoint(L_2) \cdot L_4^{(4)} \quad = \quad adjoint(L_4^{(4)}) \cdot L_2, \tag{4.43}$$

where L_2 is the order-two intertwinner:

$$\begin{aligned} L_2 \ &= \ \Big(D_t - \frac{d}{dt} \ln(r(t))\Big) \cdot D_t \qquad \text{where:} \\ r(t) \ &= \ \frac{(t^2 - 10t + 1)(t + 1)}{t \cdot (t-1)^3}. \end{aligned} \tag{4.44}$$

The remarkable equivalence of (4.41) with its adjoint is related to the fact that the exterior square of (4.41) has a rational function solution, that is, that the exterior square factors into an order-five operator L_5 and an order-one operator with a rational function solution (which coincides with $r(t)$ in (4.44)).

$$Ext^2(L_4^{(4)}) \quad = \quad L_5 \cdot \Big(D_t - \frac{d}{dt} \ln(r(t))\Big). \tag{4.45}$$

In other words, the (irreducible) order-four operator (4.41) is not only globally nilpotent (*"Derived from Geometry"* [47]) it is a "special" G-operator [255] (Special Geometry): its *differential Galois group* becomes "special" (symplectic of orthogonal groups, see for instance [139]).

This highly selected character of the order-four operator (4.41) is further confirmed by the *"integrality property"* [46] of the series expansion of its analytical solution at $t = 0$:

$$\begin{aligned} Sol(L_4^{(4)}) \ = \ \ & t \ + 11/8\, t^2 \ + 27/16\, t^3 \ + 2027/1024\, t^4 \\ & +9269/4096\, t^5 \ + 83297/32768\, t^6 \ + \ \cdots \end{aligned} \tag{4.46}$$

which, in one rescaling $t = 16\,u$, becomes a series with *integer* coefficients:

$$Sol(L_4^{(4)}) = 16\,u + 352\,u^2 + 6912\,u^3 + 129728\,u^4 + 2372864\,u^5$$
$$+42648064\,u^6 + 756609024\,u^7 + 13286784384\,u^8 \qquad (4.47)$$
$$+231412390144\,u^9 + 4002962189824\,u^{10} + 68843688570880\,u^{11}$$
$$+1178125203260416\,u^{12} + 20074611461902336\,u^{13}$$
$$+340769765322760192\,u^{14} + 5765304623564259328\,u^{15}$$
$$+97249731220784896768\,u^{16} + 1636034439292348588288\,u^{17} + \cdots$$

This *integrality property* [143] suggests a *modularity* [46, 153, 262] of this order-four operator (4.41). The simplest scenario would correspond to (4.46) being elliptic integrals or, beyond, modular forms that would typically be, up to differential equivalence, a ${}_2F_1$ hypergeometric function with *not one but two pullbacks* (the relation bewteen these two pullbacks being a modular curve). More involved scenarios would correspond to (4.41) being a *Calabi-Yau ODE* [7, 6] or some other *mirror map* (see [46]). We have first explored the simplest scenarios (elliptic integrals, *modular forms*), which, as far as differential algebra is concerned, amounts to seeing if this order-four operator (4.41) corresponds, up to differential operator equivalence, to symmetric powers of a second order operator. This simple scenario is ruled out[1]. We are now forced to explore the much more complex Calabi-Yau framework, with two possible scenarios: a general Calabi-Yau order-four ODE [7, 6], or a Calabi-Yau order-four ODE that is ${}_4F_3$ solvable, the solution like (4.46) being expressed, up to operator equivalence, in term of a ${}_4F_3$ hypergeometric function *up to a pullback that remains to be discovered.* This last situation would correspond to the ${}_4F_3$ Calabi-Yau situation we already encountered in $\tilde{\chi}^{(6)}$ (see [46]). The ${}_4F_3$ solvability is clearly a desirable situation, because everything can be much more explicit.

In constrast with the (globally nilpotent) order-two operators, finding that a given order-four operator corresponds to a given ${}_4F_3$ operator up to a pullback (and up to homomorphisms) is an extremely difficult task, because the necessary techniques have not yet been developed. Quite often, it goes the other way (no go result): one can rule out a given order-four operator being a ${}_4F_3$ operator with a rational pullback (up to differential operator equivalence).

In fact, and fortunately, operator (4.41) turns out to be, a nice example. It has singularities at $0, 1, -1, \infty$, and these points have to be mapped to $0, 1, \infty$ (the singularities of ${}_4F_3$ hypergeometric functions) by the pullback. *Assuming a rational pullback of degree two*, there is a systematic algorithm to find all of the rational pullback mapping $0, 1, -1, \infty$ onto $0, 1, \infty$. This systematic algorithm is described in [89] for order-two operators, but the same approach works (with little change) for fourth order operators as well[5]. The rational

[1] See for instance, van Hoeij's program [112] from ISSAC'2007.

[5] For order-two equations with four singularities (HeunG ...), there are already hundreds of cases (now all found), see [114]. Looking at the size of that table [114] it is clear that providing an algorithm for finding pullbacks will be quite hard.

pullback function can actually be obtained (with some trial and error) from this mapping of singularities constraint and from the exponent-differences, in the same way as in section 2.6 in [49]. The reader who is just interested in the surprisingly simple final result and not the mathematical structures, in particular the interesting relations between some Calabi-Yau ODEs and selected ${}_4F_3$, can skip the next three subsections[1] and jump directly to the solution of (4.41) given by (4.63) with (4.61).

4.3.2 Simplification of $L_4^{(4)}$

As a “warm up”, let us, for the moment, try to simplify the order-four operator (4.41), getting rid of the apparent singularities $t^2 - 10t + 1 = 0$, and trying to take into account all the symmetries of (4.41): for instance, one easily remarks that (4.41) is actually invariant by the involutive symmetry $t \leftrightarrow 1/t$.

Let us introduce the order-four operator

$$\mathcal{L}_4 \;=\; D_x^4 + \frac{10\,x^2 - 2\,x - 5}{(x-1)\,(1+2\,x)\,x} \cdot D_x^3 + \frac{1}{4} \cdot \frac{(5x+4)\cdot(6\,x^2 - 13\,x + 4)}{(x-1)^2\,(1+2\,x)\,x^2} \cdot D_x^2 + \frac{1}{4} \cdot \frac{x+8}{(x-1)^2\,(1+2\,x)\,x^2} \cdot D_x - \frac{3}{4\cdot(x-1)\,(1+2\,x)\,x^3}, \tag{4.48}$$

where $1 + 2\,x = 0$ is an apparent singularity. One can easily verify that the order-four operator (4.41) is the previous operator (4.48), where we have performed the $t \leftrightarrow 1/t$ invariant pullback:

$$x \;=\; -\frac{4\,t}{(1-t)^2}, \qquad L_4^{(4)} \;=\; \mathcal{L}_4\Big[x \rightarrow -\frac{4\,t}{(1-t)^2}\Big]. \tag{4.49}$$

The operator (4.48) is homomorphic to another order-four operator with *no apparent singularities*

$$\mathcal{M}_4 \;=\; D_x^4 + 2\cdot\frac{5\,x - 4}{(x-1)\cdot x} \cdot D_x^3 + \frac{1}{4}\cdot\frac{(95\,x^2 - 160\,x + 56)}{(x-1)^2\cdot x^2} \cdot D_x^2 + \frac{1}{4}\cdot\frac{45\,x^3 - 124\,x^2 + 104\,x - 16}{(x-1)^3\cdot x^3} \cdot D_x - \frac{2\,x - 5}{4\cdot(x-1)^3\cdot x^3}, \tag{4.50}$$

as can be seen by the (very simple) intertwinning relation:

$$\mathcal{M}_4 \cdot D_x \;=\; \Big(D_x + \frac{10\,x^2 - 4\,x - 3}{(x-1)\,(1+2\,x)\cdot x}\Big) \cdot \mathcal{L}_4. \tag{4.51}$$

This last operator with no apparent singularities, is homomorphic to its adjoint in a very

[1]Which correspond, in fact, to the way we originally found the result.

simple way:

$$adjoint(\mathcal{M}_4) \cdot x^4 \cdot (1-x) \quad = \quad x^4 \cdot (1-x) \cdot \mathcal{M}_4. \tag{4.52}$$

Do note that, remarkably, the exterior square of $\mathcal{M}_4$, *is an order five operator* and not the order six operator one could expect generically from an intertwinning relation like (4.51) (the exterior square of the order-four operator (4.48) is of order six with the rational function solution $(1 + 2x)/x$). Taking into account all these last results, no apparent singularities, the singularities being the standard $0,\ 1,\ \infty$ singularities, the intertwinning relation (4.51), the fact that the exterior square is of order five, the order-four operator (4.50) looks like a *much simpler* operator to study than the original operator (4.41).

4.3.3 k-balanced ${}_4F_3$ hypergeometric function

Let us make here an important preliminary remark on the ${}_4F_3$ linear differential operators. Let us consider a ${}_4F_3$ hypergeometric function

$${}_4F_3([a_1,\, a_2,\, a_3,\, a_4],\, [b_1,\, b_2,\, b_3]; t), \tag{4.53}$$

with *rational values* of the parameters a_i and b_j. Its exponents at $x = 0$ are $0,\ 1 - b_1,\ 1 - b_2,\ 1 - b_3$, its exponents at $x = \infty$ are $a_1,\ a_2,\ a_3,\ a_4$, and its exponents at $x = 1$ are $0,\ 1,\ 2$ and $\mathcal{S}$ where $\mathcal{S}$ is the *Saalschützian difference*:

$$\mathcal{S} \;=\; (b_1 + b_2 + b_3) \; - (a_1 + a_2 + a_3 + a_4). \tag{4.54}$$

The Saalschützian condition [205, 206, 207, 242] $\mathcal{S} = 1$ is thus a condition of confluence of two exponents at $x = 1$.

The linear differential order-four operators annihilating the ${}_4F_3$ hypergeometric function (4.53) are necessarily globally nilpotent, and *they will remain globally nilpotent up to pullbacks and up to differential operator equivalence*[2]. In contrast, the corresponding order-four operators are not, for generic (rational) values of the parameters a_i and b_j, such that they are homomorphic to their formal adjoint ("special geometry"), or such that their exterior square, of order-six, has a rational function solution (a degenerate case corresponding to the exterior square being of order *five*).

These last "special geometry" conditions (see (4.43) and (4.45)), correspond to selected algebraic subvarieties in the parameters a_i and b_j. In the particular case of *the exterior square of the order-four operator being of order five*[1], we will show, in forthcoming publications, that the parameters a_i and b_j of the hypergeometric functions are necessarily

[2] Global nilpotence is preserved by pullback (change of variables) and by homomorphisms (operator equivalence).

[1] This condition is seen by some authors, see (11) in [108], as a condition for the ODE to be a *Picard-Fuchs equation* of a Calabi-Yau manifold. These conditions, namely (11) in [108], are preserved by pullback, not operator equivalence.

restricted to three sets of algebraic varieties: a *codimension-three algebraic variety* included in the Saalschützian condition [205, 206, 207, 242] $\mathcal{S} = 1$ and two (self-dual for the adjoint) *codimension-four algebraic varieties*, respectively included in the two hyperplanes $\mathcal{S} = -1$ and $\mathcal{S} = 3$.

Imagine that one is lucky enough to see the order-four operator (4.50) (which is such that its exterior square is of order five) as a ${}_4F_3$ solvable Calabi-Yau situation: one is, thus, exploring particular ${}_4F_3$ hypergeometric functions corresponding to these (narrow sets of) algebraic varieties which single out particular ($k = -1, 1, 3$) *k-balanced* hypergeometric functions[5] (rather than the well-poised hypergeometric functions, or very well-poised[8] hypergeometric functions [164, 165] one could have imagined[1]). We are actually working up to operator equivalence, which amounts to performing derivatives of these hypergeometric functions. It is straightforward to see that the n-th derivative of a hypergeometric function shifts the Saalschützian difference (4.54) by an integer, and that this does not preserve the condition for the exterior square of the corresponding order-four operator to be order five: it becomes an order-six operator, homomorphic to its formal adjoint, with a rational function solution. The natural framework for seeking ${}_4F_3$ hypergeometric functions (if any) for our order-four operators (4.41), (4.48), (4.50) is thus (selected) k-balanced hypergeometric functions (rather than the well-poised, or very well-poised, hypergeometric functions [165] ...).

4.3.4 $L_4^{(4)}$ is ${}_4F_3$ solvable, up to a pullback

Let us restrict ourselves to the, at first sight, simpler order-four operators (4.48), (4.50): even if we know exactly the rational values of the parameters a_i and b_j, finding that a given order-four operator corresponds to this given ${}_4F_3$ operator, up to a pullback (and up to homomorphisms), remains a quite difficult task. We have first studied the case where the pullback in our selected ${}_4F_3$ hypergeometric functions is a rational function. This first scenario has been ruled out on arguments based on the matching of the singularities and of the exponents of the singularities.

We thus need to start exploring pullbacks that are *algebraic functions*. Algebraic functions can branch at certain points (this can, for instance, turn a regular point into a singular point). The set of algebraic functions is a very large one, so we started[2] with the simplest algebraic function situation, namely, *square roots singularities*. A first examination of the

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[5] k-balanced hypergeometric functions correspond to the Saalschützian difference being an integer : $\mathcal{S} = k$, k an integer.

[8] Note that very well-poised hypergeometric series are known [193] to be related with $\zeta(2), \zeta(3)$, ..., which are constants known to occur in the Ising model [265].

[1] Note that the conditions to be well-poised hypergeometric series are actually preserved by the transformation $a_i \rightarrow 1 - a_i$, $b_j \rightarrow 2 - b_j$, which corresponds to changing the linear differential operator, associated with hypergeometric functions, into its formal adjoint.

[2] And also because we had a Ising model prejudice in favour of square roots [50] ...

matching of the singularities, and of the exponents of the singularities, indicates that we should have square roots at $x = 1$ only.

Along this square root line, let us recall the well-known *inverse Landen transformation* in terms of k, the *modulus of the elliptic functions parametrizing the Ising model*:

$$k \quad \longrightarrow \quad \frac{1 - \sqrt{1-k^2}}{1 + \sqrt{1-k^2}}. \tag{4.55}$$

In terms of the variable $x = k^2$, this inverse Landen transformation reads:

$$\begin{aligned} x \quad \longrightarrow \quad P(x) \quad &= \quad \Bigl(\frac{1 - \sqrt{1-x}}{1 + \sqrt{1-x}}\Bigr)^2 \\ &= \quad \frac{x^2 - 8x + 8}{x^2} \quad - 4 \cdot (2-x) \cdot \frac{(1-x)^{1/2}}{x^2}. \end{aligned} \tag{4.56}$$

Using this pullback $P(x)$, we have actually been able to obtain the solution of the order-four differential operator (4.50) in terms of four terms like

$${}_4F_3\Bigl([\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}], [1, 1, 1], P(x)\Bigr). \tag{4.57}$$

This slightly involved solution is given in 4.B.

We can now get the solution of (4.41), the original operator $L_4^{(4)}$, from this slightly involved result, since (4.41) is (4.50) up to a simple pullback, namely the change of variable (4.49). Going back from (4.49) to the original variable t in $L_4^{(4)}$, the previous pullback (4.56) simplifies remarkably:

$$P\Bigl(-\frac{4t}{(1-t)^2}\Bigr) \quad = \quad \frac{1+t^4}{2 \cdot t^2} \; - \; \frac{1-t^4}{2 \cdot t^2} \quad = \quad t^2, \tag{4.58}$$

the Galois conjugate of (4.56) giving $1/t^2$. Of course, once this key result is known, namely that a t^2 pullback works, it is easy to justify after the fact this simple monomial result: after all, $L_4^{(4)}$ has singularities at $0, 1, -1, \infty$, and these points can be mapped (under t^2) to $0, 1, \infty$ (i.e. the singularities of ${}_4F_3$ hypergeometric functions).

Pullbacks have a natural structure with respect to *composition of functions*[1]. It is worth noting that (4.58) describes the *composition of two well-known isogenies of elliptic curves*, the *inverse Landen transformation* (4.56) and the *rational isogeny* $-4t/(1-t)^2$ underlined by R. Vidunas [239] and in [48], giving the simple quadratic transformation $t \rightarrow t^2$.

All this means that the solution of $L_4^{(4)}$ can be expressed in terms of the hypergeometric

[1]Suppose that an operator O_2 is a pullback of an operator O_1, where the pullback f is a rational function and that O_3 is also a pullback of O_1, where the pullback is a rational function g. Then O_3 is also a pullback of O_2. To compute this pullback function, one has to compose g and the inverse of f.

function

$$ {}_4F_3\Big([\frac{1}{2},\, \frac{1}{2},\, \frac{1}{2},\, \frac{1}{2}],\, [1,\, 1,\, 1],\, t^2\Big) \qquad (4.59) $$

and its derivatives. Actually considering the hypergeometric operator $\mathcal{H}$ having (4.59) as a solution, it can be seen to be homomorphic to (4.41)

$$ \mathcal{A}_3 \cdot \mathcal{H} \;\; = \;\; L_4^{(4)} \cdot A_3, \qquad (4.60) $$

where the order-three intertwinners A_3 and $\mathcal{A}_3$ read, respectively, (with $d_3(t) \, = \, t \cdot (t+1) \cdot (t-1)^2 \cdot (t^2 - 10\,t + 1)$):

$$ \begin{aligned} A_3 \;\; &= \;\; 2 \cdot (1+t) \cdot t^3 \cdot D_t^3 \; + \frac{2}{3} \cdot \frac{16t^2 - t - 11}{t-1} \cdot t^2 \cdot D_t^2 \\ &+ \frac{1}{3} \cdot \frac{31t^2 - 4t - 11}{t-1} \cdot t \cdot D_t \; + t, \end{aligned} \qquad (4.61) $$

$$ \begin{aligned} \mathcal{A}_3 \;\; = \;\; & \frac{2}{t\,-1} \cdot D_t^3 \; + \frac{2}{3} \cdot \frac{1}{d_3(t)} \cdot (10\,t^4 - 107\,t^3 - 225\,t^2 + 163\,t - 17) \cdot D_t^2 \\ & + \frac{1}{3} \cdot \frac{1}{t \cdot d_3(t)} \cdot \, (5\,t^4 - 66\,t^3 - 900\,t^2 + 290\,t - 33) \cdot D_t \\ & + \frac{1}{3} \cdot \frac{1}{t \cdot d_3(t)} \cdot \, (t^3 - 21\,t^2 \, + 99\,t - 23). \end{aligned} \qquad (4.62) $$

From the intertwinning relation (4.60), one easily finds that the solution of $L_4^{(4)}$ which is analytic at $t \, = \, 0$ is A_3 acting on (4.59):

$$ \tilde{\chi}^{(4)}_{d;3} \;\; = \;\; A_3 \Big[{}_4F_3([1/2,\, 1/2,\, 1/2,\, 1/2], [1,\, 1,\, 1];\, t^2) \Big]. \qquad (4.63) $$

Having with (4.63) a normalization for $\tilde{\chi}^{(4)}_{d;3}$, we can now fix the values of the coefficients a_i in the sum (4.34) for $\tilde{\chi}^{(4)}_d(t)$. They can be fixed by expanding and matching the rhs with (4.34) and $\tilde{\chi}^{(4)}_d(t)$, and solving for the expressions in front of three t^n, with $n \, \ge \, n_0$, n_0 being the highest local exponent of $\mathcal{L}_8^{(4)}$. This gives

$$ \tilde{\chi}^{(4)}_d \;\; = \;\; \frac{1}{2^3} \cdot \tilde{\chi}^{(4)}_{d;1} \; + \frac{1}{3 \cdot 2^3} \cdot \tilde{\chi}^{(4)}_{d;2} \; - \frac{1}{2^3} \cdot \tilde{\chi}^{(4)}_{d;3}. \qquad (4.64) $$

Remark: It is quite surprising to find exactly the same ${}_4F_3$ hypergeometric function (4.59) with the exact *same*, remarkably simple pullback t^2 as the one we already found in the order-four Calabi-Yau operator L_4 in $\tilde{\chi}^{(6)}$ [46].

Comment: Of course, from a mathematical viewpoint, when looking for a pullback one can in principle always ignore all apparent singularities. These calculations displayed here look a bit paradoxical: the calculations performed with the (no apparent singularities) operator (4.50), which looks *simpler* (it has an exterior square of order five, and is very simply homomorphic to its adjoint, ...) turns out to have a more complicated pullback (4.56), than the amazingly simple pullback (namely t^2) we finally discover for the original operator (4.41) (see (4.63)). The "complexity" of the original operator (4.41) is mostly encapsulated in the order-three intertwinner A_3 (see (4.61)). The "${}_4F_3$-solving" of the operator amounts to reducing the operator, up to operator equivalence (4.60), to a ${}_4F_3$ hypergeometric operator up to a pullback. Finding the pullback is the difficult step: as far as "${}_4F_3$-solving" of an operator is concerned, what matters is the *complexity of the pullback*, not the complexity of the operator equivalence.

Ansatz: Of course, knowing the key ingredient in the final result (4.63), namely that the pullback is just t^2, it would have been much easier to get this result. Along this line one may recall the conjectured existence of a natural boundary at unit circle $|t| = 1$ for the full susceptibility of the Ising model, and, more specifically for the diagonal suscpetibility n-fold integrals we study here, the fact that the singularities are all N-th root of unity (N integer). Consequently, one may have, for the Ising model, a t^N prejudice for pullbacks.

In forthcoming studies of linear differential operators occurring in the next (bulk) $\tilde{\chi}^{(n)}$'s or (diagonal) $\tilde{\chi}_d^{(n)}$'s, when trying to see if these new (Calabi-Yau like, special geometry) operators are ${}_{q+1}F_q$ reducible up to a pullback, we may save some large amount of work by assuming that the corresponding pullbacks are of the simple form t^N where N is an integer.

4.4 The linear differential equation of $\tilde{\chi}_d^{(5)}$ in mod. prime and exact arithmetics

The first terms of the series expansion of $\tilde{\chi}_d^{(5)}(x)$ read:

$$\tilde{\chi}_d^{(5)}(x) \; = \; \frac{3}{262144} \cdot x^{12} \; + \; \frac{39}{1048576} \cdot x^{14} \; + \; \frac{5085}{67108864} \cdot x^{16} \\ + \frac{9}{67108864} \cdot x^{17} \; + \; \frac{33405}{268435456} \cdot x^{18} \; + \; \frac{315}{536870912} \cdot x^{19} \; + \cdots \qquad (4.65)$$

where $x = t^{1/2} = \sinh 2E_v/kT \, \sinh 2E_h/kT$ is our independent variable.

In order to obtain the linear differential equation for $\tilde{\chi}_d^{(5)}(x)$, we have used in [57] a "mod. prime" calculation which amounts to generating large series *modulo a given prime*, and then deduce, the linear differential operator for $\tilde{\chi}_d^{(5)}(x)$ *modulo that prime*.

With 3000 coefficients for the series expansion of $\tilde{\chi}_d^{(5)}(x)$ modulo a prime, we have obtained linear differential equations of order 25, 26, $\cdots$. The smallest order we have reached is 19, and we have assumed that the linear differential equation of $\tilde{\chi}_d^{(5)}(x)$ is of minimal order 19.

In [50], we have introduced a method to obtain the minimal order of the ODE by producing some (≥ 4) non minimal order ODE and then using the "ODE formula" (see [45, 51, 50] for details and how to read the ODE formula). The ODE formula for $\tilde{\chi}_d^{(5)}(x)$ reads

$$31\,Q \,+ 19\,D \,-302 \;\;=\;\; (Q+1)\cdot(D+1) \,\,-f, \qquad (4.66)$$

confirming that the minimal order of the ODE for $\tilde{\chi}_d^{(5)}(x)$ is 19. Note that the degree of the polynomial carrying apparent singularities should be 237 (see Appendix B in [45]). Call $\mathcal{L}_{19}^{(5)}$ the differential operator (known mod prime) for $\tilde{\chi}_d^{(5)}(x)$.

The singularities and local exponents of $\mathcal{L}_{19}^{(5)}$ are[1]

$$\begin{aligned}
x &= 0, & \rho &= \, 0^5, 1/2, 1^4, 2^3, 4^3, 3, 7, 12, \\
x &= \infty, & \rho &= \, 1^5, 3/2, 2^4, 3^3, 4, 5^3, 8, 13, \\
x &= 1, & \rho &= \, -3, -2, -1, 0^4, 2^3, 4^2, \, \cdots, \\
x &= -1, & \rho &= \, 0^5, 2^4, 4^3, 6^2, 8^2, 10^2, \, \cdots, \\
x &= x_0, & \rho &= \, 5/2, 7/2, 7/2, \, \cdots, \\
x &= x_1, & \rho &= \, 23/2, \, \cdots
\end{aligned} \qquad (4.67)$$

where x_0 (resp. x_1) is any root of $1+x+x^2 = 0$ (resp. $1+x+x^2+x^3+x^4 = 0$), and the trailing $\cdots$ denote integers not in the list.

Note that, in practice, we do not deal with is the minimal order differential operator $\mathcal{L}_{19}^{(5)}$ but with an operator of order 30 (that $\mathcal{L}_{19}^{(5)}$ rightdivides): order 30 is what we have called in [45, 51, 50] the "optimal order", namely the order for which finding the differential operator annihilating the series requires the minimum number of terms in the series. With the tools and methods developed in [45, 51, 170], we are now able to factorize the differential operator and *recognize some factors in exact arithmetic*. This way, we may see whether some factors occurring $\mathcal{L}_{19}^{(5)}$ follow the "special geometry" line we encountered for $\tilde{\chi}_d^{(3)}$ and $\tilde{\chi}_d^{(4)}$.

Our first step in the factorization of $\mathcal{L}_{19}^{(5)}$ is to check whether $\mathcal{L}_{6}^{(3)}$ (the differential operator for $\tilde{\chi}_d^{(3)}$) is a right factor of $\mathcal{L}_{19}^{(5)}$, meaning that the solutions of $\mathcal{L}_{6}^{(3)}$ (and in particular the integral $\tilde{\chi}_d^{(3)}$) are also solution of $\mathcal{L}_{19}^{(5)}$. This is indeed the case.

Using the methods developed in [45, 51, 170], we find that the series for the difference $\tilde{\chi}_d^{(5)}(x) - \alpha\, \tilde{\chi}_d^{(3)}(x)$ requires an ODE of minimal order 17 for the value[5] $\alpha \, = \, 8$. This confirms that $\mathcal{L}_{6}^{(3)}$ is in direct sum of $\mathcal{L}_{19}^{(5)}$, and that some (order-four) factors of $\mathcal{L}_{6}^{(3)}$ are *still* in $\mathcal{L}_{17}^{(5)}$:

$$\mathcal{L}_{19}^{(5)} \;\;=\;\; \mathcal{L}_{6}^{(3)} \,\oplus\, \mathcal{L}_{17}^{(5)} \qquad (4.68)$$

This order four factor is obviously $L_1^{(3)} \oplus L_3^{(3)}$. Since these factors are in direct sum in $\mathcal{L}_{6}^{(3)}$, the order-seventeen operator $\mathcal{L}_{17}^{(5)}$ is also the annihilator of $\tilde{\chi}_d^{(5)}(x) - \beta\, \tilde{\chi}_{d,2}^{(3)}(x)$ for

[1] The local exponents are given as (e.g.) 2^3 meaning $2, 2, 2$

[5] Comparing with eq.(58) in [57], one should not expect a $1/2$ contribution, since the sum on the $g^5(N,t)$'s still contains $\tilde{\chi}_d^{(3)}$.

$\beta = 4$, meaning that we also have

$$\mathcal{L}_{19}^{(5)} \;=\; L_2^{(3)} \oplus \mathcal{L}_{17}^{(5)} \qquad (4.69)$$

At this step, the differential operator $\mathcal{L}_{17}^{(5)}$ is known in prime. To go further in the factorization, we use the method developped in [45, 51] along various singularities and local exponents of $\mathcal{L}_{17}^{(5)}$ which read[1]:

$$\begin{array}{rll}
x = 0, & \rho = 0^5, 1/2, 1^4, 2^3, 4^2, 3, 7, & \ln(z)^4,\; z^{1/2}, \\
x = \infty, & \rho = 1^5, 3/2, 2^4, 3^3, 4, 5^2, 8, & \ln(z)^4,\; z^{3/2}, \\
x = 1, & \rho = -3, -2, -1, 0^4, 2^3, \cdots, & \ln(z)^3,\; z^{-3}, z^{-2}, z^{-1}, \\
x = -1, & \rho = 0^5, 2^4, 4^3, 6^2, 8^2, \cdots, & \ln(z)^4, \\
x = x_0, & \rho = 5/2, 7/2, 7/2, \cdots, & z^{5/2}, z^{7/2}, z^{7/2}\ln(z), \\
x = x_1, & \rho = 23/2, \cdots, & z^{23/2}
\end{array} \qquad (4.70)$$

where x_0 and x_1 are again the roots of $1 + x + x^2 = 0$ and $1 + x + x^2 + x^3 + x^4 = 0$, and the trailing $\cdots$ denote integers not in the list. The last column shows the maximum $\ln(z)$ occurring in the formal solutions of $\mathcal{L}_{17}^{(5)}$, z being the local variable of the expansion.

Use is made of section 5 of [57] to recognize exactly some factors. This is completed by an usual rational reconstruction [170].

We are now able to give new results completing what was given in Section 5 of [57]. The linear differential operator $\mathcal{L}_{17}^{(5)}$ has the factorization:

$$\mathcal{L}_{17}^{(5)} \;=\; L_6^{(5)} \cdot \mathcal{L}_{11}^{(5)}. \qquad (4.71)$$

The linear differential operator $\mathcal{L}_{11}^{(5)}$ has been fully factorized and the factors *are known in exact arithmetic* (the indices are the orders)

$$\mathcal{L}_{11}^{(5)} \;=\; L_1^{(3)} \oplus L_3^{(3)} \oplus \Big(W_1^{(5)} \cdot U_1^{(5)}\Big) \oplus \Big(L_4^{(5)} \cdot V_1^{(5)} \cdot U_1^{(5)}\Big), \qquad (4.72)$$

and are given in 4.C.

The factor $L_6^{(5)}$ is the only one which is known in primes and it is irreducible. The irreducibility has been proven with the method presented in section 4 of [45]. This is technically tractable since there are only two free coefficients (see (4.76), (4.77)) that survive in the expansion of the analytical series at $x = 0$ of $L_6^{(5)}$.

In the factorization (4.71), (4.72) of $\mathcal{L}_{11}^{(5)}$ and $\mathcal{L}_{17}^{(5)}$, the factors are either known and occurring elsewhere ($L_1^{(3)}$, $L_3^{(3)}$) or simple order-one linear differential operators ($U_1^{(5)}$, $V_1^{(5)}$, $W_1^{(5)}$), *except* the order-four operator $L_4^{(5)}$ and the order-six operator $L_6^{(5)}$. It is then for these specific operators that we examine whether they are "Special Geometry".

---

[1] There are solutions analytic at $x = 0$ with exponents 0, 1, 2, 4, 7.

4.4.1 The linear differential operator $L_4^{(5)}$

The order-four linear differential operator $L_4^{(5)}$ has the following local exponents

$$
\begin{aligned}
x \,&=\, 0, \qquad && \rho = -2, -2, -1, \, 0, \\
x \,&=\, \infty, \qquad && \rho = \, 3, \, 3, \, 4, \, 5, \\
x \,&=\, 1, \qquad && \rho = -2, -2, -2, -2, \\
x \,&=\, -1, \qquad && \rho = -2, -2, \, 0, \, 0, \\
1 \, + x \, + x^2 \,&=\, 0, \qquad && \rho = -1, 0, 1, 2,
\end{aligned}
\tag{4.73}
$$

At all these singularities x_0, the solutions have the maximum allowed degree of log's (i.e. $\ln(x - x_0)^3$), except at the singularities roots of $1 \, + x \, + x^2 \, = \, 0$, where the solutions carry no log's.

If we consider the linear differential operator $L_4^{(5)} \cdot d(x)$, where

$$
d(x)^{-1} \;\; = \;\; x^2 \cdot (1 - x)^2 \cdot (1 + x)^2 \cdot (1 \, + x \, + x^2), \tag{4.74}
$$

nothing prevents (as far as the ρ's and log's are concerned) to check whether this conjugated operator is homomorphic to a symmetric cube of the order-two linear differential operator of an elliptic integral.

We find the solution of $L_4^{(5)}$ as

$$
\begin{aligned}
Sol(L_4^{(5)}) \;\; = \;\; d(x)^{-1} \cdot \Bigl(& 3\,x \cdot E(x)^3 \, - (2\,x^4 + 3\,x^3 - 4\,x^2 - 6\,x + 2)\,(1 + x)^2 \cdot K(x)^3 \\
& +(1 + x)\,(5\,x^4 - 23\,x^2 - 10\,x + 4) \cdot K(x)^2 \cdot E(x) \\
& -(2 - x - 17\,x^2 - 10\,x^3 + 2\,x^4) \cdot K(x) \cdot E(x)^2 \Bigr),
\end{aligned}
\tag{4.75}
$$

where E and K are the usual complete elliptic integrals ${}_2F_1([1/2, -1/2], [1], x^2)$ and ${}_2F_1([1/2, 1/2], [1], x^2)$. Again the occurrence of (very simple) elliptic integrals is underlined.

4.4.2 On the order-six linear differential operator $L_6^{(5)}$: "Special Geometry"

Let us write the formal solutions $L_6^{(5)}$ at $x = 0$, where the notation $[x^p]$ means that the series begins as $x^p \, (const. + \cdots)$. There is one set of five solutions and one analytical solution

$$
\begin{aligned}
& S_1 = [x^7] \, \ln(x)^4 \, + [x^4] \, \ln(x)^3 \, + [x^2] \, \ln(x)^2 \, + [x^0] \, \ln(x) \, + [x^0], \\
& S_2 = [x^7] \, \ln(x)^3 \, + [x^4] \, \ln(x)^2 \, + [x^2] \, \ln(x) \, + [x^0], \\
& S_3 = [x^7] \, \ln(x)^2 \, + [x^4] \, \ln(x) \, + [x^3], \qquad\qquad\qquad (4.76) \\
& S_4 = [x^7] \, \ln(x) \, + [x^4], \qquad S_5 = [x^7], \qquad \text{and:} \\
& S_6 = [x^2], \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (4.77)
\end{aligned}
$$

In view of this structure, the linear differential operator $L_6^{(5)}$ cannot be (homomorphic to) a symmetric fifth power of the linear differential operator corresponding to the elliptic integral.

The next step is to see whether the exterior square of $L_6^{(5)}$ has a rational solution, which means that $L_6^{(5)}$ corresponds to "Special Geometry". With the six solutions (4.76), seen as series obtained mod. primes, one can easily built the general solution of $Ext^2(L_6^{(5)})$ as

$$\sum_{k,p} d_{k,p} \cdot (S_k \frac{dS_p}{dx} - S_p \frac{dS_k}{dx}), \qquad k \neq p = 1, \cdots, 6, \tag{4.78}$$

which should not contain log's, fixing then some of the coefficients $d_{k,p}$.

For a rational solution of $Ext^2(L_6^{(5)})$ to exist, the form (free of log's)

$$D(x) \cdot \sum_{k,p} d_{k,p} \cdot (S_k \frac{dS_p}{dx} - S_p \frac{dS_k}{dx}), \tag{4.79}$$

should be a polynomial, where the denominator $D(x)$ reads

$$D(x) \; = \; x^{n_1} \cdot (x+1)^{n_2} \cdot (x-1)^{n_3} \cdot (1+x+x^2)^{n_4} \cdot (1+x+x^2+x^3+x^4)^{n_5},$$

the order of magnitude of the exponents n_j being obtained from the local exponents of the singularities. With series of length 700, we have found no rational solution for $Ext^2(L_6^{(5)})$.

Even if $L_6^{(5)}$ is an irreducible operator of *even* order, we have looked for a rational solution for its *symmetric square*. The general solution of $Sym^2(L_6^{(5)})$ is built from (4.76) as

$$\sum_{k,p} f_{k,p} \cdot S_k \, S_p, \qquad k \, \geq \, p \, = \, 1, \cdots, 6, \tag{4.80}$$

and the same calculations are performed. With some 300 terms, we actually found that $Sym^2(L_6^{(5)})$ *has a rational solution* of the form[1] (with $P_{196}(x)$ a polynomial of degree 196):

$$\frac{x^4 \cdot P_{196}(x)}{(x+1)^{10} \cdot (x-1)^{14} \cdot (1+x+x^2)^{21} \cdot (1+x+x^2+x^3+x^4)^9}, \tag{4.81}$$

thus showing that $L_6^{(5)}$ does correspond to "Special Geometry".

Note that the occurrence (4.76), (4.77) of *two analytic* solutions at $x \, = \, 0$, for $L_6^{(5)}$, which is irreducible, is a situation we have encountered in Ising integrals [45, 170]. The order twelve differential operator (called L_{12}^{left} in [170]) has four analytical solutions at $x \, = \, 0$ and it has been demonstrated that it is irreducible [170].

---

[1]Note that this form occurs, for a non minimal representative of $L_6^{(5)}$, in the factorization (4.71). On this point, see the details around (43), (44) in [45].

4.5 Singular behavior of $\tilde{\chi}_d^{(3)}(x)$

Now we have obtained all the analytic solutions at the origin of the linear differential equations of $\tilde{\chi}_d^{(3)}$ and $\tilde{\chi}_d^{(4)}$, we turn to the exact computation of their singular behavior at the finite singular points.

To obtain the singular behavior of $\tilde{\chi}_d^{(3)}(x)$ amounts to calculating the singular behavior of each term in (4.18). The details are given in 4.D.

4.5.1 The behavior of $\tilde{\chi}_d^{(3)}(x)$ as $x \rightarrow 1$

The evaluation of the singular behavior as $x \rightarrow 1$ corresponds to straightforward calculations that are given by (4.12) (see (4.122) and (4.128)):

$$\begin{aligned} sol(L_6^{(3)})(Singular, x=1) \; &= \; {{2} \over {\pi}} \cdot {{3\, a_3 \, + a_2} \over {(1\, -x)^2}} \; + \Bigl(-\Bigl({{3a_3 + a_2} \over {\pi}} \Bigr) \; + a_1 \\ +3\, a_2 \cdot \Bigl({{5\pi} \over {9\Gamma^2(5/6)\Gamma^2(2/3)}} \; &- {{8\pi} \over {\Gamma^2(1/6)\Gamma^2(1/3)}} \Bigr) \Bigr) \cdot {{1} \over {1-x}} \; + {{a_2} \over {2\pi}} \cdot \ln(1-x). \qquad (4.82) \end{aligned}$$

When specialized to the combination (4.18) defining $\tilde{\chi}_d^{(3)}(x)$, the singular behavior reads

$$\begin{aligned} \tilde{\chi}_d^{(3)}(x)(Singular, x=1) \; = \; \Bigl({{1} \over {3}} \; - {{5\pi} \over {18\Gamma^2(5/6)\Gamma^2(2/3)}} \; + {{4\pi} \over {\Gamma^2(1/6)\Gamma^2(1/3)}} \Bigr) \cdot {{1} \over {1\, -x}} \\ + {{1} \over {4\, \pi}} \cdot \ln(1\, -x). \quad (4.83) \end{aligned}$$

This result agrees with the result determined numerically in appendix B of [57].

One remarks, for the particular combination (4.18) giving $\tilde{\chi}_d^{(3)}(x)$, that the *most divergent term disappears*. Note that this is what has been obtained [59] for the susceptibility $\tilde{\chi}^{(3)}$ where the singularity $(1-4w)^{-3/2}$ of the ODE is not present in $\tilde{\chi}^{(3)}$.

4.5.2 The behavior of $\tilde{\chi}_d^{(3)}(x)$ as $x \rightarrow -1$

The calculations of the singular behavior as $x \rightarrow -1$ rely mostly on connection formulae of ${}_2F_1$ hypergeometric functions, and the results are given below in (4.129) and (4.159). For the combination (4.18), the singular behavior reads

$$\tilde{\chi}_d^{(3)}(x)(Singular, x=-1) \; = \; {{1} \over {4\pi^2}} \cdot \ln(1+x)^2 \; + \Bigl({{1} \over {4\pi}} \; - {{2\ln(2) - 1} \over {2\,\pi^2}} \Bigr) \cdot \ln(1+x),$$

which agrees with the result of appendix B of [57].

4.5.3 The behavior of $\tilde{\chi}_d^{(3)}(x)$ as $x \rightarrow e^{\pm 2\pi i/3}$

The result for the singular behaviour $\tilde{\chi}_d^{(3)}(x)$ as $x \rightarrow x_0 = e^{\pm 2\pi i/3}$ reads:

$$\begin{aligned}
\tilde{\chi}_d^{(3)}(Singular, x = x_0) \quad &= \quad -\frac{8 \cdot 3^{1/4}}{35\pi}\, e^{\pi i/12} \cdot (x - x_0)^{7/2} \\
&= \quad -0.0957529 \cdots\ e^{\pi i/12} \cdot (x - x_0)^{7/2}.
\end{aligned} \tag{4.84}$$

This agrees with the numerical result of Appendix B of [57]

$$-\frac{1}{3}\sqrt{2}\, e^{\pi i/12} \cdot b \cdot (x - x_0)^{7/2}, \tag{4.85}$$

with $b = 0.203122784 \cdots$

4.6 Singular behaviour of $\tilde{\chi}_d^{(4)}(x)$

To obtain the singular behavior of $\tilde{\chi}_d^{(4)}(x)$ amounts to obtaining the singular behavior of each term in (4.34).

4.6.1 Behavior of $\tilde{\chi}_d^{(4)}(t)$ as $t \rightarrow 1$

The calculations of the singular behavior of $\tilde{\chi}_{d;2}^{(4)}(t)$ as $t \rightarrow 1$ are displayed in 4.E, and read

$$\begin{aligned}
\tilde{\chi}_{d;2}^{(4)}(t)(Singular, t = 1) \quad &= \quad \frac{8}{\pi^2(1-t)^2} \quad - \frac{8}{\pi^2(1-t)} \\
&+ \frac{5}{2\pi^2} \cdot \ln\frac{16}{1-t} \quad - \frac{3}{2\pi^2} \cdot \ln^2\frac{16}{1-t}.
\end{aligned} \tag{4.86}$$

To compute the singular behavior of $\tilde{\chi}_{d;3}^{(4)}(t)$ as $t \rightarrow 1$ we need the expression of the hypergeometric function ${}_4F_3([1/2,\, 1/2,\, 1/2,\, 1/2], [1,\, 1,\, 1]; z)$ as $z \rightarrow 1$. This hypergeometric function is an example of solution of a Calabi-Yau ODE, and explicit computations of its monodromy matrices have been given [80].

The differential equation for ${}_4F_3([1/2,\, 1/2,\, 1/2,\, 1/2], [1,\, 1,\, 1]; z)$ is Saalschützian and well-poised (but not very-well-poised). At $z = 1$ it has one logarithmic solution and three analytic solutions of the form

$$\sum_{n=0}^{\infty} c_n \cdot (1 - z)^n. \tag{4.87}$$

The c_n satisfy the fourth order recursion relation

$$16\, n \cdot (n-1)^2\, (n-2) \cdot c_n \quad - 24\, (n-1)(n-2)(2n^2-6n+5) \cdot c_{n-1} \\ +16\, (n-2)^2\, (3n^2-12n+13) \cdot c_{n-2} \quad - (2n-5)^4 \cdot c_{n-3} \quad = \quad 0, \qquad (4.88)$$

where $c_n \, = \, 0$ for $n \, \le \, -1$. The vanishing of the coefficient c_n at $n \, = \, 0, \, 1, \, 2,$ of c_{n-1} at $n-1, \, 2$ and c_{n-2} at $n = \, 2$ guarantees that $c_0, \; c_1, \; c_2$ may be chosen arbitrarily.

The behaviour at $z \, = \, 1$ of ${}_4F_3([1/2, 1/2, 1/2, 1/2], [1, 1, 1]; z)$, which is the solution of the ODE that is analytic at $z \, = \, 0$, is given in theorem 3 of Bühring [64] with the parameter

$$s \;=\; \sum_{j=1}^{3} b_j \; - \sum_{j=1}^{4} a_j \;=\; 1, \qquad (4.89)$$

(i.e. the *Saalschützian condition* [205, 206, 207, 242]). For completeness we quote this theorem which is valid for all ${}_{p+1}F_p([a_1, \, \cdots \, , \, a_{p+1}], \, [b_1, \, \cdots \, , \, b_p]; \, z)$ when the parameter s of (4.89) is *any integer*[2] $s \ge 0$:

$$\frac{\Gamma(a_1) \cdots \Gamma(a_{p+1})}{\Gamma(b_1) \cdots \Gamma(b_p)} \cdot \; {}_{p+1}F_p([a_1, \cdots, a_{p+1}]; [b_1, \cdots, b_p]; \, z) \\ = \quad \sum_{n=0}^{s-1} I_n^{<} \cdot (1-z)^n \; + \sum_{n=s}^{\infty} I_n^{>} \cdot (1-z)^n \\ +(1-z)^s \cdot \sum_{n=0}^{\infty} [w_n \, + q_n \cdot \ln(1-z)] \cdot (1-z)^n, \qquad (4.90)$$

for $|1-z| \, < \, 1, \, -\pi \, < \, arg(1-z) \, < \, \pi$ and $p \, = \, 2, \, 3, \, \cdots$ where for $0 \, \le \, n \, \le \, s-1$

$$I_n^{<} \;=\; (-1)^n \cdot \frac{\Gamma(a_1+n)\Gamma(a_2+n)(s-n-1)!}{\Gamma(a_1+s)\Gamma(a_2+s) n!} \cdot \sum_{k=0}^{\infty} \frac{(s-n)_k}{(a_1+s)_k (a_2+s)_k} \cdot A_k^{(p)}, \qquad (4.91)$$

for $s \le n$

$$I_n^{>} \;=\; (-1)^n \cdot \frac{(a_1+s)_{n-s})(a_2+s)_{n-s}}{n!} \cdot \sum_{k=n-s+1}^{\infty} \frac{(k-n+s)!}{(a_1+s)_k (a_2+s)_k} \cdot A_k^{(p)}, \qquad (4.92)$$

[2] Again we emphasise the role of k-balanced hypergeometric functions.

and

$$w_n \; + q_n \cdot \ln(1-z) \;\; = \;\; (-1)^s \cdot \frac{(a_1+s)_n (a_2+s)_n}{(s+n)!n!}$$

$$\times \;\; \Bigl(\sum_{k=0}^{n} \frac{(-n)_k}{(a_1+s)_k (a_2+s)_k} \cdot A_k^{(p)} [\psi(1+n-k) + \psi(1+s+n)$$

$$-\psi(a_1+s+n) \, - \psi(a_2+s+n) \, - \ln(1-z)] \Bigr) \, , \qquad (4.93)$$

where $(a)_n \; = \; a\,(a+1) \, \cdots \, (a+n-1)$ is the Pochhammer's symbol. The $A_k^{(p)}$ are computed recursively in [64] as $p-1$ fold sums. In particular

$$A_k^{(2)} \;\; = \;\; \frac{(b_2-a_3)_k \, (b_1-a_3)_k}{k!}, \qquad (4.94)$$

and

$$A_k^{(3)} \;\; = \;\; \sum_{k_2=0}^{k} \frac{(b_3+b_2-a_4-a_3+k_2)_{k-k_2} \, (b-1-a_3)_{k-k_2} \, (b_3-a_4)_{k_2} \, (b_2-a_4)_{k_2}}{(k-k_2)! \, k_2!}$$

$$= \;\; \frac{(b_1+b_3-a_3-a_4)_k (b_2+b_3-a-3-a_4)_k}{k!} \qquad (4.95)$$

$$\times \, {}_3F_2([b_3-a_3, \, b_3-a_4, \, -k]; [b_1+b_3-a_{-}a_4, \, b_2+b_3-a_3-a_4]; \, 1).$$

For use in (4.63) we need to specialize to $a_j \, = \, 1/2, \;\, b_j \, = \, 1$, where

$$A_k^{(3)} \;\; = \;\; \sum_{k_2}^{k} \frac{(1+k_2)_{k-k_2} \, (1/2)_{k-k_2} \, (1/2)_{k_2}^2}{(k-k_2)! \, k_2!}$$

$$= \;\; k! \cdot \, {}_3F_2([1/2, 1/2, -k], \, [1,1]; \, 1), \qquad (4.96)$$

and for respectively $n = 0$ and $n \ge 1$

$$I_0^{<} \; = \; 4 \sum_{k=0}^{\infty} \frac{k!}{(3/2)_k^2} \cdot A_k^{(3)}, \qquad I_n^{>} \; = \; (-1)^n \, \frac{(3/2)_{n-1}^2}{(n)!} \cdot \sum_{k=n}^{\infty} \frac{(k-n)!}{(3/2)_k^2} \cdot A_k^{(3)}. \qquad (4.97)$$

We note, in particular, the terms

$$A_0^{(3)} \; = \; 1, \qquad A_1^{(3)} \; = \; 3/4, \qquad A_2^{(3)} \; = \; 41/32. \qquad (4.98)$$

Using these specializations in (4.90) we compute the terms in $\tilde{\chi}_{d;3}^{(4)}(t)$ which diverge as $t \, \rightarrow \, 1$.

The term $(1-t)^{-1} \cdot \ln(1-t^2)$ cancels and we are left with

$$\tilde{\chi}_{d;3}^{(4)}(t)(Singular, t=1) \;=\; \frac{1}{\pi^2} \cdot \Bigl(\frac{8}{3\,(1-t)^2} \;+ \frac{56}{3\,(1-t)} + \frac{16}{3 \cdot (1-t)} \cdot (3\,I_1^{>} \;-4\,I_2^{>}) \Bigr) + \frac{8}{3\,\pi^2} \cdot \ln \frac{1-t^2}{16} \tag{4.99}$$

Thus, using (4.35), (4.86) and (4.99), we find the terms in $sol(L_8^{(4)})$, which diverge as $t \to 1$, are

$$sol(L_8^{(4)})(Singular, t=1) \;=\; \frac{8\,(a_3+3a_2)}{8\,\pi^2} \cdot \frac{1}{(1-t)^2} + \Bigl(a_1 \;-\frac{8(3a_2-7a_3)}{3\pi^2} \;+\frac{16\,a_3}{3\pi^2} \cdot (3I_1^{>} \;-4I_2^{>}) \Bigr) \cdot \frac{1}{1-t} + \frac{15a_2-16a_3}{\pi^2} \cdot \ln(\frac{16}{1-t}) \;-\frac{3a_2}{2\pi^2} \cdot \ln^2(\frac{16}{1-t}), \tag{4.100}$$

where the constant $3I_1^{>} \;-4I_2^{>}$ reads (with 200 digits):

$$3I_1^{>} \;-4I_2^{>} \;= \tag{4.101}$$

$$-2.2128121289308219235479768149860500214813592933574677661716308473602321648549649858153751858425263240493587926169320613312976710769503767043582482649611010077309255782127142418255205323181711923135264 \cdots \tag{4.102}$$

When specializing to the particular combination (4.64), the singular behavior of the integral $\tilde{\chi}_d^{(4)}(t)$ reads

$$\tilde{\chi}_d^{(4)}(t)(Singular, t=\;1) \;=\; \frac{1}{8\,(1-t)} \cdot \Bigl(1 \;-\frac{1}{3\pi^2}[64\;+16 \cdot (3I_1^{>} \;-4I_2^{>})] \Bigr) + \frac{7}{16\pi^2} \cdot \ln \frac{16}{1-t} \;-\frac{1}{16\pi^2} \cdot \ln^2 \frac{16}{1-t}, \tag{4.103}$$

This agrees[2] with the result determined numerically in Appendix B of [57].

We find again and similarly to $\tilde{\chi}_d^{(3)}(t)$ that the most divergent term disappears for the particular combination giving $\tilde{\chi}_d^{(4)}(t)$. And here again, this is what has been observed [59] for the susceptibilty $\tilde{\chi}^{(4)}$ at the singularity $x=\;16w^2=\;1$ which occurs in the ODE as $x^{-3/2}$ and cancels in the integral $\tilde{\chi}^{(4)}$.

[2]Note that there is an overall factor of 2 between this result and the results given in Appendix B of [57] which comes from a multiplicative factor of 2 in the series (around $t=\;0$) of $\tilde{\chi}_d^{(4)}(t)$ used in [57]. This applies also to the result of the singular behavior at $t=\;-1$.

Remark: It is worth recalling that similar calculations for $\tilde{\chi}^{(4)}$, also based on the evaluation of a connection matrix (see section 9 of [265]), require to evaluate a constant I_4^- that is actually expressed in terms of $\zeta(3)$:

$$I_4^- \;=\; \frac{1}{16\,\pi^3}\cdot\Bigl(\frac{4\,\pi^2}{9}\,-\,\frac{1}{6}\,-\,\frac{7}{2}\cdot\zeta(3)\Bigr), \tag{4.104}$$

when the bulk $\tilde{\chi}^{(3)}$ requires some Clausen constant [265] that can be written as:

$$Cl(\pi/3) \;=\; \frac{3^{1/2}}{108}\cdot(3\cdot\psi(1,\,1/3)\,+3\cdot\psi(1,\,1/6)\,-8\,\pi^2). \tag{4.105}$$

It is quite natural to see if the constant $3I_1^> - 4I_2^>$ given with 200 digits in (4.101), can also be obtained exactly in terms of known transcendental constants ($\zeta(3), \cdots$), or evaluations of hypergeometric functions that naturally occur in connection matrices [265] (see (4.185) in 4.F). This question is sketched in 4.F.

4.6.2 Behavior of $\tilde{\chi}_d^{(4)}(t)$ as $t \rightarrow -1$

When $t \rightarrow -1$ the only singular terms come from $\tilde{\chi}_{d;3}^{(4)}(t)$. Furthermore the operator A_3 of (4.61) is non-singular at $t = -1$. Therefore, the only singularities in $\tilde{\chi}_d^{(4)}(t)$ come from the terms with $\ln(1-t^2)$ in the expansion (4.90) of ${}_4F_3([1/2,1/2,1/2,1/2],[1,1,1];\,t^2)$ at $t \rightarrow -1$. Thus, from (4.64) we find that the singular part of $\tilde{\chi}_d^{(4)}(t)$ at $t = -1$ reads

$$\tilde{\chi}_{d;sing}^{(4)}(t) \;=\; -\frac{1}{8}\,\tilde{\chi}_{d;3;sing}^{(4)}(t) \;=\; -\frac{1}{8}\ln(1-t^2)\cdot A_3\cdot\sum_{n=0}^{\infty} q_n\cdot(1-t^2)^{n+1}, \tag{4.106}$$

with q_n obtained from (4.93) as

$$q_n \;=\; \frac{(3/2)_n^2}{(n+1)!\,n!}\cdot\sum_{k=0}^{n}\frac{(-n)_k}{(3/2)_k^2}\cdot\,A_k^{(3)}, \tag{4.107}$$

where $A_k^{(3)}$ is given by (4.95). We know from the exponents of $L_4^{(4)}$ at $t = -1$ that the result has the form $(t+1)^7\cdot\ln(t+1)$. Therefore to obtain this term in a straight forward way we need to expand the coefficient of $\ln(1-t^2)$ to order $(1+t)^9$ in order that the term from $(1+t)\cdot D_t^3$ be of order $(1+t)^7$. This is tedious by hand but is easily done on Maple and we find that the leading singularity in $\tilde{\chi}_d^{(4)}(t)$ at $t = -1$ is

$$\tilde{\chi}_d^{(4)}(Singular, t=-1) \;=\; \frac{1}{26880}\cdot(1+t)^7\cdot\,\ln(1+t), \tag{4.108}$$

which agrees with Appendix B of [57].

4.7 Conclusion: is the Ising model "modularity" reducible to selected ${}_{(q+1)}F_q$ hypergeometric functions ?

In this paper we have derived the exact analytic expressions for $\tilde{\chi}_d^{(3)}(t)$ and $\tilde{\chi}_d^{(4)}(t)$ and from them have computed the similar behaviour at all singular points. We have also obtained some additional exact results for $\tilde{\chi}_d^{(5)}(t)$ (see section 4.4). This completes the program initiated in [57] where the singularities were studied by means of formal solutions found on Maple and numerical studies of the connection problem [265]. In this sense we have a complete solution to the problem. However, in another sense, there are still most interesting open questions.

In section 4.3.1 we used the solution of the hypergeometric connection problem [64] which gave the connection constants $I_n^{<}$ and $I_n^{>}$ as multiple sums. However there are special cases, as mentioned in [65], where it is known by indirect means that the series can be simplified, but for which a direct simplification of the series has not been found. One example is given by the computation in section 4.2 of the singularity of $\tilde{\chi}_d^{(3)}(t)$ at $t = 1$ which we accomplished by means of the reduction (4.19) of a ${}_3F_2$ function to a product of ${}_2F_1$ functions. This produced the gamma function evaluation of the singularity at $x = 1$ of (4.128). This singularity could also have been computed directly from the ${}_3F_2$ function in (4.16) by use of the Bühring formula (4.90) but a reduction of the sums for the required I_n to the gamma function form is lacking. There are two suggestions that such a reduction may exist for $\tilde{\chi}_d^{(4)}(t)$ at $t = 1$. The first is that, by analogy with the corresponding calculation for $\tilde{\chi}^{(4)}(t)$ in the bulk [234], the amplitude could be evaluated in terms of $\zeta(3)$. The second is that evaluations of Calabi-Yau [80] hypergeometric functions like ${}_4F_3([1/2, 1/2, 1/2, 1/2], [1, 1, 1]; z)$ take place. The larger question, of course, is how much the structure seen in $\tilde{\chi}_d^{(n)}(t)$ and $\tilde{\chi}^{(n)}(t)$ for $n = 1, 2, 3, 4$ can be expected to generalize to higher values of n. It is the opinion of the authors that there is a great deal of mathematical structure of deep significance remaining to be discovered.

These new exact results for the diagonal susceptibility of the Ising model confirm that the linear differential operators that emerge in the study of these Ising n-fold integrals, are not only "Derived From Geometry" [47], but actually correspond to "Special Geometries" (they are homomorphic to their adjoint, which means [139] that their differential Galois group is "special", their symmetric square, exterior square has rational function solutions, ...). More specifically, when we are able to get the exact expressions of these linear differential operators, we find out that they are associated with elliptic function theory (*elliptic functions [12] or modular forms*), and, in more complicated cases, *Calabi-Yau* ODEs [7, 6]. This totally confirms what we already saw [47] on $\tilde{\chi}^{(5)}$ and $\tilde{\chi}^{(6)}$. We see in particular, with $\chi_d^{(5)}$, the emergence of a remarkable order-six operator which is such that *its symmetric square has a rational solution.*

Let us recall that it is, generically, extremely difficult to see that a linear differential operator corresponding to a Calabi-Yau ODE [7, 6], is homomorphic to a ${}_{q+1}F_q$ hypergeometric linear differential operator up to an algebraic pullback. Worse, it is not impossible that many of the Calabi-Yau ODEs are actually reducible (up to operator equivalence) to ${}_{q+1}F_q$ hypergeometric functions up to algebraic pullbacks that have not been found yet. Let us assume that this is not the case, and that the Calabi-Yau world is not reducible to the hypergeometric world (up to involved algebraic pullback), we still have to see if the "Special Geometry" operators that occur for the Ising model, are "hypergeometric" ones, reducing, in fact systematically to (selected k-balanced) ${}_{q+1}F_q$ hypergeometric functions, or correspond to the more general solutions of Calabi-Yau equations.

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Appendix

4.A Miscellaneous comments on the modular curve (4.27)

Let us introduce other rational expressions, similar to (4.17) and (4.26):

$$Q_2(x) \;=\; \frac{27\,x^4\cdot(1+x)}{(x\,+\,2)^6}, \qquad\qquad Q_3(x) \;=\; -\,\frac{27\,x\cdot(1+x)^4}{(x-1)^6},$$

where recalling the expression of (4.26) one has (for instance):

$$Q_2(x) \;=\; Q_1\Bigl(\frac{1}{x}\Bigr) \;=\; Q_1\Bigl(-\,\frac{1\,+x}{x}\Bigr), \qquad\qquad Q_3(x) \;=\; Q_1\Bigl(-\,\frac{1}{1\,+\,x}\Bigr)$$
$$=\; Q_1\Bigl(-\,\frac{x}{1\,+\,x}\Bigr) \;=\; Q_2(-1\,-\,x) \;=\; Q_2\Bigl(-\,\frac{1+x}{x}\Bigr).$$

Remarkably the elimination of x between the Hauptmodul $Q \,=\, Q(x)$ and $Q_2 \,=\, Q_2(x)$ (or $Q \,=\, Q(x)$ and $Q_3 \,=\, Q_3(x)$) also gives the *same* modular curve (4.27).

We also have remarkable identity on the *same* hypergeometric function with these new Hauptmodul pullbacks (4.109):

$$(x\,+2)\cdot\,{}_2F_1\Bigl([\frac{1}{6},\,\frac{1}{3}],\,[1];\,Q(x)\Bigr)$$
$$=\;\; 2\cdot(1+x+x^2)^{1/2}\cdot\,{}_2F_1\Bigl([\frac{1}{6},\,\frac{1}{3}],\,[1];\,Q_2(x)\Bigr), \qquad (4.109)$$

and:

$$(1 - x) \cdot {}_2F_1\Big([\frac{1}{6}, \frac{1}{3}], [1]; Q(x)\Big)$$
$$= (1 + x + x^2)^{1/2} \cdot {}_2F_1\Big([\frac{1}{6}, \frac{1}{3}], [1]; Q_3(x)\Big). \qquad (4.110)$$

The (modular [46]) curve (4.27) should not be confused with the fundamental modular curve [46]

$$5^9 v^3 u^3 - 12 \cdot 5^6 u^2 v^2 \cdot (u+v) + 375\, u v \cdot (16 u^2 + 16 v^2 - 4027 v u)$$
$$-64 (v+u) \cdot (v^2 + 1487 v u + u^2) + 2^{12} \cdot 3^3 \cdot u v = 0, \qquad (4.111)$$

corresponding to the elimination of the variable x between the previous Hauptmodul (4.17) and another Hauptmodul[4] $Q_L(x)$:

$$Q_L(x) = -108 \cdot \frac{(1+x)^4 \cdot x}{(x^2 - 14 x + 1)^3}. \qquad (4.112)$$

The new modular curve (4.27) also has a rational parametrization, $(u, v) = (Q_L(x), Q_4(x))$, between this last new Hauptmodul (4.112) and a new simple Hauptmodul:

$$Q_4(x) = 108 \cdot \frac{(1+x)^2 \cdot x^2}{(1-x)^6}. \qquad (4.113)$$

4.B Solution of $\mathcal{M}_4$ analytical at $x = 0$

The solution of $\mathcal{M}_4$, analytical at $x = 0$, reads:

$$Sol(x) = (1-x)^{3/4} \cdot \rho(x) \cdot sol(x), \qquad (4.114)$$

where $sol(x)$ reads:

$$Z_1 \cdot {}_4F_3\Big([\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}], [1, 1, 1]; P(x)\Big) + Z_2 \cdot {}_4F_3\Big([\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}], [2, 2, 2]; P(x)\Big)$$
$$+ Z_3 \cdot {}_4F_3\Big([\frac{5}{2}, \frac{5}{2}, \frac{5}{2}, \frac{5}{2}], [3, 3, 3]; P(x)\Big) + Z_4 \cdot {}_4F_3\Big([\frac{7}{2}, \frac{7}{2}, \frac{7}{2}, \frac{7}{2}], [4, 4, 4]; P(x)\Big),$$

with

$$Z_1 = -512 \cdot \frac{n_1}{d_1}, \quad Z_2 = 128 \cdot \frac{n_2}{d_2}, \quad Z_3 = -54 \cdot \frac{n_3}{d_3}, \quad Z_4 = -625 \cdot \frac{n_4}{d_4},$$

[4]Related by a Landen transformation on $x^{1/2}$ see [46].

and

$$
\begin{aligned}
n_1 \;&=\; (7\,x^3 \,-56\,x^2 \,+112\,x \,-64) \,\cdot\, (1 \,-x)^{1/2} \\
&\quad +(x-1)\,(x^3 \,-24\,x^2 \,+80\,x \,-64), \\
n_2 \;&=\; (2352\,x^2 \,-472\,x^3 \,-3904\,x \,+2048 \,+19\,x^4) \,\cdot\, (1 \,-x)^{1/2} \\
&\quad +x^5 \,-125\,x^4 \,+1288\,x^3 -4048\,x^2 \,+4928\,x \,-2048, \\
n_3 \;&=\; (x^6 \,-28080\,x^3 \,-355\,x^5 \,-52992\,x \,+17920 +5750\,x^4 \,+57760\,x^2)\cdot\, (1 \,-x)^{1/2} \\
&\quad -2\,(x-1)\,(20\,x^5 \,-855\,x^4 \,+6736\,x^3 \,-18992\,x^2 \,+22016\,x \,-8960), \\
n_4 \;&=\; (x^2 \,-8\,x \,+8)\,(x^4 \,-64\,x^3 \,+320\,x^2 \,-512\,x \,+256)\cdot\, (1 \,-x)^{1/2} \\
&\quad -4\,(x-1)\,(x-2)\,(3\,x \,-4)\,(x \,-4)\,(x^2 \,-16\,x \,+16),
\end{aligned}
$$

and

$$
\begin{aligned}
d_1 \;&=\; (1-x)\cdot x^2\cdot((x-2)\cdot(x^2 \,-16\,x \,+16)\cdot(1 \,-x)^{1/2} \\
&\quad -2\,(x-1)\,(3\,x-4)\,(x-4)), \\
d_2 \;&=\; (1-x)\cdot x^4\cdot(4\cdot(x-2)\cdot(1 \,-x)^{1/2} \,+\, x^2 \,-8\,x \,+8), \\
d_3 \;&=\; (1-x)\cdot x^6\cdot(2\,(x-1) \,-(x-2)\cdot(1 \,-x)^{1/2}), \\
d_4 \;&=\; (1-x)\cdot x^8,
\end{aligned}
$$

and

$$
\rho(x) \;=\; \Big((2-x)\cdot(1 \,-x)^{1/2} \,+2\cdot(x \,-1)\Big)^{1/2},
$$

and where $P(x)$ denotes the pullback (4.56):

$$
P(x) \;=\; {{x^2 \,-8\,x \,+8} \over {x^2}} \;-4\cdot(2-x)\cdot{{(1-x)^{1/2}} \over {x^2}}. \qquad (4.115)
$$

This solution has the integrality property [143]. Changing x into $64\,x$ the series expansion of the previous solution (4.114) has *integer coefficients*:

$$
\begin{aligned}
Sol(64\,x) \;&=\; 128 \,+2560\,x \,+116736\,x^2 \,+6072320\,x^3 \,+335104000\,x^4 \\
&\quad +19117744128\,x^5 +1114027622400\,x^6 +65874638708736\,x^7 \\
&\quad +3937277209282560\,x^8 \,+\,\cdots
\end{aligned}
$$

4.C The linear differential operator $\mathcal{L}_{11}^{(5)}$ in exact arithmetic

The factors occurring in the differential operator $\mathcal{L}_{11}^{(5)}$ read

$$U_1^{(5)} \;=\; D_x \;-\; \frac{d}{dx}\ln\Big(\frac{x}{(1-x)^3}\Big), \tag{4.116}$$

$$V_1^{(5)} \;=\; D_x \;-\; \frac{1}{2}\cdot\frac{d}{dx}\ln\Big(\frac{(1+x+x^2)^3}{(1+x)^2\cdot(1-x)^6\cdot x^2}\Big), \tag{4.117}$$

$$W_1^{(5)} \;=\; D_x \;-\; \frac{1}{2}\cdot\frac{d}{dx}\ln\Big(\frac{(x^2+1)^2}{(1+x)^2\cdot(1-x)^6\cdot x}\Big), \tag{4.118}$$

$$L_4^{(5)} \;=\; D_x^4 \;+\frac{p_3}{p_4}\cdot D_x^3 \;+\frac{p_2}{p_4}\cdot D_x^2 \;+\frac{p_1}{p_4}\cdot D_x \;+\frac{p_0}{p_4}, \tag{4.119}$$

with:

$$\begin{aligned} p_4 \;=\; & x^3\cdot(1+x+x^2)\cdot(x+1)^3\cdot(x-1)^4\Big(160+3148\,x+24988\,x^2+86008\,x^3 \\ & +141698\,x^4+69707\,x^5-141750\,x^6-358707\,x^7-356606\,x^8-1071\,x^9+347302\,x^{10} \\ & +510214\,x^{11}+347302\,x^{12}-1071\,x^{13}-356606\,x^{14}-358707\,x^{15}-141750\,x^{16} \\ & +69707\,x^{17}+141698\,x^{18}+86008\,x^{19}+24988\,x^{20}+3148\,x^{21}+160\,x^{22}\Big), \end{aligned}$$

$$\begin{aligned} p_3 \;=\; & 2\,x^2\cdot(x+1)^2\cdot(x-1)^3\cdot\Big(-880-16620\,x-126586\,x^2-421558\,x^3-520547\,x^4 \\ & +733378\,x^5+3794648\,x^6+6252130\,x^7+3922367\,x^8-4349032\,x^9-12817741\,x^{10} \\ & -12881692\,x^{11}-2612141\,x^{12}+10986996\,x^{13}+16830947\,x^{14}+12283572\,x^{15} \\ & +729267\,x^{16}-8919176\,x^{17}-10905121\,x^{18}-5398478\,x^{19}+866024\,x^{20} \\ & +3665682\,x^{21}+3069821\,x^{22}+1351818\,x^{23}+323590\,x^{24}+36308\,x^{25}+1680\,x^{26}\Big), \end{aligned}$$

$$p_2 = 2\,x\cdot(x-1)^2\cdot\Big(2400+38692\,x+228422\,x^2+366806\,x^3-1591741\,x^4-8948446\,x^5$$
$$-18137183\,x^6-10301088\,x^7+31576074\,x^8+82978356\,x^9+80098415\,x^{10}$$
$$-8308172\,x^{11}-123518048\,x^{12}-158759046\,x^{13}-65285821\,x^{14}+78248130\,x^{15}$$
$$+152708392\,x^{16}+124727752\,x^{17}+26488355\,x^{18}-65301174\,x^{19}-90679899\,x^{20}$$
$$-47527872\,x^{21}+4032496\,x^{22}+27473954\,x^{23}+23107094\,x^{24}+9927812\,x^{25}$$
$$+2288564\,x^{26}+245416\,x^{27}+10800\,x^{28}\Big),$$

$$p_1 = 2\,(x-1)\cdot\Big(-1440-15176\,x-3552\,x^2+632252\,x^3+3988986\,x^4+11012538\,x^5$$
$$+10122851\,x^6-31358640\,x^7-125311964\,x^8-166380144\,x^9+20063039\,x^{10}$$
$$+375202188\,x^{11}+523233277\,x^{12}+189830162\,x^{13}-422078559\,x^{14}-747281488\,x^{15}$$
$$-440223099\,x^{16}+161161298\,x^{17}+530901457\,x^{18}+491902752\,x^{19}+168466049\,x^{20}$$
$$-168274188\,x^{21}-282329480\,x^{22}-158906808\,x^{23}-754525\,x^{24}+72189798\,x^{25}$$
$$+61435092\,x^{26}+25677392\,x^{27}+5672988\,x^{28}+577984\,x^{29}+24000\,x^{30}\Big),$$

$$p_0 = -3600-52880\,x-324108\,x^2-1147996\,x^3-1575180\,x^4+8228874\,x^5$$
$$+52977905\,x^6+108476130\,x^7-739178\,x^8-371064711\,x^9-563202298\,x^{10}$$
$$-29824206\,x^{11}+842725375\,x^{12}+1075242362\,x^{13}+273493047\,x^{14}-909934423\,x^{15}$$
$$-1189246308\,x^{16}-414338515\,x^{17}+420114304\,x^{18}+702981552\,x^{19}+447865799\,x^{20}$$
$$+30467322\,x^{21}-270639170\,x^{22}-233990685\,x^{23}-67035676\,x^{24}+45089100\,x^{25}$$
$$+61580064\,x^{26}+29851532\,x^{27}+7030080\,x^{28}+714400\,x^{29}+28800\,x^{30}.$$

4.D Analysis of the singular behavior of $\tilde{\chi}^{(3)}_d(x)$

Let us give a detailed analysis of the singularity behaviour of $\tilde{\chi}^{(3)}_{d;2}(x)$ and $\tilde{\chi}^{(3)}_{d;3}(x)$ around the three singularities: $x = +1, -1, e^{\pm 2\pi i/3}$.

4.D.1 The behavior as $x \to 1$

To evaluate $\tilde{\chi}^{(3)}_{d;2}(x)$ for $x \to 1$ we use

$$_2F_1(1/2,1/2;1;x^2) = \frac{2}{\pi}\cdot\ln\left[\frac{4}{(1-x^2)^{1/2}}\right], \qquad \text{and:} \tag{4.120}$$

$$_2F_1(1/2,-1/2;1;x^2) = \frac{2}{\pi}\cdot\left(1+\frac{1-x^2}{2}[\ln\frac{4}{(1-x^2)^{1/2}}-\frac{1}{2}]\right), \tag{4.121}$$

to find, from (4.13), that

$$\tilde{\chi}^{(3)}_{d;2}(x)(Singular, x = 1) \; = \; \frac{2}{\pi(1-x)^2} \; - \frac{1}{\pi(1-x)} + \frac{1}{2\pi} \ln(1-x) \tag{4.122}$$

To evaluate $\tilde{\chi}^{(3)}_{d;3}(x)$ as $x \to 1$ we use (1) on page 108 of [21]

$$\begin{aligned} {}_2F_1([1/6, 1/3],\, [1],\, Q) \; &= \; \frac{\Gamma(1)\Gamma(1/2)}{\Gamma(5/6)\Gamma(2/3)}\, {}_2F_1([1/6, 1/3],\, [1/2],\, 1-Q) \\ &+ \frac{\Gamma(1)\Gamma(-1/2)}{\Gamma(1/6)\Gamma(1/3)} \cdot (1-Q)^{1/2}\, {}_2F_1([5/6, 2/3],\, [3/2],\, 1-Q), \end{aligned} \tag{4.123}$$

$$\begin{aligned} {}_2F_1([7/6, 4/3], [2],\, Q) \; &= \; 18\, \frac{\partial}{\partial Q} \cdot {}_2F_1(1/6, 1/3; 1; Q) \\ &= \frac{\Gamma(2)\Gamma(-1/2)}{\Gamma(5/6)\Gamma(2/3)} \cdot {}_2F_1([7/6, 4/3],\, [3/2];\, 1-Q) \\ &+ \frac{\Gamma(2)\Gamma(1/2)}{\Gamma(7/6)\Gamma(4/3)} \cdot (1-Q)^{-1/2} \cdot {}_2F_1([5/6, 2/3],\, [1/2]; 1-Q). \end{aligned} \tag{4.124}$$

Then as $x \to 1$ one has

$$(1-Q)^{-1/2} \; = \; \frac{2}{\sqrt{3}} \frac{1}{1-x} \; - \frac{1}{\sqrt{3}} \; + O(1-x), \tag{4.125}$$

$${}_2F_1([1/6, 1/3], [1],\, Q)^2 \;\; \longrightarrow \;\; \frac{\pi}{\Gamma^2(5/6)\Gamma^2(2/3)}, \tag{4.126}$$

$$\begin{aligned} &\frac{2\,Q}{9} \cdot {}_2F_1([1/6, 1/3],\, [1],\, Q) \cdot {}_2F_1([7/6, 4/3], [2],\, Q) \\ &\quad \longrightarrow \;\; \frac{2}{\pi(1-x)} \; - \frac{1}{\pi} - \frac{4\pi}{9\Gamma^2(5/6)\Gamma^2(2/3)} - \frac{8\pi}{\Gamma^2(1/6)\Gamma^2(1/3)}, \end{aligned} \tag{4.127}$$

and, thus, one deduces

$$\begin{aligned} \tilde{\chi}^{(3)}_{d;3}(x)(Singular, x = 1) \;\; &= \;\; \frac{6}{\pi} \cdot \frac{1}{(1-x)^2} \\ + \frac{3}{(1-x)} \cdot \Big[-\frac{1}{\pi} \; &+ \; \frac{5\pi}{9\Gamma^2(5/6)\Gamma^2(2/3)} \; - \frac{8\pi}{\Gamma^2(1/6)\Gamma^2(1/3)} \Big]. \end{aligned} \tag{4.128}$$

4.D.2 The behavior as $x \to -1$

When $x \to -1$ it is straightforward from (4.13) to obtain

$$\tilde{\chi}^{(3)}_{d;2}(Singular, x = -1) \;=\; \frac{1}{2\pi} \cdot \ln(1+x). \qquad (4.129)$$

To evaluate $\tilde{\chi}^{(3)}_{d;3}$ we note, when $x \to -1$, that Q vanishes as $Q \sim \frac{27}{4}(1+x)^2$. However, we cannot directly set $Q = 0$ in (4.16) or (4.19) because we must analytically connect the solution analytic at $x = 0$ to the proper solution at $x = -1$. To do this we need further connection formulas.

We first do the general case with no logs and then specialize to our case of $c = 1$ by taking the limit.

There are two solutions (1) on page 74 of [21], u_1 and u_2 and they connect to $z = 1$ using (1) on page 108 of [21] as

$$\begin{aligned} u_1 \;&=\; {}_2F_1([a,b],[c];\, z) \qquad (4.130)\\ &= \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \cdot {}_2F_1([a,b],[a+b-c+1];\, 1-z)\\ &+\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} \cdot (1-z)^{c-a-b} \cdot {}_2F_1([c-a,c-b],\, [c-a-b+1];\, 1-z), \end{aligned}$$

$$\begin{aligned} u_2 \;=&\; z^{1-c} \cdot {}_2F_1([a+1-c,b+1-c],[2-c];\, z) \qquad (4.131)\\ =&\; z^{1-c} \cdot \{\frac{\Gamma(2-c)\Gamma(c-a-b)}{\Gamma(1-a)\Gamma(1-b)} \cdot {}_2F_1([a+1-c,b+1-c],\, [a+b-c+1];\, 1-z)\\ &+\frac{\Gamma(2-c)\Gamma(a+b-c)}{\Gamma(a+1-c)\Gamma(b+1-c)} \cdot (1-z)^{c-a-b} \cdot {}_2F_1([1-a,1-b],\, [c-a-b+1];\, 1-z)\} \end{aligned}$$

Furthermore by use of

$$\begin{aligned} &z^{1-c} \cdot {}_2F_1([a+1-c,b+1-c],\, [a+b-c+1];\, 1-z)\\ &\qquad = \;{}_2F_1([a,b],\, [a+b-c+1];\, 1-z), \end{aligned} \qquad (4.132)$$

and the companion equation obtained by the replacement $a \to c-a$ and $b \to c-b$

$$\begin{aligned} &z^{1-c} \cdot {}_2F_1([1-a,1-b],\, [c-a-b+1];\, 1-z)\\ &\qquad = \;{}_2F_1([c-a,c-b],\, [c-a-b+1];\, 1-z), \end{aligned} \qquad (4.133)$$

we rewrite (4.131) as

$$\begin{aligned} u_2 &= z^{1-c} \cdot {}_2F_1([a+1-c, b+1-c], [2-c];\, z) \\ &= \frac{\Gamma(2-c)\Gamma(c-a-b)}{\Gamma(1-a)\Gamma(1-b)} \cdot {}_2F_1([a,b],\, [a+b-c+1], 1-z) \\ &+ \frac{\Gamma(2-c)\Gamma(a+b-c)}{\Gamma(a+1-c)\Gamma(b+1-c)} \cdot (1-z)^{c-a-b} \cdot {}_2F_1([c-a, c-b], [c-a-b+1];\, 1-z). \end{aligned} \tag{4.134}$$

Thus we have the connection matrix for $c \neq 1$

$$\left[\begin{array}{c} u_1 \\ u_2 \end{array}\right] = C \cdot \left[\begin{array}{c} {}_2F_1([a,b], [a+b-c+1];\, 1-z) \\ (1-z)^{c-a-b} \cdot {}_2F_1([c-a, c-b],\, [c-a-b+1];\, 1-z) \end{array}\right],$$

with

$$C = \left[\begin{array}{cc} C_{11} & C_{12} \\ C_{21} & C_{22} \end{array}\right], \qquad \text{where:} \tag{4.135}$$

$$\begin{aligned} C_{11} &= \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}, & C_{12} &= \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}, \\ C_{21} &= \frac{\Gamma(2-c)\Gamma(c-a-b)}{\Gamma(1-a)\Gamma(1-b)}, & C_{22} &= \frac{\Gamma(2-c)\Gamma(a+b-c)}{\Gamma(a+1-c)\Gamma(b+1-c)}. \end{aligned} \tag{4.136}$$

Furthermore, using

$$C_{11}\, C_{22} - C_{12}\, C_{21} = \frac{1-c}{c-a-b}, \tag{4.137}$$

we have for $c \neq 1$

$$C^{-1} \left[\begin{array}{c} u_1 \\ u_2 \end{array}\right] = \left[\begin{array}{c} {}_2F_1([a,b],\, [a+b-c+1];\, 1-z) \\ (1-z)^{c-a-b} \cdot {}_2F_1([c-a, c-b],\, [c-a-b+1];\, 1-z) \end{array}\right], \tag{4.138}$$

with:

$$C^{-1} = \frac{c-a-b}{1-c} \cdot \left[\begin{array}{cc} C_{22} & -C_{12} \\ -C_{21} & C_{11} \end{array}\right]. \tag{4.139}$$

We now need to take the limit $c \rightarrow 1$ where the connection matrix becomes singular. In this limit we write

$$u_2 = u_1 + (1-c) \cdot \tilde{u}_2, \tag{4.140}$$

where

$$\tilde{u}_2 = \ln z\, {}_2F_1([a,b], [1];\, z) - \frac{\partial}{\partial c}\, {}_2F_1([a+1-c, b+1-c],\, [2-c];\, z)|_{c=1}. \tag{4.141}$$

Then, by subtracting (4.130) from (4.135) we find

$$\left[\begin{array}{c} u_1 \\ \tilde{u}_2 \end{array} \right] \;=\; \tilde{C} \cdot \left[\begin{array}{c} {}_2F_1([a,b],[a+b];\, 1\,-z) \\ (1-z)^{1-a-b}\, {}_2F_1([1-a,1-b],[2-a-b];\, 1\,-z) \end{array} \right],$$

with

$$\tilde{C} \;=\; \left[\begin{array}{cc} C_{11} & C_{12} \\ \tilde{C}_{21} & \tilde{C}_{22} \end{array} \right], \qquad\qquad \text{where:} \tag{4.142}$$

$$\begin{aligned} \tilde{C}_{21} \;&=\; \lim_{c\to 1} \frac{C_{21}-C_{11}}{1-c} \\ &=\; \frac{\Gamma(1-a-b)}{\Gamma(1-a)\Gamma(1-b)} \cdot (2\psi(1)-\psi(1-a)-\psi(1-b)), \qquad (4.143) \\ \tilde{C}_{22} \;&=\; \lim_{c\to 1} \frac{C_{22}-C_{12}}{1-c} \;=\; \frac{\Gamma(a+b-1)}{\Gamma(a)\Gamma(b)} \cdot (2\psi(1)\,-\psi(a)\,-\psi(b)), \end{aligned}$$

where $\psi(z) \;=\; \Gamma'(z)/\Gamma(z)$. Similarly from (4.138) we find

$$\tilde{C}^{-1} \left[\begin{array}{c} u_1 \\ \tilde{u}_2 \end{array} \right] \;=\; \left[\begin{array}{c} {}_2F_1([a,b],[a+b];\, 1\,-z) \\ (1-z)^{1-a-b} \cdot\, {}_2F_1([1-a,1-b],\, [2-a-b];\, 1\,-z) \end{array} \right], \tag{4.144}$$

with

$$\tilde{C}^{-1} \;=\; (1-a-b) \cdot \left[\begin{array}{cc} \tilde{C}_{22} & -C_{12} \\ -\tilde{C}_{21} & C_{11} \end{array} \right]. \tag{4.145}$$

We may now use (4.142) and (4.144) to study $\tilde{\chi}^{(3)}_{d;3}(x)$ as given by (4.19) as $x \to -1$. To do this we note that, as x goes from $x \;=\; 0$ to $x \;=\; -1$ on the real axis, $Q(x)$ increases monotonically from zero to one as x goes from 0 to $-1/2$, and decreases monotonically from one to zero as x goes from $-1/2$ to -1. On the segment $0 \;\geq\; x \;>\; -1/2$ the connection formula (4.142) with for u_1 is the same as (4.123) and (4.124) which we recall are

$$\begin{aligned} &{}_2F_1([1/6,1/3],[1];\, Q) \;=\; \frac{\Gamma(1)\Gamma(1/2)}{\Gamma(5/6)\Gamma(2/3)} \cdot\, {}_2F_1([1/6,1/3],\, |1/2];\, 1\,-Q) \\ &+\frac{\Gamma(1)\Gamma(-1/2)}{\Gamma(1/6)\Gamma(1/3)} \cdot (1-Q)^{1/2} \cdot\, {}_2F_1([5/6,2/3],\, [3/2];\, 1\,-Q), \qquad (4.146) \\ &{}_2F_1([7/6,4/3],\, [2];\, Q) \;=\; 18 \frac{\partial}{\partial Q}\, {}_2F_1([1/6,1/3],[1];\, Q) \\ &=\; \frac{\Gamma(2)\Gamma(-1/2)}{\Gamma(5/6)\Gamma(2/3)}\, {}_2F_1([7/6,4/3],\, [3/2];\, 1\,-Q) \\ &+\frac{\Gamma(2)\Gamma(1/2)}{\Gamma(7/6)\Gamma(4/3)} (1-Q)^{-1/2}\, {}_2F_1([5/6,2/3],\, [1/2];\, 1\,-Q). \qquad (4.147) \end{aligned}$$

From (4.17) one easily gets:

$$1 - Q \;=\; \frac{(1-x)^2\,(1+2x)^2\,(2+x)^2}{4\cdot(1+x+x^2)^3}. \tag{4.148}$$

Using (4.148), and the fact that there is no singularity at $x = -1/2$, we see that we must choose near $x = -1/2$

$$(1-Q)^{1/2} \;=\; \frac{(1-x)\cdot(1+2x)\cdot(2+x)}{2\cdot(1+x+x^2)^{3/2}}, \tag{4.149}$$

which is positive for $0 > x > -1/2$ and negative for $-1/2 > x > -1$. Therefore, for $-1/2 > x > -1$, we see that

$$u_1 \;=\; {}_2F_1([1/6,1/3],\,[1];\,Q) \;\longrightarrow\; \frac{\Gamma(1)\Gamma(1/2)}{\Gamma(5/6)\Gamma(2/3)}\cdot\,{}_2F_1([1/6,1/3],[1/2],\,1-Q)$$
$$-\frac{\Gamma(1)\Gamma(-1/2)}{\Gamma(1/6)\Gamma(1/3)}\cdot\,(1-Q)^{1/2}\,{}_2F_1([5/6,2/3],[3/2];\,1-Q). \tag{4.150}$$

We now can use (4.144) in the right hand side of (4.150) to find that for $-1/2 > x > -1$

$${}_2F_1([1/6,1/3],\,[1],\,Q) \;\to\; \frac{\sqrt{3}}{2\pi}\,\tilde{u}_2 + \frac{1}{2}\left(\frac{\Gamma(1/2)}{\Gamma(5/6)\Gamma(2/3)}\cdot\tilde{C}_{22} + \frac{\Gamma(-1/2)}{\Gamma(1/6)\Gamma(1/3)}\,\tilde{C}_{21}\right)\cdot u_1$$
$$=\; \frac{\sqrt{3}}{2\pi}\left({}_2F_1([1/6,1/3],\,[1];\,Q)\,\ln Q - \frac{\partial}{\partial c}\,{}_2F_1([7/6-c,4/3-c],\,[2-c];\,Q)|_{c=1}\right)$$
$$+\frac{1}{2}\left(\frac{\Gamma(1/2)}{\Gamma(5/6)\Gamma(2/3)}\cdot\tilde{C}_{22} + \frac{\Gamma(-1/2)}{\Gamma(1/6)\Gamma(1/3)}\cdot\,\tilde{C}_{21}\right)\cdot\,{}_2F_1([1/6,1/3],\,[1];\,Q). \tag{4.151}$$

We note that

$$\frac{\Gamma(1/2)}{\Gamma(5/6)\Gamma(2/3)}\cdot\tilde{C}_{22} \;+ \frac{\Gamma(-1/2)}{\Gamma(1/6)\Gamma(1/3)}\cdot\tilde{C}_{21} \tag{4.152}$$
$$=\; \frac{\Gamma(1/2)\Gamma(-1/2)}{\Gamma(5/6)\Gamma(1/6)\Gamma(2/3)\Gamma(1/3)}\cdot\,(4\psi(1) - \psi(1/3) - \psi(2/3) - \psi(1/6) - \psi(5/6)),$$

with $\psi(z) \;=\; \Gamma'(z)/\Gamma(z)$ and from page 19 of [21] that

$$\psi(1) \;=\; -\gamma, \qquad \psi(1/3) + \psi(2/3) \;=\; -2\gamma - 3\ln 3, \tag{4.153}$$
$$\psi(1/6) + \psi(5/6) \;=\; -2\gamma - 3\ln 3 - 4\ln 2, \tag{4.154}$$

so that we have

$$\frac{\Gamma(1/2)}{\Gamma(5/6)\Gamma(2/3)}\cdot\tilde{C}_{22} \;+ \frac{\Gamma(-1/2)}{\Gamma(1/6)\Gamma(1/3)}\cdot\tilde{C}_{21} \;=\; -\frac{\sqrt{3}}{2\pi}\cdot(6\ln 3 + 4\ln 2), \tag{4.155}$$

and thus as $x \to -1$

$$
\begin{aligned}
{}_2F_1([1/6, 1/3],\, [1];\, Q) \;&=\; \frac{\sqrt{3}}{2\pi}\,(\ln Q \,-(3\ln 3\, + 2\ln 2)) \; + O(Q \ln Q) \\
&=\; \frac{\sqrt{3}}{\pi}\,(\ln(1+x) \,- 2\ln 2) \;\; + O[(1+x)\ln(1+x)].
\end{aligned}
\tag{4.156}
$$

Similarly

$$
\begin{aligned}
{}_2F_1(7/6, 4/3; 2; Q) \;&=\; 18\,\frac{\partial}{\partial Q} \cdot {}_2F_1([1/6, 1/3], [1];\, Q) \\
&\to \qquad \frac{9\sqrt{3}}{\pi} \cdot Q^{-1},
\end{aligned}
\tag{4.157}
$$

so as $x \to -1$

$$
Q \cdot {}_2F_1([7/6, 4/3], [2];\, Q) \;\; \longrightarrow \;\; \frac{9\sqrt{3}}{\pi} \;\; + O(1). \tag{4.158}
$$

Thus, using (4.156) and (4.158) in (4.19), we find, as $x \to -1$, that

$$
\tilde{\chi}^{(3)}_{d;3}\,(Singular, x = -1) \;=\; -\frac{3}{2\pi^2} \cdot \ln^2(1+x) \;\; + 3\,\frac{2\ln 2 - 1}{\pi^2} \cdot \ln(1+x). \tag{4.159}
$$

4.D.3 The behavior as $x \to e^{\pm 2\pi i/3}$

When $x \to e^{\pm 2\pi i/3}$ then $Q \to \infty$ and $\tilde{\chi}^{(3)}_{d;3}$ becomes singular. Thus to extract this singularity we to connect that solution analytic at $x = 0$ to the singularity at $x = e^{\pm 2\pi i/3}$. To do this it is convenient to notice that Q is symmetric about $x = -1/2$. This is seen by letting

$$
x \;=\; -1/2 \, + iy, \tag{4.160}
$$

to obtain

$$
Q(y) \;=\; \frac{(1+4y^2)^2}{(1-\frac{4}{3}y^2)^3}, \tag{4.161}
$$

and we define z by

$$
z \;=\; (1 - Q(y))^{1/2} \;=\; \frac{i\,y \cdot (9/4 + y^2)}{(3/4 - y^2)^{3/2}}. \tag{4.162}
$$

Furthermore, as y goes from 0 to $\sqrt{3}/2$, $Q(y)$ goes from 1 to ∞. In the previous section we have already connected the solution analytic at $x = 0$ with the solution analytic at $x = -1/2$.

We rewrite the solutions (4.146) and (4.147) using (4.162) as

$$
\begin{aligned}
{}_2F_1([1/6,1/3],\,[1];\,Q) \;&=\; \frac{\Gamma(1)\Gamma(1/2)}{\Gamma(5/6)\Gamma(2/3)}\cdot\,{}_2F_1([1/6,1/3],\,[1/2];\,z^2)\\
&+\frac{\Gamma(1)\Gamma(-1/2)}{\Gamma(1/6)\Gamma(1/3)}\cdot z\cdot\,{}_2F_1([5/6,2/3],\,[3/2];\,z^2) \qquad (4.163)\\
{}_2F_1(7/6,4/3;2;Q) \;&=\; 18\frac{\partial}{\partial Q}\cdot\,{}_2F_1([1/6,1/3],\,[1];\,Q)\\
&= \frac{\Gamma(2)\Gamma(-1/2)}{\Gamma(5/6)\Gamma(2/3)}\cdot\,{}_2F_1([7/6,4/3],[3/2];\,z^2)\\
&\quad+\frac{\Gamma(2)\Gamma(1/2)}{\Gamma(7/6)\Gamma(4/3)}\cdot z^{-1}\cdot\,{}_2F_1([5/6,2/3],[1/2];\,z^2). \qquad (4.164)
\end{aligned}
$$

These solutions must be connected from $y = 0$ to $y = \sqrt{3}/2$ along the straight line path (4.160). On this path z^2 is on the negative real axis and, hence, we may use the connection formula (2) on page 109 of [21]

$$
\begin{aligned}
{}_2F_1([a,b],\,[c];\,z^2) \;&=\; \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)}\cdot(-z^2)^{-a}\cdot\,{}_2F_1([a,1-c+a],[1-b+a];\,z^{-2})\\
&+\frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)}\cdot\,(-z^2)^{-b}\,\cdot\,{}_2F_1([b,1-c+b],[1-a+b];\,z^{-2}). \qquad (4.165)
\end{aligned}
$$

Thus using (4.165) in (4.163) and (4.164) we find

$$
\begin{aligned}
{}_2F_1([1/6,1/3],\,[1/2],\,z^2) \;&=\; \frac{\Gamma(1/2)\Gamma(1/6)}{\Gamma(1/3)\Gamma(1/3)}(-z^2)^{-1/6}\,\cdot\,{}_2F_1([1/6,2/3],\,[5/6];\,z^{-2})\\
&+\frac{\Gamma(1/2)\Gamma(-1/6)}{\Gamma(1/6)\Gamma(1/6)}\cdot(-z^2)^{-1/3}\,{}_2F_1([1/3;5/6],\,[7/6];\,z^{-2}) \qquad (4.166)
\end{aligned}
$$

$$
\begin{aligned}
{}_2F_1([5/6,2/3];\,[3/2];\,z^2) \;&=\; \frac{\Gamma(3/2)\Gamma(-1/6)}{\Gamma(2/3)\Gamma(2/3)}\cdot(-z^2)^{-5/6}\,\cdot\,{}_2F_1([5/6,1/3],\,[7/6];\,z^{-2})\\
&+\frac{\Gamma(3/2)\Gamma(1/6)}{\Gamma(5/6)\Gamma(5/6)}\cdot\,(-z^2)^{-2/3}\cdot\,{}_2F_1([2/3,1/6],\,[5/6];\,z^{-2}), \qquad (4.167)
\end{aligned}
$$

$$
\begin{aligned}
{}_2F_1([7/6,4/3],\,[3/2];\,z^2) \;&=\; \frac{\Gamma(3/2)\Gamma(1/6)}{\Gamma(4/3)\Gamma(1/3)}(-z^2)^{-7/6}\,{}_2F_1([7/6,2/3],\,[5/6];\,z^{-2})\\
&+\frac{\Gamma(3/2)\Gamma(-1/6)}{\Gamma(7/6)\Gamma(1/6)}\cdot(-z^2)^{-4/3}\cdot\,{}_2F_1([4/3,5/6],\,[7/6];\,z^{-2}), \qquad (4.168)
\end{aligned}
$$

$$ {}_2F_1([5/6, 2/3],\ [1/2];\ z^2) \ = \ \frac{\Gamma(1/2)\Gamma(-1/6)}{\Gamma(2/3)\Gamma(-1/3)} \cdot (-z^2)^{-5/6} \cdot {}_2F_1([5/6, 4/3],\ [7/6];\ z^{-2}) $$
$$ + \frac{\Gamma(1/2)\Gamma(1/6)}{\Gamma(5/6)\Gamma(-1/6)} \cdot (-z^2)^{-2/3} \cdot {}_2F_1([2/3, 7/6],\ [5/6];\ z^{-2}). \tag{4.169} $$

Thus we obtain

$$ {}_2F_1([1/6, 1/3],\ [1];\ Q) \ = \ \frac{3}{2}\frac{\Gamma(2/3)}{\Gamma(5/6)^2} \cdot (-z^2)^{-1/6} \cdot {}_2F_1([1/6, 2/3],\ [5/6];\ z^{-2}) $$
$$ - \frac{3}{2}\frac{\Gamma(5/6)^2}{\pi\Gamma(2/3)}(-z^2)^{-1/3} \cdot {}_2F_1([1/3; 5/6], [7/6];\ z^{-2}) $$
$$ + \frac{3\sqrt{3}}{2}\frac{\Gamma(5/6)^2}{\pi\Gamma(2/3)} \cdot z \cdot (-z^2)^{-5/6} \cdot {}_2F_1([5/6, 1/3],\ [7/6];\ z^{-2}) $$
$$ - \frac{\sqrt{3}}{2}\frac{\Gamma(2/3)}{\Gamma(5/6)^2} \cdot z \cdot (-z^2)^{-2/3} \cdot {}_2F_1([2/3, 1/6],\ [5/6];\ z^{-2}), \tag{4.170} $$

and

$$ {}_2F_1([7/6, 4/3], [2];\ Q) \ = \ -\frac{9}{2}\frac{\Gamma(2/3)}{\Gamma(5/6)^2} \cdot (-z^2)^{-7/6}\, {}_2F_1([7/6, 2/3],\ [5/6];\ z^{-2}) $$
$$ +9\frac{\Gamma(5/6)^2}{\pi\Gamma(2/3)} \cdot (-z^2)^{-4/3} \cdot {}_2F_1([4/3, 5/6], [7/6];\ z^{-2}) $$
$$ +9\sqrt{3}\frac{\Gamma(5/6)^2}{\pi\Gamma(2/3)}z^{-1} \cdot (-z^2)^{-5/6} \cdot {}_2F_1([5/6, 4/3], [7/6];\ z^{-2}) $$
$$ -\frac{3\sqrt{3}}{2}\frac{\Gamma(2/3)}{\Gamma(5/6)^2} \cdot z^{-1} \cdot (-z^2)^{-2/3} \cdot {}_2F_1([2/3, 7/6],\ [5/6];\ z^{-2}). \tag{4.171} $$

Then setting

$$ z \ = \ i\,\bar{z} \tag{4.172} $$

with $\bar{z}$ real and nonnegative we obtain

$$ {}_2F_1([1/6, 1/3],\ [1];\ Q) \ = \ \frac{\sqrt{3}}{2}(\sqrt{3} - i)\frac{\Gamma(2/3)}{\Gamma(5/6)^2} \cdot \bar{z}^{-1/3} \cdot {}_2F_1([1/6, 2/3],\ [5/6];\ -\bar{z}^{-2}) $$
$$ +\frac{3}{2}\,(i\sqrt{3}\ - 1)\ \frac{\Gamma(5/6)^2}{\pi\Gamma(2/3)} \cdot \bar{z}^{-2/3} \cdot {}_2F_1([1/3, 5/6],\ [7/6];\ -\bar{z}^{-2}), \tag{4.173} $$

and

$$ {}_2F_1([7/6, 4/3],\ [2];\ Q) = -\frac{3\sqrt{3}}{2}(\sqrt{3} - i)\frac{\Gamma(2/3)}{\Gamma(5/6)^2} \cdot \bar{z}^{-7/3} \cdot {}_2F_1([7/6, 2/3],\ [5/6];\ -\bar{z}^{-2}) $$
$$ +9\,(1 - i\sqrt{3})\,\frac{\Gamma(5/6)^2}{\pi\Gamma(2/3)} \cdot \bar{z}^{-8/3} \cdot {}_2F_1([4/3, 5/6],\ [7/6];\ -\bar{z}^{-2}). \tag{4.174} $$

Now we note that

$$Q \;=\; 1 - z^2 \;=\; 1 + \bar{z}^2, \tag{4.175}$$

and thus

$${}_2F_1([1/6,1/3],\,[1];\,Q)^2 \;+\frac{2Q}{9}\,{}_2F_1([1/6,1/3],\,[1];\,Q)\cdot\,{}_2F_1([7/6,4/3],\,[2];\,Q)$$

$$= \;(\sqrt{3}-i)^2\,\frac{\Gamma(2/3)^2}{\Gamma(5/6)^4}\cdot\bar{z}^{-2/3}\cdot\,{}_2F_1([1/6,2/3],\,[5/6];\,-\bar{z}^{-2})$$
$$\times\left(\frac{3}{4}\cdot\,{}_2F_1([1/6,2/3],[5/6];\,-\bar{z}^{-2}) - \frac{1}{2}(1+\bar{z}^{-2})\cdot\,{}_2F_1([7/6,2/3],\,[5/6];\,-\bar{z}^{-2})\right)$$

$$+(i\sqrt{3}-1)^2\,\frac{\Gamma(5/3)^4}{\pi^2\Gamma(2/3)^2}\cdot\bar{z}^{-4/3}\cdot\,{}_2F_1([1/3,5/6],\,[7/6];\,-\bar{z}^{-2})$$
$$\times\left(\frac{9}{4}\,{}_2F_1([1/3,5/6],\,[7/6];\,-\bar{z}^{-2}) - 3\,(1+\bar{z}^{-2})\cdot\,{}_2F_1([4/3,5/6],\,[7/6];\,-\bar{z}^{-2})\right)$$
$$+\frac{6\sqrt{3}}{\pi}\,i\,\bar{z}^{-1}\cdot\,{}_2F_1([1/6,2/3],\,[5/6];\,-\bar{z}^{-2})\cdot\,{}_2F_1([1/3,5/6],\,[7/6];\,-\bar{z}^{-2})$$
$$-4\,\frac{\sqrt{3}}{\pi}\,i\,\bar{z}^{-1}\,(1+\bar{z}^{-2})\cdot\,{}_2F_1([1/6,2/3],\,[5/6];\,-\bar{z}^{-2})\,{}_2F_1([4/3,5/6],\,[7/6];\,-\bar{z}^{-2})$$
$$-2\frac{\sqrt{3}}{\pi}\,i\,\bar{z}^{-1}\,(1+\bar{z}^{-2})\cdot\,{}_2F_1([7/6,2/3]\,[5/6];\,-\bar{z}^{-2})\cdot\,{}_2F_1([1/3,5/6],\,[7/6];\,-\bar{z}^{-2}).$$

As $\bar{z} \,\to\, \infty$ the last three terms go as

$$-\,\frac{54\sqrt{3}}{\pi 35}\cdot\, i\;\bar{z}^{-3} \tag{4.176}$$

Thus, noting, as $x \,\to\, e^{2\pi i/3}$, that

$$\bar{z} \;\;\longrightarrow\;\;\; \frac{3^{3/4}}{2}\,e^{-3\pi i/4}\cdot\,(x-x_0)^{-3/2}, \tag{4.177}$$

and

$$\frac{(1\,+2x)\cdot(x\,+2)}{(1-x)\cdot(x^2+x+1)} \;\;\longrightarrow\;\;\; \frac{e^{\pi i/3}}{x-x_0}, \tag{4.178}$$

we find that the leading singularity at $x_0 \,=\, e^{2\pi i/3}$ in $\tilde{\chi}^{(3)}_{d,3}$ is

$$\tilde{\chi}^{(3)}_{d;3}(Singular, x=x_0) \quad=\quad \frac{16\cdot 3^{5/4}}{35\pi}\cdot\, e^{\pi i/12}\cdot(x-x_0)^{7/2}. \tag{4.179}$$

4.E Analysis of the singular behavior of $\tilde{\chi}^{(4)}_{d;2}(t)$ as $t \rightarrow 1$

To get the singular behaviour of $\tilde{\chi}^{(4)}_{d;2}(t)$ as $t \rightarrow 1$, we use (12) of page 110 of [21]

$$
\begin{aligned}
{}_2F_1([1/2, -1/2], [1]; t) \; &= \; \frac{2}{\pi} \qquad\qquad (4.180)\\
+\frac{1-t}{2\pi} \cdot [\psi(1) \, + \psi(2) \, - \psi(3/2) \, &- \psi(1/2) \, - \ln(1-t)] \, + O((1-t)^2 \ln(1-t)),
\end{aligned}
$$

and

$$
\begin{aligned}
{}_2F_1([1/2, 1/2], [1]; t) \; &= \; \frac{1}{\pi} \cdot [2\psi(1) \, - 2\psi(1/2) \, - \ln(1-t)] \\
+\frac{1}{\pi} \cdot [\frac{1-t}{4}(2\psi(2) \, - 2\psi(3/2) \, &- \ln(1-t))] \, + O((1-t)^2 \ln(1-t) \qquad (4.181)
\end{aligned}
$$

we have

$$
\begin{aligned}
&{}_2F_1([1/2, -1/2], |1]; t) \\
&= \; \frac{2}{\pi} \; - \frac{1-t}{2\pi}\big(1 \, - 4\ln 2 \, + \ln(1-t^2)\big) \; + O((1-t)^2 \ln(1-t^2) \\
&= \; \frac{2}{\pi} \cdot \left(1 + \frac{1-t}{4}(\ln \frac{16}{1-t} \, - 1)\right) \, + O((1-t)^2 \, \ln(1-t), \qquad (4.182)
\end{aligned}
$$

and

$$
\begin{aligned}
&{}_2F_1([1/2, 1/2], [1], t) \; = \qquad\qquad (4.183)\\
&= \; \frac{1}{\pi} \cdot \left(\ln \frac{16}{1-t} \; + \frac{1-t}{4} \cdot \, (\ln \frac{16}{1-t}) - 2\right) \; + O((1-t)^2 \ln(1-t).
\end{aligned}
$$

Using these in (4.13) we find the result quoted in the text in (4.86).

4.F Towards an exact expression for $3I_1^{>} - 4I_2^{>}$

The constant $3I_1^{>} \, - 4I_2^{>}$ occurs for $\tilde{\chi}^{(4)}_d(t)$ through $\tilde{\chi}^{(4)}_{d;3}$ which is obtained (4.63) by the action of the differential operator A_3 on ${}_4F_3([1/2,\, 1/2,\, 1/2,\, 1/2], [1,\, 1,\, 1];\, t^2)$.

The constant $3I_1^{>} \, - 4I_2^{>}$ can then be deduced from the 4×4 connection matrix for ${}_4F_3([1/2,\, 1/2,\, 1/2,\, 1/2], [1,\, 1,\, 1];\, t^2)$. The line of the connection matrix relating the solutions at $t \, = \, 0$ to the solutions at $t \, = \, 1$ is

$$
[A_{4,1}, \;\; -1/2 \cdot A_{4,1} \, + 2/\pi^2, \;\; A_{4,3} \, - 2\, i/\pi, \;\; A_{4,4} \, + i/\pi],
$$

and the constant $3I_1^> - 4I_2^>$ reads

$$\frac{4}{3\pi^2} \cdot (3\, I_1^> \, - 4\, I_2^>) \quad = \quad -\frac{16}{\pi^2} \, + \, \frac{17}{108} \cdot A_{4,1} \, - \frac{2}{3} \cdot A_{4,3} \, - \, \frac{4}{3} \cdot A_{4,4}, \qquad (4.184)$$

The entry $A_{4,1}$ of the connection matrix is actually the *evaluation of the hypergeometric function* (4.59) at $t \, = \, 1$:

$$A_{4,1} \; = \; -2 \cdot {}_4F_3\Big([\frac{1}{2}, \, \frac{1}{2}, \, \frac{1}{2}, \, \frac{1}{2}], \, [1, \, 1, \, 1], \, 1\Big). \qquad (4.185)$$

There is, at first sight, a "ln(2)" coming from the terms in the Buhring formula [64] involving the ψ function. This is the "same" log 2 which appears in the connection formulas for $E(k)$ and $K(k)$. However, numerically, these $\ln(2)$ contributions in $A_{4,3}$ and $A_{4,4}$ read respectively ($\alpha = -1.9453040783 \cdots$, $\gamma = 0.5274495683 \cdots$):

$$A_{4,3} \; = \; \alpha \, + \, 2 \cdot \beta \cdot \ln(2), \qquad A_{4,4} \; = \; \gamma \, - \, \beta \cdot \ln(2), \qquad (4.186)$$
$$\beta \; = \; 0.101321183 \; \cdots$$

The fact that these two entries occur through the linear combination $A_{4,3} + 2 \cdot A_{4,4}$ actually cancel a $\ln(2)$ contribution in the expression of the constant $3I_1^> - 4I_2^>$.

Similar constants (see (4.104) for the bulk $\tilde{\chi}^{(4)}$, (4.105) for the bulk $\tilde{\chi}^{(3)}$) can be deduced from entries of the connection matrices (occurring in the exact calculation of the differential Galois group [265]), such entries being often closely related to evaluation, at selected singular points, of the holonomic solutions we are looking at. When hypergeometric functions like (4.59) pop out, it is not a surprise to have entries that can be simply expressed as these hypergeometric functions at $x \, = \, 1$ (see (4.185)). Along this line, it is worth recalling that $\zeta(3)$ (or $\zeta(5)$, ...) can be simply expressed in terms of a simple evaluation at $x \, = \, 1$ of a ${}_{q+1}F_q$ hypergeometric function [144] (see also [192]):

$$\zeta(3) \; = \; {}_4F_3([1, 1, 1, 1], [2, 2, 2]; \, 1), \qquad (4.187)$$
$$\zeta(5) \; = \; \frac{32}{31} \cdot {}_6F_5([\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1], [\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}]; \, 1).$$

It is thus quite natural to ask if the sums in $I_1^>$ and $I_2^>$ can be evaluated in terms of known constants such as $\zeta(3)$ or evaluations (for instance at $t \, = \, 1$) of hypergeometric functions.

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Chapter 5

Paper 3

Hard hexagon partition function for complex fugacity

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Abstract

We study the analyticity of the partition function of the hard hexagon model in the complex fugacity plane by computing zeros and transfer matrix eigenvalues for large finite size systems. We find that the partition function per site computed by Baxter in the thermodynamic limit for positive real values of the fugacity is not sufficient to describe the analyticity in the full complex fugacity plane. We also obtain a new algebraic equation for the low density partition function per site.

5.1 Introduction

The hard hexagon model was solved by Baxter over 30 years ago [22, 29, 30]. More precisely Baxter computed the thermodynamic limit of the grand partition function per site for real positive values of the fugacity z

$$\lim_{L_v,L_h\to\infty} Z_{L_v,L_h}^{1/L_vL_h}(z) \qquad \text{with} \qquad 0 < L_v/L_h < \infty \qquad \text{fixed.} \tag{5.1}$$

Even more precisely Baxter computed the limit

$$\kappa(z) = \lim_{L_h\to\infty} \lambda_{\max}(z;L_h)^{1/L_h}, \tag{5.2}$$

where $\lambda_{\max}(z;L_h)$ is the largest eigenvalue of the transfer matrix. Baxter found that there are two distinct regions of positive fugacity

$$0 \le z < z_c \qquad \text{and} \qquad z_c < z < \infty, \tag{5.3}$$

with

$$z_c = \frac{11+5\sqrt{5}}{2} = 11.0901699473 \cdots, \tag{5.4}$$

where in each separate region the partition function per site has separate analytic expressions, which we denote by $\kappa_-(z)$ for the low density, and by $\kappa_+(z)$ for the high density intervals respectively. The low density function $\kappa_-(z)$ has branch points at z_c and

$$z_d = -\frac{1}{z_c} = \frac{11-5\sqrt{5}}{2} = -0.0901699473 \cdots, \tag{5.5}$$

is real and positive in the interval $z_d \le z \le z_c$ and is analytic in the plane cut along the real axis from z_d to $-\infty$ and z_c to $+\infty$. Conversely the high density function $\kappa_+(z)$ is real and positive for $z_c \le z < +\infty$ and is analytic in the plane cut along the real axis from z_c to $-\infty$.

For the purpose of thermodynamics it is sufficient to restrict attention to positive values of the fugacity. However, it is of considerable interest to investigate the behavior of the partition function for complex values of z as well. For finite size systems the partition function is, of course, a polynomial and as such can be specified by its zeros.

In the thermodynamic limit the free energy will be analytic in all regions which are the limit of the zero free regions of the finite system [260]. In general there will be several such regions. One such example with three regions is given by Baxter [23]. There appears to be no general theorem stating when the free energy of a system can be continued through the locus of zeros.

The analytic structure of the free energy in the complex fugacity plane is not in general determined by the the free energy on the positive z axis and for hard hexagons it is only for the positive z axis that a complete analysis has been carried out. In this paper we address the problem of determining analyticity in the complex z plane by computing the partition function zeros on lattices as large as 39×39 and comparing these zeros with the locus computed from the limiting partition functions per site computed by Baxter for real positive value for the fugacity $0 \leq z \leq \infty$. We will see that the two functions $\kappa_{\pm}(z)$ are not sufficient to describe the location of the zeros in the complex z plane. There is, of course, no reason that $\kappa_{\pm}(z)$ should be sufficient to represent the partition function in the entire complex z plane. We propose in section 5.6.2 an extension of Baxter's methods which can explain our results in the portion of the complex plane not covered by $\kappa_{\pm}(z)$.

In section 5.2 we present the relation between partition function zeros and the eigenvalues of the transfer matrix with special attention to the differences between cylindrical and toroidal boundary conditions.

In section 5.3 we begin by recalling the results of Baxter [22] for $\kappa_{\pm}(z)$ and the subsequent analysis of Joyce [133] for the high density regime for the polynomial relation between z and $\kappa_{+}(z)$. For the low density regime we derive a new polynomial relation between z and $\kappa_{-}(z)$. Some details of the analysis of $\kappa_{\pm}(z)$ and the associated density $\rho_{-}(z)$ are presented in 5.A and 5.B.

In section 5.4 we compute transfer matrix eigenvalues and equimodular curves for the maximum eigenvalues for values of L_h as large as 30. We demonstrate the difference between the equimodular curves of the full transfer matrix and the equimodular curves for eigenvalues restricted to the sector $P = 0$. These equimodular curves are compared with the partition functions per site $\kappa_{\pm}(z)$.

In section 5.5 we present the results for partition function zeros for both toroidal and cylindrical boundary conditions for a variety of $L_h \times L_v$ lattices. For $L_h = L_v$ the largest sizes are 39×39 for cylindrical and 27×27 for toroidal boundary conditions. We compare the zeros with $\kappa_{\pm}(z)$ and with the equimodular eigenvalue curves of section 5.4 for both the cases $L_v = L_h$ and $L_v \gg L_h$ and we analyze the density of zeros on the negative z axis. We analyze the dependence of the approach as $L \to \infty$ of the endpoints $z_d(L)$ and $z_c(L)$ to z_d and z_c by means of finite size scaling and identify several correction to scaling exponents.

In section 5.6 we use our results to discuss the relation of the free energy on the positive real fugacity axis to the partition function in the full complex fugacity plane and some concluding remarks are made in section 5.7. A description of the methods used for the numerical computations of eigenvalues and zeros are given in 5.E and the numerical details of the finite size scaling are given in 5.F.

5.2 Preliminaries

In this section we review the concepts of partition function, transfer matrix, free energy and partition function zeros and highlight the properties we discuss in later sections.

5.2.1 Partition function

The hard hexagon model is defined on a triangular lattice, which is conveniently viewed as a square lattice with an added diagonal on each face as shown in figure 5.1. Particles are placed on the sites of the lattice with the restriction that if there is a particle at one site no particle is allowed at the six nearest neighbor sites. The grand canonical partition function on the lattice with L_v rows and L_h columns is computed as

$$Z_{L_v,L_h}(z) \;=\; \sum_{N=0}^{\infty} g(N)\cdot\, z^N, \tag{5.6}$$

where $g(N)$ is the number of allowed configurations with N particles. By definition on a finite lattice the partition function is a polynomial which can be described by its zeros z_k as $\prod(1-z/z_k)$. For hard hexagons the order of the polynomial is bounded above by $L_vL_h/3$ which becomes an equality when it is an integer.

5.2.2 Transfer matrices

An alternative and quite different representation of the partition function on the finite lattice is given in terms of a transfer matrix $T(z;L_h)$ computed in terms of the local Boltzmann weights in figure 5.1 as

$$T_{\{b_1,\cdots b_{L_h}\},\{a_1,\cdots .a_{L_h}\}} \;=\; \prod_{j=1}^{L_h} W(a_j,\, a_{j+1};\, b_j,\, b_{j+1}), \tag{5.7}$$

where the occupation numbers a_j and b_j take the values 0 and 1 and for periodic boundary conditions in the horizontal direction we use the convention that $L_h+1\equiv 1$. Then the hard hexagon weights $W(a_j,a_{j+1};b_j,j_{j+1})$ are written (see page 403 of [29, 30]) in the form

$$\begin{aligned} &W(a_j,a_{j+1};b_j,b_{j+1}) \;=\; 0 \\ &\text{for} \qquad a_ja_{j+1} \;=\; b_jb_{j+1} \;=\; a_jb_j \;=\; a_{j+1}b_{j+1} \;=\; a_{j+1}b_j \;=\; 1, \end{aligned} \tag{5.8}$$

and otherwise:

$$W(a_j,a_{j+1};\, b_j,b_{j+1}) \;=\; z^{(a_j+a_{j+1}+b_j+b_{j+1})/4}. \tag{5.9}$$

This transfer matrix does not satisfy $T\,=\,T^t$: thus there may be complex eigenvalues even for $z\,\geq\,0$. As far as real values of z are concerned, the matrix elements are all non negative for $z\,\geq\,0$ and, thus, by the Perron-Frobenius theorem the maximum eigenvalue is real and positive.

For lattices with toroidal boundary conditions where there are periodic boundary conditions in the vertical direction

$$Z^P_{L_v,L_h}(z) \;=\; \mathrm{Tr}\; T^{L_v}(z;L_h). \tag{5.10}$$

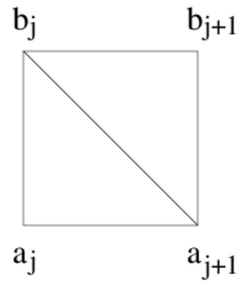


Figure 5.1: Boltzmann weights for the transfer matrix of hard hexagons

For lattices with cylindrical boundary conditions where there are free boundary condition in the vertical direction

$$Z^C_{L_v,L_h}(z) \;=\; \langle \mathbf{v}_B | T^{L_v}(z;L_h) | \mathbf{v}'_B \rangle, \tag{5.11}$$

where $\mathbf{v}_B$ and $\mathbf{v}'_B$ are suitable vectors for the boundary conditions on rows 1 and L_v. For the transfer matrix (5.7) with Boltzmann weights given by the symmetrical form (5.8) with (5.9) the components of the vectors $\mathbf{v}_B$ and $\mathbf{v}'_B$ for free boundary conditions are

$$\mathbf{v}_B(a_1, a_2, \cdots, a_{L_h}) \;=\; \mathbf{v}'_B(a_1, a_2, \cdots, a_{L_h}) \;=\; \prod_{j=1}^{L_h} z^{a_j/2}. \tag{5.12}$$

When the transfer matrix is diagonalizable (5.10) and (5.11) may be written in terms of the eigenvalues λ_k and eigenvectors $\mathbf{v}_k$ of the transfer matrix $T_{L_h}(z)$ as

$$Z^P_{L_v,L_h}(z) \;=\; \sum_k \lambda_k^{L_v}(z;L_h) \qquad \text{and} \tag{5.13}$$

$$Z^C_{L_v,L_h}(z) \;=\; \sum_k \lambda_k^{L_v}(z;L_h)\cdot c_k \quad \text{where} \quad c_k \;=\; (\mathbf{v_B}\cdot\mathbf{v_k})(\mathbf{v_k}\cdot\mathbf{v'_B}). \tag{5.14}$$

5.2.3 The thermodynamic limit

For finite size systems the hard hexagon partition function is a polynomial and the transfer matrix eigenvalues are all algebraic functions. However, for physics we must study the thermodynamic limit where $L_v,\ L_h \to \infty$ and, because both the partition function and the transfer matrix eigenvalues diverge in this limit we consider instead of the partition function the free energy

$$-F/k_BT \;=\; \lim_{L_v,L_h\to\infty} (L_vL_h)^{-1}\cdot \ln Z_{L_v,L_h}(z). \tag{5.15}$$

For real positive values of z this limit must be independent of the aspect ratio $0 < L_v/L_h < \infty$ for thermodynamics to be valid.

In terms of the transfer matrix representations of the partition function (5.13) and (5.14) we take the limit $L_v \to \infty$

$$\lim_{L_v\to\infty} L_v^{-1} \cdot \ln Z_{L_v,L_h}(z) \;=\; \ln \lambda_{\max}(z; L_h). \tag{5.16}$$

For the limiting free energy (5.15) to exist and be non zero it is required that

$$0 \;<\; \lim_{L_h\to\infty} L_h^{-1} \cdot \ln \lambda_{\max}(z; L_h) \;<\; \infty, \tag{5.17}$$

or, equivalently, that the partition function per site exists

$$\kappa(z) \;=\; \lim_{L_h\to\infty} \lambda_{\max}\,(z; L_h)^{1/L_h} \;<\; \infty, \tag{5.18}$$

(in other words the maximum eigenvalue must be exponential in L_h). This exponential behavior will guarantee that for real positive z

$$\lim_{L_h\to\infty}\, \lim_{L_v\to\infty} (L_v L_h)^{-1} \ln Z_{L_v,L_h}(z) \;=\; \lim_{L_v,L_h\to\infty} (L_v L_h)^{-1} \cdot \ln Z_{L_v,L_h}(z), \tag{5.19}$$

independent of the aspect ratio L_v/L_h. However for complex "nonphysical values" of z this independence of the ratio L_v/L_h is not obvious. In particular for hard squares at $z = -1$ *all* eigenvalues of the transfer matrix lie on the unit circle and the partition function $Z_{L_v,L_h}(-1)$ depends on number theoretic properties [90, 130, 61, 25] of L_v and L_h.

5.2.4 Partition function zeros versus transfer matrix eigenvalues

It remains in this section to relate partition function zeros to transfer matrix eigenvalues and eigenvectors. For finite lattices the partition function zeros can be obtained from (5.13) and (5.14) if all eigenvalues and eigenfunctions are known. We begin with the simplest case where

$$L_v \;\to\; \infty \qquad \text{with fixed} \qquad L_h, \tag{5.20}$$

considered by Beraha, Kahane and Weiss [34, 33, 32] as presented by Salas and Sokal [210]. This is the case of a cylinder of infinite length with L_h sites in the finite direction where the aspect ratio $L_v/L_h \to \infty$.

Generically the eigenvalues have different moduli and in the limit (5.20) the partition function will have zeros when two or more maximum eigenvalues of $T(z; L_h)$ have equal moduli

$$|\lambda_1(z; L_h)| \;=\; |\lambda_2(z; L_h)|. \tag{5.21}$$

The locus in the complex plane z is called an equimodular curve [246, 248, 250, 251]. On this curve

$$\frac{\lambda_1(z;L_h)}{\lambda_2(z;L_h)} = e^{i\phi(z)}, \tag{5.22}$$

where $\phi(z)$ is real and depends on z. The density of zeros on this curve is proportional to $d\phi(z)/dz$.

A simple example occurs for hard hexagons where on segments of the negative z-axis there is a complex conjugate pair of eigenvalues which have the maximum modulus.

However, we will see that for the hard hexagon model there are points in the complex plane where more than two eigenvalues values have equal moduli. Indeed, for hard squares at $z = -1$, we have previously noted that all eigenvalues have modulus one.

For values of z in the complex plane where the interchange of (5.19) holds the limiting locus of partition function zeros for the square $L_v = L_h$ lattice will coincide with the transfer matrix equimodular curves. However there is no guarantee that the interchange (5.19) holds in the entire complex z plane.

Our considerations are somewhat different for toroidal and cylindrical boundary conditions and we treat these two cases separately.

Cylindrical boundary conditions

For cylindrical boundary conditions the partition function is given by (5.14) which in addition to the eigenvalues of $T(L_h)$ depends on the boundary vector $\mathbf{v}_B$ (5.12). Because of the periodic boundary conditions in the L_h direction there is a conserved momentum P. Consequently the transfer matrix and translation operator may be simultaneously diagonalized. Therefore the transfer matrix may be block diagonalized by a transformation which is independent of z and hence the characteristic equation will factorize. Furthermore the boundary vector (5.12) for the cylindrical case satisfies

$$\mathbf{v}_B(a_1, a_2, \cdots, a_{L_h}) = \mathbf{v}_B(a_{L_h}, a_1, \cdots, a_{L_h-1}) \tag{5.23}$$

and thus is also translationally invariant. Therefore the only eigenvectors which contribute to the partition function in (5.14) lie in the translationally invariant subspace where $P = 0$. Consequently we are able to restrict our attention to the reduced transfer matrix for this translationally invariant sector where the momentum of the state is $P = 0$ because all of the scalar products c_k in (5.14) for eigenvectors in sectors with $P \neq 0$ vanish.

Toroidal boundary conditions

For toroidal boundary conditions the partition function in (5.13) is the sum over all eigenvalues and a new feature arises because for $P \neq 0, \pi$ the eigenvalues for $\pm P$ are degenerate in modulus, but may have complex conjugate phases which are independent of z.

By grouping these two eigenvalues together we see that the discussion leading to (5.21) still applies. There are now three types of equimodular curves:

1) Two eigenvalues are equal for crossings of eigenvectors with $P = 0, \pi$,

2) Three eigenvalues are equal for crossings of eigenvectors of $P = 0, \pi$ with $P \neq 0, \pi$,

3) Four eigenvalues are equal for crossing of eigenvectors with $P \neq 0, \pi$.

Nonzero finite aspect ratios L_v/L_h

We are, of course, not really interested in the limit (5.20) but rather in the case of finite nonzero aspect ratio L_v/L_h and particularly in the isotropic case $L_v = L_h$. There is apparently no general theory for finite nonzero aspect ratio in the literature and we will study this case in detail below.

5.3 The partition functions $\kappa_\pm(z)$ per site for hard hexagons

Baxter [22, 29, 30] has computed the fugacity and the partition function per site in terms of an auxiliary variable x using the functions

$$G(x) = \prod_{n=1}^{\infty} \frac{1}{(1-x^{5n-4})(1-x^{5n-1})}, \tag{5.24}$$

$$H(x) = \prod_{n=1}^{\infty} \frac{1}{(1-x^{5n-3})(1-x^{5n-2})}, \qquad Q(x) = \prod_{n=1}^{\infty} (1-x^n). \tag{5.25}$$

For high density where $0 < z^{-1} < z_c^{-1}$ the results are

$$z = \frac{1}{x} \cdot \Big(\frac{G(x)}{H(x)}\Big)^5 \qquad \text{and} \tag{5.26}$$

$$\kappa_+ = \frac{1}{x^{1/3}} \cdot \frac{G^3(x)\,Q^2(x^5)}{H^2(x)} \cdot \prod_{n=1}^{\infty} \frac{(1-x^{3n-2})(1-x^{3n-1})}{(1-x^{3n})^2}, \tag{5.27}$$

where, as x increases from 0 to 1, the value of z^{-1} increases from 0 to z_c^{-1}.

For low density where $0 \leq z < z_c$

$$z = -x \cdot \Big(\frac{H(x)}{G(x)}\Big)^5 \qquad \text{and} \tag{5.28}$$

$$\kappa_- = \frac{H^3(x)\, Q^2(x^5)}{G^2(x)} \cdot \prod_{n=1}^{\infty} \frac{(1-x^{6n-4})(1-x^{6n-3})^2(1-x^{6n-2})}{(1-x^{6n-5})(1-x^{6n-1})(1-x^{6n})^2}, \tag{5.29}$$

where, as x decreases from 0 to -1, the value of z increases from 0 to z_c.

5.3.1 Algebraic equations for $\kappa_\pm(z)$

The auxiliary variable x can be eliminated between the expressions for z and κ (5.26)-(5.29) and the resulting functions $\kappa_\pm(z)$ are in fact algebraic functions of z. To give these algebraic equations we follow Joyce [133] and introduce the functions

$$\Omega_1(z) = 1 + 11z - z^2, \tag{5.30}$$
$$\Omega_2(z) = z^4 + 228z^3 + 494z^2 - 228z + 1, \tag{5.31}$$
$$\Omega_3(z) = (z^2+1) \cdot (z^4 - 522z^3 - 10006z^2 + 522z + 1). \tag{5.32}$$

For the high density Joyce (see eqn. (7.9) in [133]) showed that the function $\kappa_+(z)$ satisfies a polynomial relation of degree 24 in the variable $\kappa_+(z)$

$$f_+(z, \kappa_+) = \sum_{k=0}^{4} C_k^+(z) \cdot \kappa_+^{6k} = 0, \qquad \text{where} \tag{5.33}$$

$$\begin{aligned}
C_0^+(z) &= -3^{27}\, z^{22} \\
C_1^+(z) &= -3^{19}\, z^{16} \cdot \Omega_3(z), \\
C_2^+(z) &= -3^{10}\, z^{10} \cdot [\Omega_3^2(z) - 2430\, z \cdot \Omega_1^5(z)], \\
C_3^+(z) &= -z^4 \cdot \Omega_3(z) \cdot [\Omega_3^2(z) - 1458\, z \cdot \Omega_1^5(z)] \\
C_4^+(z) &= \Omega_1^{10}(z).
\end{aligned} \tag{5.34}$$

Joyce has also derived an algebraic equation for the density (see eqn. (8.28) in [133]) which follows from (5.33).

For low density we have obtained by means of a Maple computation the substantially more complicated polynomial relation which was not obtained in [133]

$$f_-(z, \kappa_-) = \sum_{k=0}^{12} C_k^-(z) \cdot \kappa_-^{2k} = 0, \qquad \text{where} \tag{5.35}$$

$$
\begin{aligned}
C_0^-(z) &= -2^{32} \cdot 3^{27} \cdot z^{22}, \\
C_1^-(z) &= 0 \\
C_2^-(z) &= 2^{26} \cdot 3^{23} \cdot 31 \cdot z^{18} \cdot \Omega_2(z), \\
C_3^-(z) &= 2^{26} \cdot 3^{19} \cdot 47 \cdot z^{16} \cdot \Omega_3(z), \\
C_4^-(z) &= -2^{17} \cdot 3^{18} \cdot 5701 \cdot z^{14} \cdot \Omega_2^2(z), \\
C_5^-(z) &= -2^{16} \cdot 3^{14} \cdot 7^2 \cdot 19 \cdot 37 \cdot z^{12} \cdot \Omega_2(z)\,\Omega_3(z), \\
C_6^-(z) &= -2^{10} \cdot 3^{10} \cdot 7 \cdot z^{10} \cdot [273001 \cdot \Omega_3^2(z) + 2^6 \cdot 3^5 \cdot 5 \cdot 4933 \cdot z \cdot \Omega_1^5(z)], \\
C_7^-(z) &= -2^9 \cdot 3^{10} \cdot 11 \cdot 13 \cdot 139 \cdot z^8 \cdot \Omega_3(z)\,\Omega_2^2(z), \\
C_8^-(z) &= -3^5 \cdot z^6 \cdot \Omega_2(z) \cdot [7 \cdot 1028327 \cdot \Omega_3^2(z) - 2^6 \cdot 3^4 \cdot 11 \cdot 419 \cdot 16811 \cdot z \cdot \Omega_1^5(z)], \\
C_9^-(z) &= -z^4 \cdot \Omega_3(z) \cdot [37 \cdot 79087\,\Omega_3^2(z) + 2^6 \cdot 3^6 \cdot 5150251 \cdot z \cdot \Omega_1^5(z)], \\
C_{10}^-(z) &= -z^2 \cdot \Omega_2^2(z) \cdot [19 \cdot 139\Omega_3^2(z) - 2 \cdot 3^6 \cdot 151 \cdot 317 \cdot z \cdot \Omega_1^5(z)] \\
C_{11}^-(z) &= -\Omega_2(z)\,\Omega_3(z) \cdot [\Omega_3^2(z) - 2 \cdot 613 \cdot z \cdot \Omega_1^5(z)], \\
C_{12}^-(z) &= \Omega_1^{10}(z).
\end{aligned}
\tag{5.36}
$$

We have verified that Joyce's algebraic equation for the density (see eqn. (12.10) in [133]) follows from (5.35).

We note the symmetry

$$
z^{44} \cdot f_\pm\Big(-\frac{1}{z}, \frac{\kappa_\pm}{z}\Big) \quad = \quad f_\pm(z, \kappa). \tag{5.37}
$$

In 5.A we discuss the behavior $\kappa_\pm(z)$ at the singular points $z_c,\ z_d$.

5.3.2 Partition function for complex z

From section 5.2.4 we see that the simplest construction of the partition function of hard hexagons in the complex z plane would be if the low and high density eigenvalues in the thermodynamic limit were the only two eigenvalues of maximum modulus and that the interchange of limits (5.19) holds for z in the entire complex plane. Then the zeros would be given by the equimodular curve $|\kappa_+(z)| = |\kappa_-(z)|$. Because the partition functions per site $\kappa_\pm(z)$ satisfy algebraic equations this curve will satisfy an algebraic equation which can be found by setting $\kappa_+(z) = r\kappa_-(z)$ in the equation (5.33) for $\kappa_+(z)$ and computing the resultant between equations (5.35) and (5.33). The solutions of this equation for r on the unit circle will give all the locations where $\kappa_\pm(z)$ have equimodular solutions. We have produced this equation using Maple but unfortunately is it too large to print out. However, we are only interested in the crossings of the maximum modulus eigenvalues. Consequently we have computed this curve not from its algebraic equation but directly from the parametric representations (5.26)-(5.29). We plot this curve in figure 5.2. The curve crosses the positive real axis at z_c and the negative real axis at $z = -5.9425104 \cdots$ which is exactly determined from the algebraic equation of the equimodular curve given in 5.C. The tangent to the equimodular curve is discontinuous at this negative value of z.

We will see in the next section that this two eigenvalue assumption is insufficient to account for our finite size computations in some regions of the plane.

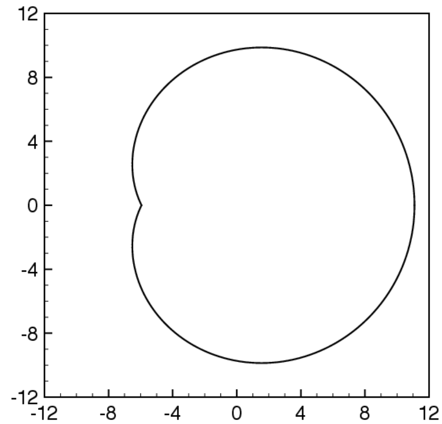


Figure 5.2: The equimodular curve for $|\kappa_-(z)| = |\kappa_+(z)|$ in the complex z plane. The crossing of the positive z axis is at z_c and the crossing of the negative z axis is at $z = -5.925104\cdots$

5.4 Transfer matrix eigenvalues

To obtain further information on the partition function in the complex z plane we compute, in this section, the eigenvalues for finite sizes of the transfer matrix $T(z; L_h)$ for the case of periodic boundary conditions in the L_h direction.

There are two ways to study the eigenvalues of the transfer matrix; analytically and numerically. Numerical computations can be carried out on matrices which are too large for symbolic computer programs to handle. However, analytic computations reveal properties which cannot be seen in numerical computations. Consequently we begin our presentation with analytic results before we present our numerical results.

5.4.1 Analytic results

The eigenvalues of a matrix are obtained as the solutions of its characteristic equation. For the transfer matrices of the hard hexagon model this characteristic equation is a polynomial in the parameter z and the eigenvalue λ with integer coefficients. Consequently the eigenvalues λ are algebraic functions of z. In general such characteristic polynomials will be irreducible (i.e. they will not factorize into products of polynomials with integer coefficients).

There are two important analytic non-generic features of the hard hexagon eigenvalues: factorization of the characteristic equation and the multiplicity of the roots of the resultant.

Factorization of the characteristic equation

For a transfer matrix with cylindrical boundary conditions the characteristic equation factorizes into subspaces characterized by a momentum eigenvalue P. In general the characteristic polynomial in the translationally invariant $P = 0$ subspace will be irreducible. We have found that this is indeed the case for hard squares. However, for hard hexagons we find that for $L_h = 12, 15, 18$, the characteristic polynomial, for $P = 0$, factors into the product of two irreducible polynomials with integer coefficients. We have not been able to study the factorization for larger values of L_h but we presume that factorization always occurs and is a result of the integrability of hard hexagons. What is unclear is if for larger lattices a factorization into more than two factors can occur.

Multiplicity of the roots of the resultant

An even more striking non-generic property of hard hexagons is seen in the computation of the resultant of the characteristic polynomial in the translationally invariant sector. The zeros of the resultant locate the positions of all potential singularities of the solutions of the polynomials.

We have been able to compute the resultant for $L_h = 12, 15, 18$, and find that almost all zeros of the resultant have multiplicity two which indicates that there is in fact no singularity at those points and that the two eigenvalues cross. This very dramatic property will almost certainly hold for all L_h and must be a consequence of the integrability (although to our knowledge no such theorem is in the literature).

5.4.2 Numerical results in the sector $P = 0$

For the partition function with cylindrical boundary conditions only the transfer matrix eigenvalues with $P = 0$ contribute. In this sector we have numerically computed eigenvalues of the transfer matrix, in the $P = 0$ sector, for systems of size as large as $L_h = 30$ which has dimension 31836. For such large matrices brute force computations will obviously not be sufficient and we have developed algorithms specific to this problem which we sketch in 5.E. We restrict our attention to values of L_h being a multiple of three, to minimize boundary effects which will occur when the circumference L_h is incompatible with the three-sublattice structure of the triangular lattice.

In figure 5.3 we plot the equimodular curves for the crossing of the largest transfer matrix eigenvalues in the $P = 0$ sector for $L_h = 12, 15, 18, 21, 24, 27$, and in figure 5.4 we plot $L_h = 30$. It is obvious from these curves that more than two eigenvalues of the transfer matrix contribute to the partition function because of the increasing number of regions in the left half plane which we refer to as the "necklace". A striking feature is that there is a pronounced mod 6 effect where for $L_h \equiv 3 \pmod 6$ there is a level crossing curve in the necklace on the negative real z axis which is not present for $L_h \equiv 0 \pmod 6$. The level crossing curves separate the necklace into well defined regions. The number of these regions is $L_h/3 - 4$ for $L \leq 27$. The number of regions for $L_h = 30$ is the same as for $L_h = 24$. For $L_h = 21, 27$ all the branch points of the necklace are given in table 5.1 and in table 5.2 for $L_h = 18, 24, 30$.

There are further features in figures 5.3 and 5.4 which deserve a more detailed discussion.

Comparison with the equimodular curve of $\kappa_\pm(z)$

If the two eigenvalues $\kappa_\pm(z)$ computed in [22] were sufficient to describe the $L_h \to \infty$ thermodynamic limit of these finite size computations then the equimodular curves of figures 5.3 and 5.4 must approach the equimodular curve of $\kappa_\pm(z)$ of figure 5.2. We make this comparison for $L_h = 30$ in figure 5.4.

In figure 5.4 the agreement of the $\kappa_\pm(z)$ level crossing curve with the eigenvalue equimodular curve for $L_h = 30$ is exceedingly good in the entire portion of the plane which does not include the necklace. However, in the necklace region the $\kappa_\pm(z)$ curve does not agree with either the inner or outer boundaries of the necklace but rather splits the necklace region into two parts.

A more quantitative argument follows from the values of the leftmost crossing with the negative real axis of the necklace given in table 5.1 for $L_h \equiv 0 \pmod 6$ and in table 5.2 for $L_h \equiv 3 \pmod 6$. In both cases the left most crossing moves to the left to a value which if extrapolate in terms of $1/L_h$ lies between 9 and 10. The Y branching in tables 5.1 and 5.2 also moves to the left but does not extrapolate to a value to the left of $z = -5.9425104 \cdots$ where the $\kappa_\pm(z)$ equimodular curve crosses the negative real axis. We interpret this as implying that the necklace persists in the thermodynamic limit and that at least one more transfer matrix eigenvalue is needed to explain the analyticity of the free energy in the complex z plane.

$L_h = 21$	$L_h = 27$	comment
-3.7731	-4.1138	Y branching
$-5.5898 \pm 5.8764i$	$-4.6228 \pm 7.2480i$	necklace end
	$-5.2737 \pm 6.5159i$	
	$-5.2321 \pm 6.3840i$	
$-5.2264 \pm 1.3949i$	$-5.3175 \pm 1.4134i$	
$-7.2883 \pm 2.4533i$	$-7.6848 \pm 2.4225i$	
-7.9020	-8.2803	leftmost crossing

Table 5.1: The branch points of the necklace of the equimodular curves of hard hexagons with cylindrical boundary conditions for $L_h = 21, 27$.

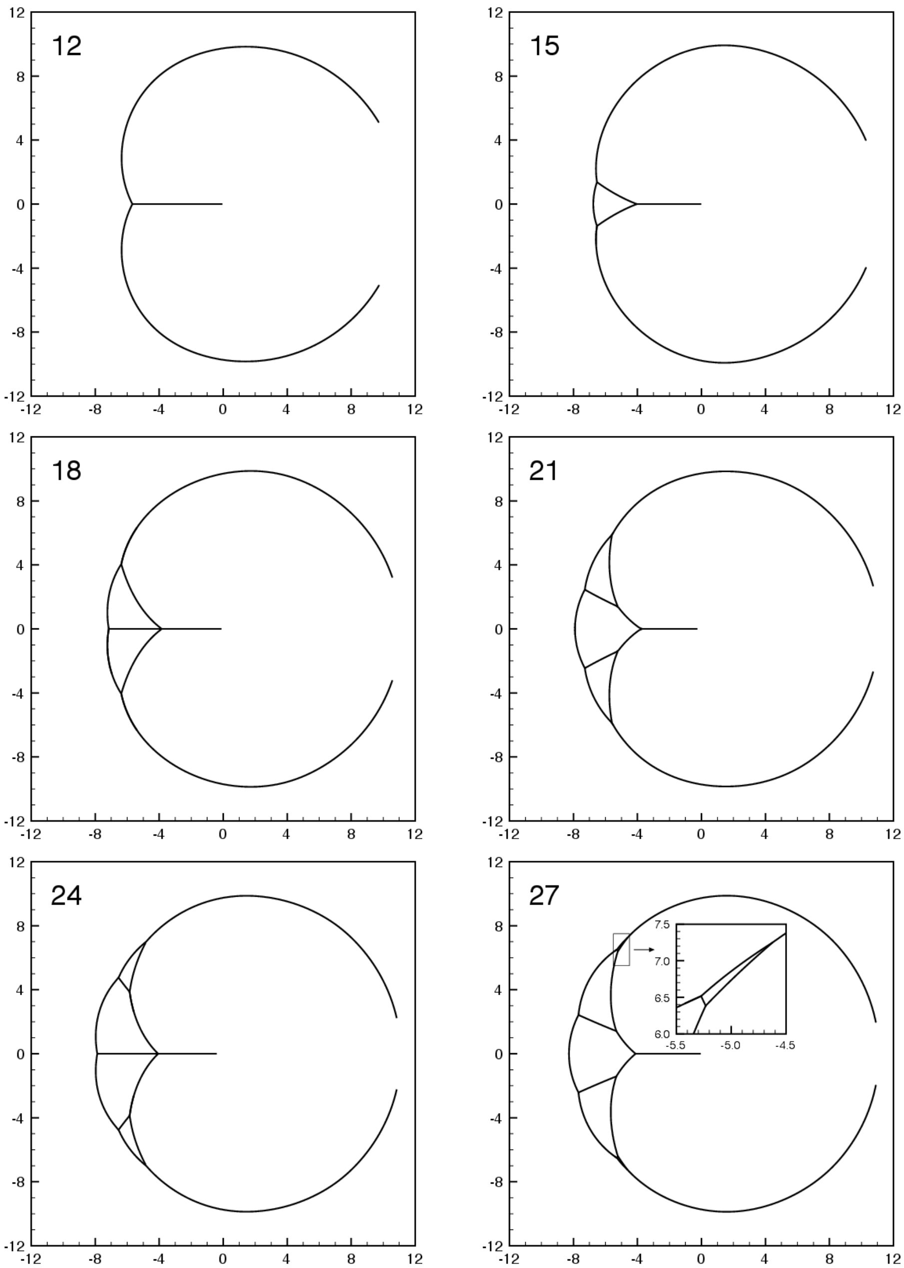


Figure 5.3: Plots in the complex fugacity plane z of the equimodular curves of hard hexagon eigenvalues with cylindrical boundary conditions of size $L_h = 12, 15, 18, 21, 24, 27$. The value of L_h is given in the upper left hand corner of the plots.

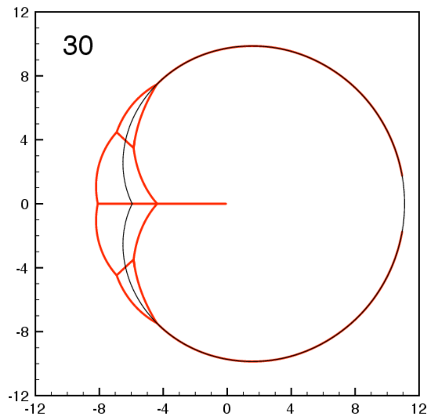


Figure 5.4: Comparison of the dominant eigenvalue crossings $L_h = 30$ shown in red with the equimodular curve $|\kappa_+(z)| = |\kappa_-(z)|$ of figure 5.2 shown in black. Color online.

$L_h = 18$	$L_h = 24$	$L_h = 30$	comment
-3.8370	-4.0637	-4.3794	Y branching
$-6.3703 \pm 4.0485i$	$-4.8079 \pm 7.0090i$	$-4.4043 \pm 7.4623i$	necklace end
	$-6.5389 \pm 4.7519i$	$-6.9134 \pm 4.4771i$	
	$-5.8477 \pm 3.8460i$	$-5.8526 \pm 3.4864i$	
-7.1499	-7.8663	-8.0937	leftmost crossing

Table 5.2: The branch points of the necklace of the equimodular curves of hard hexagons with cylindrical boundary conditions for $L_h = 18, 24, 30$.

The endpoints $z_d(L_h)$ and $z_c(L_h)$

In table 5.3 we give the endpoints which approach the unphysical and the physical singular points of the free energy z_d and z_c. We also give in this table the ratio of the largest to the next largest eigenvalue at $z_d(L_h)$ and $z_c(L_h)$ as determined from eigenvalue crossings. In the limit $L_h \to \infty$ this ratio must go to unity so the deviation from one is a measure of how far the finite size L_h is from the thermodynamic limit.

5.4.3 Eigenvalues for the toroidal lattice partition function

For lattices with toroidal boundary conditions the eigenvalues of all momentum sectors, not just $P = 0$, contribute to the partition function. In particular, in the thermodynamic limit for $P = \pm 2\pi/3$, it is shown in [27] that there is an eigenvalue $\lambda_{\pm 2\pi/3}(z; L_h)$ such that

L_h	$z_d(L_h)$	$\lambda_1/\lambda_{\max}$	$z_c(L_h)$	$\lambda_1/\lambda_{\max}$
12	-0.09051765	0.45085	$9.7432 \pm 5.0712i$	0.55487
15	-0.09037303	0.53048	$10.2971 \pm 3.9465i$	0.54278
18	-0.09030007	0.59046	$10.5753 \pm 3.2016i$	0.58463
21	-0.09026034	0.63709	$10.7340 \pm 2.6730i$	0.62006
24	-0.09023555	0.67431	$10.8310 \pm 2.2852i$	0.65030
27	-0.09021968	0.70467	$10.8955 \pm 1.9834i$	0.67582
30	-0.09020833	0.72989	$10.9389 \pm 1.7499i$	0.69827
∞	-0.09016994	1.00000	11.09016994	1.00000

Table 5.3: The values of the endpoints $z_d(L)$, $z_c(L)$ for hard hexagons on the cylindrical lattice with length L_h as determined from the equimodular eigenvalue curves and the ratios of the first excited state λ_1 to the largest eigenvalue $\lambda_{\max}$ at $z_d(L_h)$ and $z_c(L_h)$.

for $z \geq z_c$

$$\lim_{L_h \to \infty} \frac{\lambda_{\pm 2\pi/3}(z; L_h)}{\lambda_{\max}(z; L_h)} = e^{\pm 2\pi i/3}. \tag{5.38}$$

These two eigenvalues with $P = \pm 2\pi/3$ cause significant differences from the equimodular curves for $P = 0$ for finite values of L_h. We illustrate this in figures 5.5 and 5.6. In figure 5.5 we plot the equimodular curves for toroidal boundary conditions for $L_h = 9, 12, 15, 18, 21$.

In these figures level crossings of 2 eigenvalues are shown in red, of 3 eigenvalues in green and 4 eigenvalues in blue. For sectors separated by a red boundary, both sectors have momentum $P = 0$. For sectors separated by a green boundary, one sector has momentum $P = 0$, and the other has two eigenvalues of equal modulus and fixed phases of $e^{\pm 2\pi i/3}$. For sectors separated by a blue boundary, each sector has two eigenvalues of equal modulus, and fixed phases of $e^{\pm 2\pi i/3}$. The equimodular curve $|\kappa_-(z)| = |\kappa_+(z)|$ is plotted in black for comparison.

It is instructive to compare the necklace regions of the plots of figure 5.5 with the corresponding plots of figure 3 where the momentum of the eigenvalues is restricted to $P = 0$. We do this in figure 6 where in the necklace region we have added in dotted red lines the $P = 0$ level crossing of figure 5.3 which are, now, crossings of sub-dominant eigenvalues.

There are two important observations to make concerning these plots.

The rays out to infinity

The most striking difference between the equimodular curves for cylindrical and toroidal boundary conditions is that there are "rays" of equimodular curves which go to infinity. These rays all have three equimodular eigenvalues which separate a sector
with $P = 0$ from a sector with $P = \pm 2\pi/3$. In the limit $L_h \to \infty$ these three eigenvalues

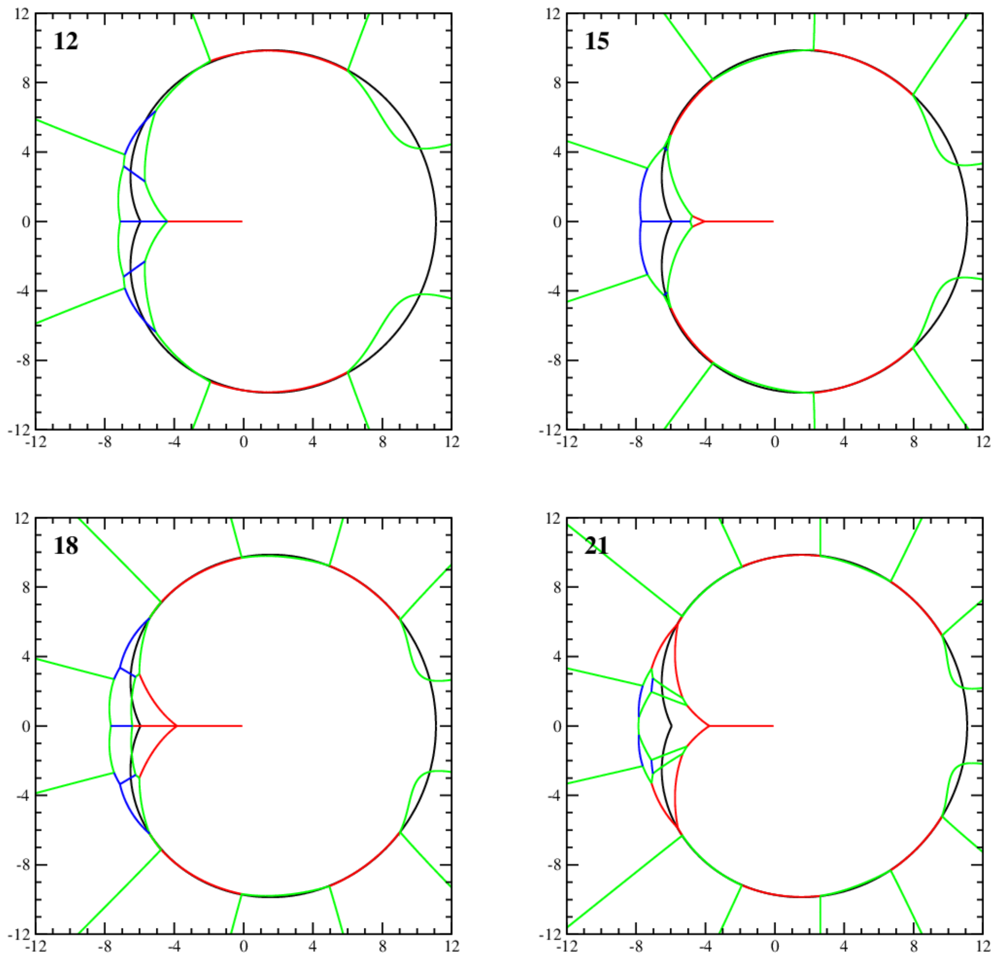


Figure 5.5: Plots in the complex fugacity plane z of the equimodular curves of hard hexagon eigenvalues for toroidal lattices for $L = 12, 15, 18, 21$. On the red lines 2 eigenvalues are equimodular, on the green lines 3 eigenvalues are equimodular and on the blue lines 4 eigenvalues are equimodular. The equimodular curve $|\kappa_-(z)| = |\kappa_+(z)|$ is given in black for comparison. Color online.

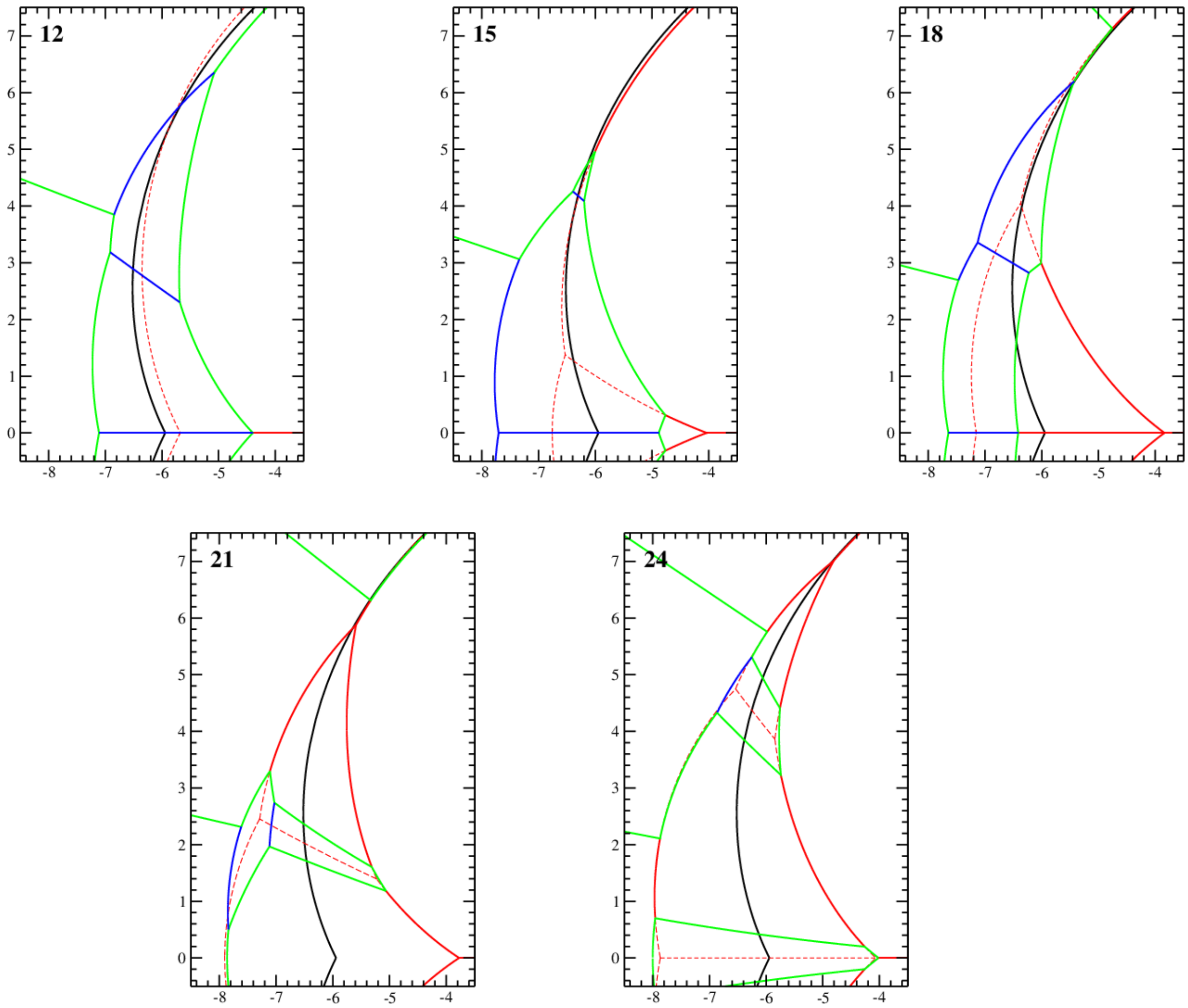


Figure 5.6: Comparison in the complex fugacity plane z of the necklace region of the equimodular curves of hard hexagon maximal eigenvalues for toroidal lattices for $L_h = 12,\ 15,\ 18,\ 21,\ 24$ with the eigenvalue crossing in the $P = 0$ sector of figure 5.3. On the red lines 2 eigenvalues are equimodular, on the green lines 3 eigenvalues are equimodular and on the blue lines 4 eigenvalues are equimodular. The dotted red curves are the additional crossings in the $P = 0$ sector from figure 5.3 which are now sub-dominant. The equimodular curve $|\kappa_{-}(z)| = |\kappa_{+}(z)|$ is given in black for comparison. Color online.

on the rays become equimodular independent of z, and thus there will be no zeros on these rays in the thermodynamic limit.

Dominance of $P = 0$ as $L_h \to \infty$

We see in figure 5.6 that for the smaller values of L_h, such as 12 and 15, a sizable portion the region in the necklace has momentum $P = \pm 2\pi/3$. However, as seen in the plots for $L_h = 18$, 21 and 24 as L_h increases the regions with $P = 0$ grow and squeeze the regions with $P = \pm 2\pi/3$ down to a very small area. It is thus most natural to conjecture that, in the limit $L_h \to \infty$, only momentum $P = 0$ survives, except possibly on the equimodular curves themselves.

5.5 Partition function zeros

We now turn to zeros of the partition function $Z_{L,L}(z)$ on the lattices of size $L \times L$. Just as we required the creation of specialized algorithms to compute the eigenvalues of the transfer matrix so we need specialized algorithms to compute the polynomials. We have studied both cylindrical and toroidal boundary conditions.

5.5.1 Cylindrical boundary conditions

We have computed partition function zeros for lattices with cylindrical boundary conditions for sizes up to 39×39. We plot these zeros in figure 5.7. These plots share with the equimodular $P = 0$ eigenvalue curves of figure 5.3 the feature of having a necklace in the left half plane beyond the Y branching. These plots also have the feature that as the size increases the number of zeros inside the necklace region increases. However, in contrast with the equimodular $P = 0$ eigenvalue curves there is no necklace for $L = 15$.

Branching of the necklace

We give the left most crossing of the necklace, the Y branching point and the necklace endpoint in table 5.4. We note that the left most crossing is to the left of the corresponding left most crossing of the transfer matrix eigenvalue equimodular crossings given in tables 5.1 and 5.2. These crossings are moving to the right with increasing L for $L \geq 27$. The Y branchings are moving to the right for $L \geq 30$. These trends are the opposite of what was found for the transfer matrix eigenvalue curves which only went up to $L_h = 27$. We note that for 15×15 through 27×27 there is only one region in the necklace. However. for 30×30 there are two regions, for 33×33 three, for 36×36 five and for 39×39 seven. It is unknown if the number of regions increases for larger lattices.

L	leftmost crossing	Y branching	necklace endpoints
15	no necklace	-6.8311	
18	-8.666	-5.6655	
21	-9.1957	-4.5411 (min)	
24	$-8.8963 \pm 0.264i$	-4.7137	
27	-9.4969	-4.8031	$-6.292287 \pm 7.325196i$
30	$-9.2717 \pm 0.541i$	-5.0851 (max)	$-5.515958 \pm 8.174231i$
33	-9.4610	-4.8875	$-4.728011 \pm 8.742729i$
36	$-9.213 \pm 0.527i$	-4.6972	$-4.797746 \pm 8.473961i$
39	-9.3221	-4.5687	$-4.270164 \pm 8.792602i$

Table 5.4: The necklace crossing and endpoints as a function of L for the $L \times L$ lattice with cylindrical boundary conditions. There is a mod 6 phenomenon apparent in both the location of the necklace crossings and the endpoint. The necklace endpoints at $L = 27,\ 33,\ 39$ and at $L = 30,\ 36$ are moving to the right.

Comparison with the eqimodular curves

In figure 5.8 we compare the equimodular curves for $L_h = 27$ with the partition function zeros of the 27×27 lattice by plotting the partition function zeros for the lattices 27×27, 27×54, 27×135 and 27×270. This comparison clearly shows how slight kinks for 27×27 grow into an equimodular curve with 5 separate regions.

The endpoints $z_d(L)$ and $z_c(L)$

In table 5.5 we give the values of the endpoints which approach z_d and z_c. We note that the values of $z_d(L_h)$ and $z_c(L_h)$ of table 5.3 as determined from the equimodular curves are significantly closer to the limiting values z_d and z_c than the corresponding values of table 5.5. We also note that, in table 5.3, $\mathrm{Re}(z_c(L_h))$ is monotonic and approaches z_c from below, while in table 5.5 $\mathrm{Re}(z_c(L_h))$ is not monotonic and approaches z_c from above.

It is clear in table 5.5 that $z_d(L)$ is converging rapidly to z_d and a careful quantitative analysis well fits the data with the form

$$z_d(L) - z_d = b_0 L^{-12/5} + b_1 L^{-17/5} + b_2 L^{-22/5} + a_3 L^{-27/5} + \cdots \tag{5.39}$$

with

$$b_0 = 1.7147(1), \quad b_1 = -9.30(2), \quad b_2 = 48(2), \quad b_3 = -180(30). \tag{5.40}$$

The exponent $12/5$ is the leading exponent of the energy operator of the Lee-Yang edge as is seen from analysis of [119] and [68]. It is expected to be the inverse of the correlation exponent ν at $z = z_d$ but a computation of this correlation length is not in the literature.

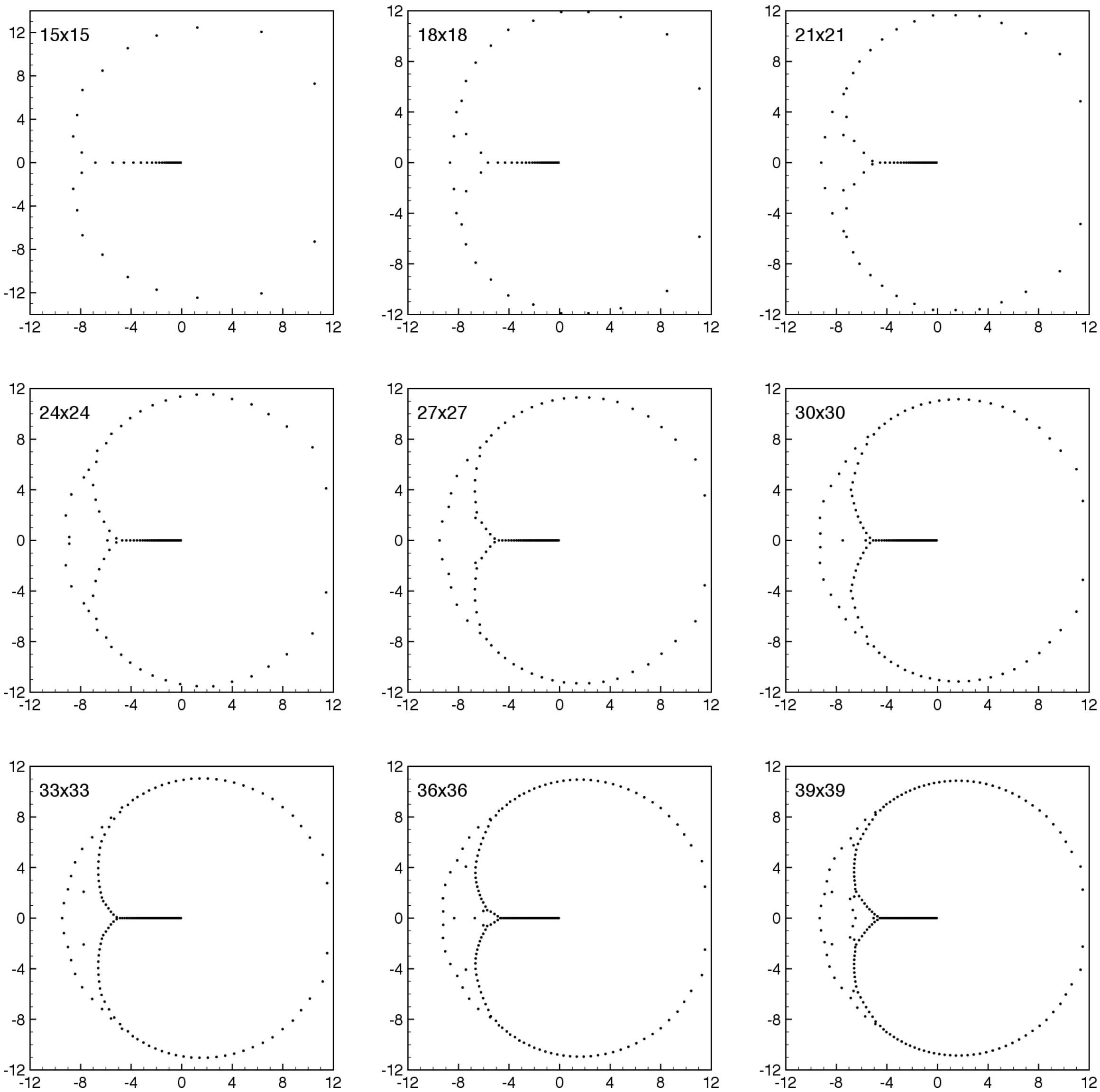


Figure 5.7: Plots of partition function zeros in the complex fugacity plane z of hard hexagon model for lattices with cylindrical boundary conditions of size $15\times15,\ 18\times18,\ 21\times21,\ 24\times24,\ 27\times27,\ 30\times30,\ 33\times33,\ 36\times36,\ 39\times39$.

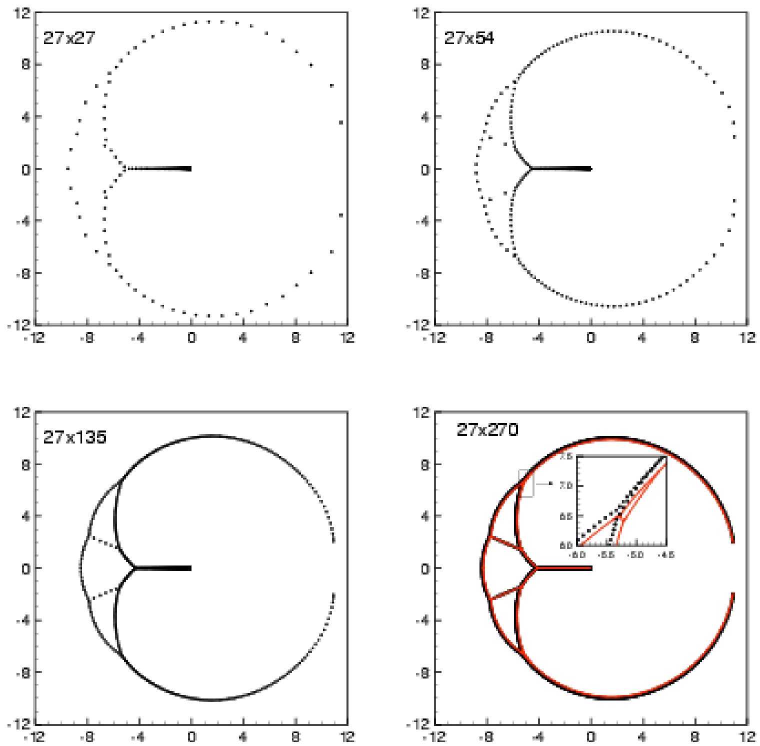


Figure 5.8: The partition function zeros for the lattices 27×27 , 27×54 27×135 and 27×270. For 27×270 the equimodular curve is shown in red. Color online

L	$z_d(L)$	$z_c(L)$
9	-0.0957417573	$5.9002937473 \pm 12.2312152474i$
12	-0.0932266680	$9.2335210855 \pm 9.3476347389i$
15	-0.0920714392	$10.5114514245 \pm 7.2812520022i$
18	-0.0914523473	$11.0571925423 \pm 5.8559364459i$
21	-0.0910853230	$11.3084528958 \pm 4.8492670401i$
24	-0.0908515103	$11.4268383658 \pm 4.1113758041i$
27	-0.0906942824	$11.4806273673 \pm 3.5521968857i$
30	-0.0905839894	$11.5012919280 \pm 3.1162734906i$
33	-0.0905039451	$11.5044258314 \pm 2.7682753249i$
36	-0.0904442058	$11.4981796564 \pm 2.4848695493i$
39	-0.0903985638	$11.4869896404 \pm 2.2501329582i$
∞	-0.0901699437	11.0901699437

Table 5.5: The values of $z_d(L)$, and $z_c(L)$ as a function of L for the $L \times L$ lattice with cylindrical boundary conditions as determined from the zeros of the partition function.

For $z_c(L)$ the data of table 5.5 is well fit by

$$|z_c(L)| - z_c = a_0 L^{-6/5} + a_1 L^{-2} + a_2 L^{-14/5} + \cdots \tag{5.41}$$

where

$$a_0 = 53.0(1), \quad a_1 = -50(5), \quad a_2 = -200(50) \tag{5.42}$$

where the exponent $y = 6/5$ is the inverse of the correlation length exponent ν of the hard hexagon model at $z = z_c$ [27]. The exponent -2 is consistent with $-y - |y'|$ where $y' = -4/5$ is the exponent for the subdominant energy operator $\phi_{(3.1)}$ for the three state Potts model [87] and the exponent $-14/5$ follows from $-y - 2|y'|$. We note that the potential exponents $-y - 1$ and $-2y$ do not appear in (5.41).

The analysis leading to (5.39) and (5.41) and the relation with conformal field theory is given in appendix F.

Comparison with the equimodular curve of $\kappa_{\pm}(z)$

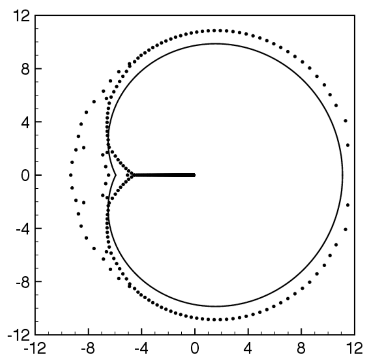


Figure 5.9: The equimodular curves for $|\kappa_-(z)| = |\kappa_+(z)|$ in the complex z plane and the partition function zeros for cylindrical boundary conditions on the 39 × 39 lattice

In figure 5.9 we compare the zeros for the 39 × 39 lattice with the equimodular curve of the $\kappa_{\pm}(z)$ of figure 5.2. Unlike the comparisons of figure 5.4 the $\kappa_{\pm}(z)$ equimodular curve does not have a region of overlap with the zeros of the 39 × 39 lattice. However, in the region to the right of the necklace, if

$$\lim_{L_h \to \infty, L_v \to \infty} Z_{L_v, L_h}(z)^{1/L_v L_h} \qquad \text{is independent of} \quad L_v/L_h,$$

then, for this region, the limiting locus of zeros will agree with the $\kappa_{\pm}$ equimodular curve. We have examined this possibility and find that we can well fit this portion of the zero locations of figure 5.7 by a shifted cardioid

$$\begin{aligned}
\mathrm{Re}(z) &= \frac{a}{2} + c \ + a\cos\theta \ + \frac{a}{2}\cdot\cos 2\theta, \\
\mathrm{Im}(z) &= a\sin\theta \ + \frac{a}{2}\cdot\sin 2\theta.
\end{aligned} \tag{5.43}$$

The fitting parameters a and c depend on L, and, when plotted versus $1/L$, these values fall very closely on a straight line which extrapolated to $L \to \infty$ gives a curve which is virtually indistinguishable from the $\kappa_\pm$ equimodular curve outside of the necklace regions. We take this to be evidence that in this non necklace region the limit (5.43) for cylindrical boundary conditions is independent of the ratio L_v/L_h. Further numerical details are given in 5.D.

5.5.2 Toroidal boundary conditions

It is numerically more difficult to compute partition function zeros for toroidal boundary conditions and the maximum size we have been able to study is 27×27. These results are plotted in figure 5.10. There is a necklace for $L \geq 12$ and there are zeros in the necklace region for 15×15 through 21×21. For 24×24 and 27×27 there are no zeros in the necklace region.

Comparison with the equimodular curve of $\kappa_\pm(z)$

In figure 5.11 we compare the partition function zeros for toroidal boundary conditions on the 27×27 lattice with the equimodular curve of $\kappa_\pm(z)$. Outside of the necklace region the agreement is much closer than it was for the cylindrical case for the 39×39 lattice. It is appealing to attribute this agreement with the absence of boundary effects.

Dependence on the aspect ratio L_v/L_h

We conclude our study of partition function zeros by examining the dependence of the zeros on the aspect ratio L_v/L_h of the $L_h \times L_v$ lattices. In figure 5.12 we plot the partition function zeros for the toroidal lattices of various ratios L_v/L_h as large as 40 for $L_h =$ 15, 18, 21. We see that the number of zeros outside the main curve increases for fixed L_h with increasing aspect ratio and for fixed aspect ratio decreases with increasing L_h. It is furthermore obvious that even for an aspect ratio of 40 there are remarkably few zeros on the rays seen in the transfer matrix equimodular curves of figure 5.5. From this we conclude, for fixed $L_v/L_h < \infty$ with $L_h \to \infty$, that the partition function zeros of the $L_h \times L_v$ on the toroidal lattice will not have any rays of zeros which extend to infinity.

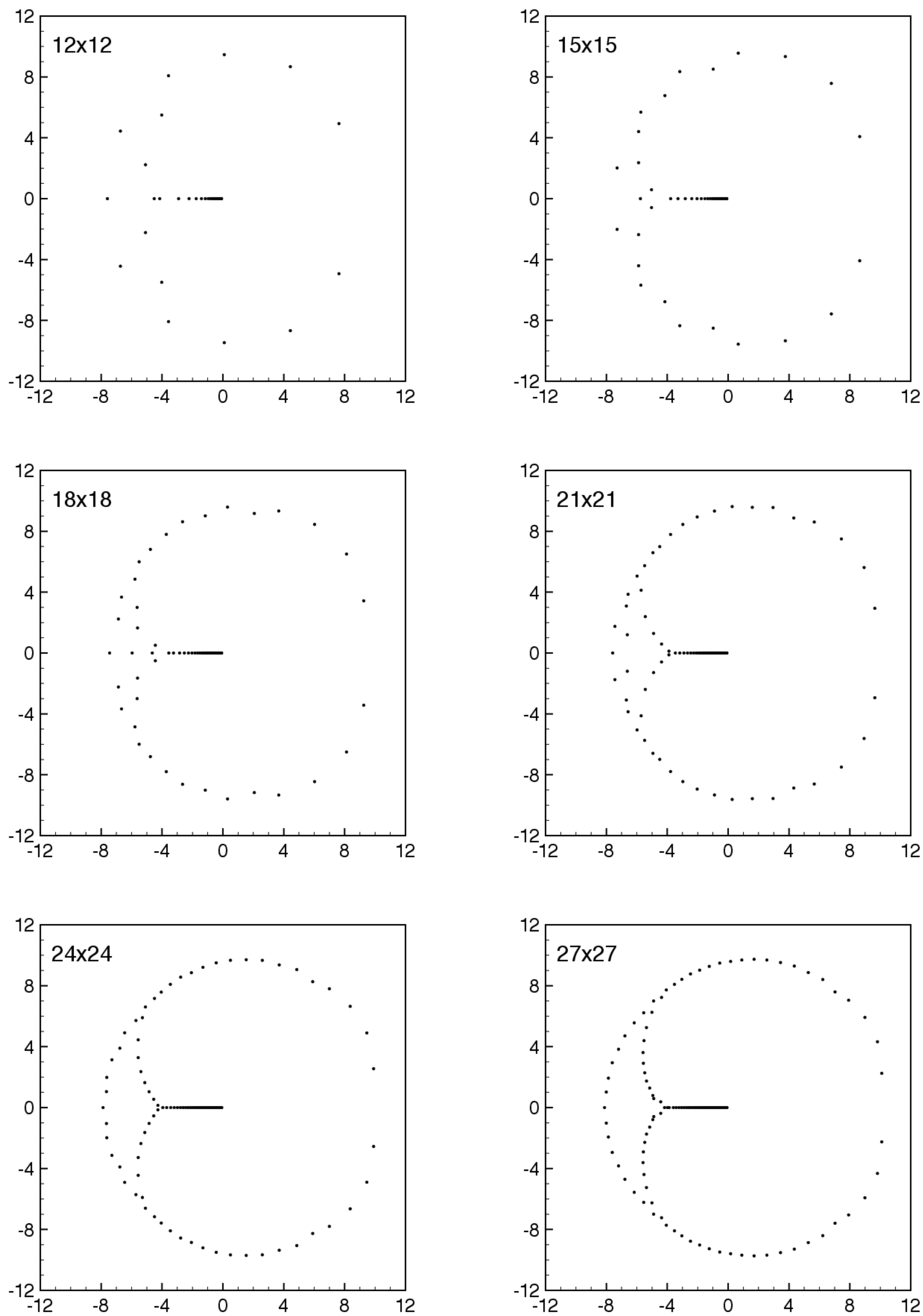


Figure 5.10: Plots of partition function zeros in the complex fugacity plane z for hard hexagon with toroidal boundary conditions of size $L \times L$ with $L = 12,\ 15,\ 18,\ 21,\ 24,\ 27$. The value of $L \times L$ is given in the upper left hand corner of the plots.

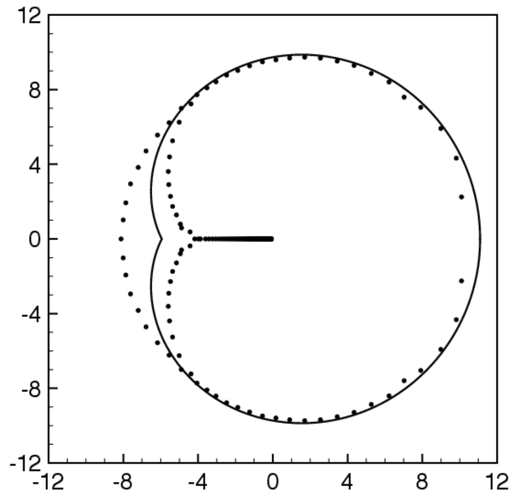


Figure 5.11: The equimodular curves for $|\kappa_-(z)| = |\kappa_+(z)|$ in the complex z plane and the partition function zeros for toroidal boundary conditions on the 27×27 lattice

5.5.3 Density of zeros for $z_y \leq z \leq z_d$

On the negative z axis we label as z_j the position of the j^{th} zero where z_1 is the zero nearest to $z = 0$ and z_y is the zero closest to the Y branching on the negative z axis. Then calling N_L the number of zeros in the interval $z_y \leq z \leq 0$ on a finite lattice of size $L \times L$ the density $D(z)$ in the thermodynamic limit is proportional to

$$D(z) \; = \; \lim_{L \to \infty} \; D_L(z_j) \qquad \text{where} \qquad D_L(z_j) \; = \; \frac{1}{N_L \cdot \, (z_j - z_{j+1})}. \tag{5.44}$$

This density of zeros will diverge at z_d as $(1 - z/z_d)^{-1/6}$, which is obtained from the leading term in the expansion of $\rho_-(z)$. This expansion is obtained, in 5.B, from the algebraic equation (see eqn. (12.10) in [133]) as

$$\begin{aligned} \rho_-(z) \quad = \quad & t_d^{-1/6} \cdot \Sigma_0(t_d) \quad + \Sigma_1(t_d) \quad + t_d^{2/3} \cdot \Sigma_2(t_d) \quad + t_d^{3/2} \cdot \Sigma_3(t_d) \\ & + t_d^{7/3} \cdot \Sigma_4(t_d) \quad + t_d^{19/6} \cdot \Sigma_5(t_d), \end{aligned} \tag{5.45}$$

where $t_d = 5^{-3/2} \cdot (1 - z/z_d)$, the fractional powers are all defined positive for positive t_d and where the $\Sigma_i(t_d)$ read

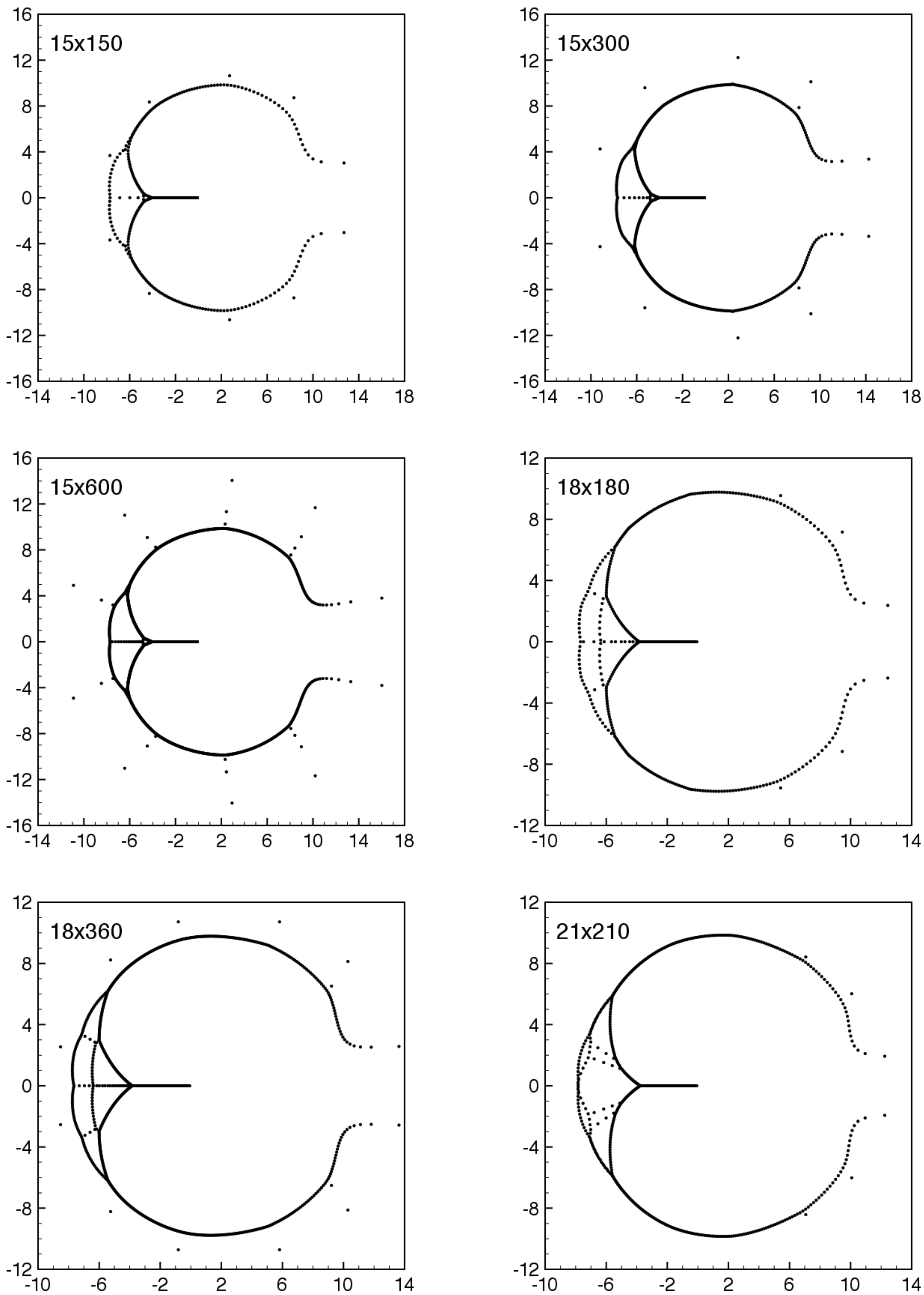


Figure 5.12: Partition function zeros for toroidal boundary conditions on the lattices 15×150, 15×300, 15×600, the lattices 18×180, 18×360 and the lattice 21×210. The number of points off of the main curve for fixed aspect ratio L_v/L_h decreases with increasing L_h.

$$
\begin{aligned}
\Sigma_0 &= -\frac{1}{\sqrt{5}} + \frac{1}{12}\left(5+\frac{11}{\sqrt{5}}\right)t_d + \frac{1}{144}\left(275+\frac{639}{\sqrt{5}}\right)t_d^2 + \frac{1}{1296}\left(17765+\frac{37312}{\sqrt{5}}\right)t_d^3 + \cdots \\
\Sigma_1 &= \frac{1}{2}\left(1+\frac{1}{\sqrt{5}}\right) + \frac{1}{\sqrt{5}}t_d + \frac{1}{2}\left(5-\frac{1}{\sqrt{5}}\right)t_d^2 - \frac{1}{2}\left(5-\frac{83}{\sqrt{5}}\right)t_d^3 + \cdots \\
\Sigma_2 &= -\frac{2}{\sqrt{5}} - \frac{2}{15}(25-4\sqrt{5})t_d + \frac{4}{45}(125-108\sqrt{5})t_d^2 - \frac{4}{405}(16775-4621\sqrt{5})t_d^3 + \cdots \\
\Sigma_3 &= -\frac{3}{\sqrt{5}} - \frac{3}{4}\left(15-\frac{7}{\sqrt{5}}\right)t_d + \frac{3}{16}\left(175-\frac{1189}{\sqrt{5}}\right)t_d^2 - \frac{21}{16}\left(705-\frac{646}{\sqrt{5}}\right)t_d^3 + \cdots \\
\Sigma_4 &= -\frac{4}{\sqrt{5}} - \frac{2}{15}(175-13\sqrt{5})t_d + \frac{2}{45}(1625-2637\sqrt{5})t_d^2 - \frac{52}{405}(22100-3499\sqrt{5})t_d^3 + \cdots \\
\Sigma_5 &= -\frac{6}{\sqrt{5}} - \frac{1}{2}\left(95-\frac{31}{\sqrt{5}}\right)t_d + \frac{1}{24}\left(3875-\frac{34641}{\sqrt{5}}\right)t_d^2 - \frac{31}{216}\left(55685-\frac{40892}{\sqrt{5}}\right)t_d^3 + \cdots
\end{aligned}
\tag{5.46}
$$

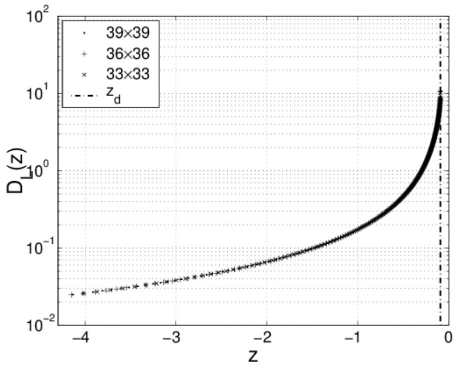
The term in $t_d^{2/3}$ was first obtained by Dhar [84] but the full expansion has not been previously reported. The form (5.45) follows from the renormalization group expansion [68] of the singular part of the free energy at $z = z_d$

$$
f_s = t_d^{2/y} \cdot \sum_{n=0}^{4} t_d^{-n(y'/y)} \cdot \sum_{m=0}^{\infty} a_{n;m} \cdot t_d^m, \tag{5.47}
$$

where $y = 12/5$ is the leading renormalization group exponent for the Yang-Lee edge, and $y' = -2$, the exponent for the contributing irrelevant operator which breaks rotational invariance on the triangular lattice, is determined from the term $t_d^{2/3}$ in (5.45).

The density $\rho_-(z)$ has singularities only at z_d and z_c in the plane cut on $\infty \leq z \leq z_d$ and $z_c \leq z \leq \infty$. However, this does not require that the series (5.46) for $\Sigma_j(t_d)$ will have t_d evaluated at z_c as their radii of convergence. We have investigated this by computing the coefficients $c_j(n)$ of z^n in the series for $\Sigma_j(t_d)$ using Maple up to $n = 1200$. For $\Sigma_0(t_d)$ these coefficients are all positive for $n > 1$ and for $\Sigma_j(t_d)$ with $j = 2, 3, 4$ all coefficients are negative. However, for $\Sigma_5(t_d)$ the coefficients are negative for $0 \leq n \leq 19$ and positive for $n \geq 20$. For $\Sigma_1(t_d)$ the coefficients are positive for $0 \leq n \leq 554$ and negative for $n \geq 555$. Furthermore the ratios $r_j = c_j(n)/c_j(n+1)$ seem to be converging to $2^{-3/2} = 0.08944271\cdots$ which corresponds to $z = 0$.

We investigate the density $\rho_-(z)$ further by plotting, in figure 5.13, $D_L(z_j)$ as a function of z computed from the zeros of the $L \times L$ lattice with cylindrical boundary conditions for $L = 33, 36, 39$. The values of $D_L(z_j)$ for all three lattices lie remarkably close to the same curve except for the region $-0.093 < z < z_d$, where some scatter is observed which is caused by the finite size of the lattice.



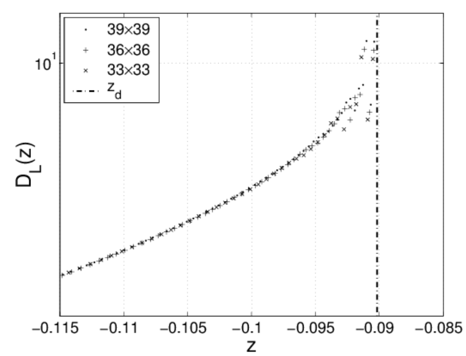


Figure 5.13: Log plots of the density of zeros $D_L(z_j)$ on the negative z axis for $L \times L$ lattices with cylindrical boundary conditions. The figure on the right is an expanded scale near the singular point z_d.

To estimate the divergence of $D(z)$, at $z = z_d$, we write for z near z_d

$$D(z) \sim A \cdot (z_d - z)^{\alpha} \qquad \text{and thus} \qquad \frac{D(z)}{D'(z)} \sim \frac{z_d - z}{\alpha}, \tag{5.48}$$

where $D'(z)$ is the derivative of $D(z)$. In figure 5.14 we plot $D_L(z_j)/D'_L(z_j)$, where we define

$$D'_L(z_j) = \frac{D_L(z_{j+1}) - D_L(z_j)}{z_{j+1} - z_j}. \tag{5.49}$$

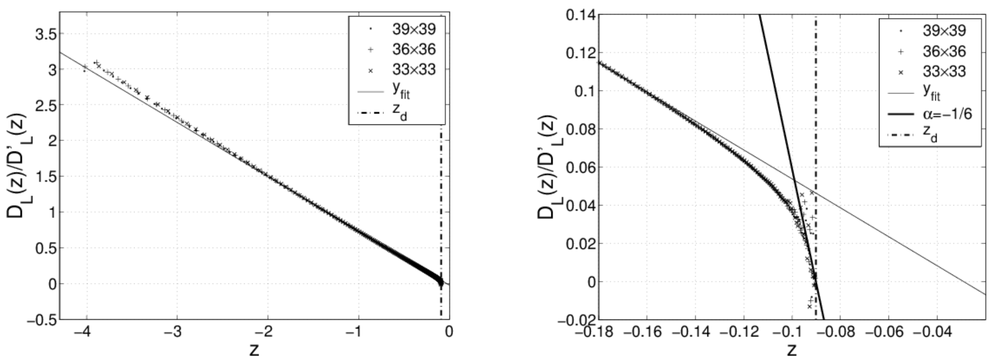


Figure 5.14: Plots of $D_L(z_j)/D'_L(z_j)$ on the negative z axis for $L \times L$ lattices with cylindrical boundary conditions. For the plot on the left it is impressive that for the range $-4.0 \leq z \leq -0.14$ the data is extremely well fitted by the power law form (5.48) with an exponent -1.32 (which corresponds to a slope of -0.76) and an intercept $z_f = -0.029$. The plot on the right is an expanded scale near z_d and the line passing through $z = z_d$ with slope of -6 is plotted for comparison which corresponds to the true exponent $= -1/6$ which only is observed in a very narrow range near z_d of $-0.095 \leq z \leq z_d = -0.0901 \cdots$.

For z, away from z_d, the plot is very well fitted by the z-line

$$\frac{D_L(z)}{D'_L(z)} \sim \frac{z_f - z}{\alpha}, \tag{5.50}$$

with $\alpha_f = -1.32 \cdots$ (or $\alpha_f^{-1} = -0.76 \cdots$), and $z_f = -0.029 \cdots$ However, for $-0.14 \leq z \leq z_d$ this fit is no longer valid. We make in figure 5.14 a comparison with the true value of $\alpha = -1/6$, which is obtained from $\kappa_-(z)$. This figure vividly illustrates the very limited range of validity for the use of perturbed conformal field theory and scaling arguments to describe systems away from critical points. The same phenomenon has been seen in [121, eqn. (4.8) and Fig. 4] for Hamiltonian chains.

5.6 Discussions

The results of the numerical studies presented above allow us to discuss in some detail the relation of the functions $\kappa_\pm(z)$, which completely describe the hard hexagon partition function per site on the positive z axis, with the partition function per site in the full complex z plane. In particular the approach to the thermodynamic limit, the existence of the necklace, the relation to the renormalization group and questions of analyticity will be addressed.

5.6.1 The thermodynamic limit

When the fugacity z is real and positive the free energy and the partition function per site is independent of the aspect ratio L_v/L_h of the $L_h \times L_v$ lattice as L_h, $L_v \to \infty$, and will be the same for both cylindrical and toroidal boundary conditions. This is a necessary condition for thermodynamics to be valid.

However, the example of hard squares at $z = -1$, where it is found [90, 130, 61, 25] that the partition function $Z_{L_v,L_h}(-1)$ depends on number theoretic properties of L_v and L_h, demonstrates that there may be places in the complex z plane where a thermodynamic limit independent of L_v/L_h does not exist. We have investigated in sections 5.4 and 5.5 the extent to which our data supports the conclusion that for complex z there is a thermodynamic limit independent of the aspect ratio L_v/L_h as stated in (5.19). If this independence holds then the limiting locus of partition function zeros will lie on the limiting locus of transfer matrix equimodular curves. However, the converse does not need to be true and there is no guarantee that zeros will lie on all limiting loci of transfer matrix eigenvalues. In particular we have argued in sections 5.4.3 and 5.5.2 that for toroidal boundary conditions there will be no zeros in the rays which go to infinity.

5.6.2 Existence of the necklace

All the data both for partition function zeros and transfer matrix eigenvalues contain a necklace in the left half plane. Such a necklace is incompatible with a partition function which only includes the functions $\kappa_\pm(z)$.

For cylindrical boundary conditions it is clear from figures 5.3 and 5.4 that the limiting locus of transfer matrix equimodular curves in the necklace region has not yet been obtained. Furthermore in figures 5.3 and 5.4 there are equimodular curves inside the necklace region beginning at $L_h = 18$ whereas in figure 5.7 partition function zeros only appear clearly inside the necklace region for lattices 30×30 and greater.

For toroidal boundary conditions the dominance of the $P = 0$ sector in the limit $L_h \to \infty$, discussed in section 5.4.3, implies that in the thermodynamic limit the necklace will be the same as for cylindrical boundary conditions.

The simplest mechanism which will account for this behavior is for there to be one (or more) extra eigenvalue(s) of the transfer matrix which becomes dominant in the necklace region. Further analytic computation is needed to verify this mechanism. However, the present data does not rule out the possibility that for sufficiently large systems the necklace region could be filled with zeros.

5.6.3 Relation to the renormalization group

The form of the singularity of the density $\rho_-(z)$ at $z = z_d$ given in section 5.5.3 in (5.47) is not the most general form, allowed by the renormalization group. The most general form allows the singular part of the free energy to have $y' = -1$, which would give a term in (5.45) with exponent $t_d^{1/4}$ (which is, in fact, not present). This may be explained by the following renormalization group argument given by Cardy [66]. The integer corrections given by ny' are conformal descendants of the identity operator. The total scaling dimension of these operators is $N + \bar{N}$. Their conformal spin is $N - \bar{N}$, where N and $\bar{N}$ are nonnegative integers, and the corresponding exponent y' is $2 - N - \bar{N}$. However, the six fold lattice symmetry of the hard hexagon model allows only operators with $N - \bar{N} \equiv 0 \pmod 6$. Therefore the dimensions y' cannot be odd which is what is observed in (5.45). The same conclusion will apply also to hard squares but not for hard triangles.

5.6.4 Analyticity of the partition function

The final property to be discussed is the relation of the analyticity of the free energy obtained by analytically continuing the free energy from the positive z axis into the complex z plane.

For hard hexagons the functions $\kappa_{\pm}(z)$ have singularities only at $z = z_d$, z_c, ∞, whereas the partition function per site in the complex plane fails to be analytic at those boundaries which are the thermodynamic limit of the equimodular curves. It is obvious for hard hexagons that these boundaries have nothing to do with the analyticity of $\kappa_{\pm}(z)$. However it is unknown if in general the partition function per site on the real axis can be continued analytically beyond the region where it corresponds to the maximum modulus of the transfer matrix eigenvalue.

The other locus where the hard hexagon model has partition function zeros is on the negative real axis for $z \leq z_d$. These zeros correspond to the complex conjugate solutions for $\kappa_{-}(z)$ alone and have no connection with $\kappa_{+}(z)$. The leading singular behavior of hard hexagons at z_d is believed to be a property shared by all systems with purely repulsive (positive) potentials and is a universal repulsive-core singularity [147, 178]. Therefore it is of considerable interest to determine whether the ability to continue through this locus of zeros, which is the case for the integrable system of hard hexagons, will hold for all the non-integrable models in the same universality class.

5.7 Conclusion

The hard hexagon model solved by Baxter [22, 29, 30] not only satisfies the Yang-Baxter equation but also as shown by Joyce [133] and Tracy *et al* [191, 235] has a remarkable structure in terms of algebraic modular functions and their associated Hauptmoduls. It is thus a good candidate for a global analysis in the whole complex plane of the partition function per site which is complementary to a local analysis based on series expansions and perturbation theory.

In this paper we have made a precision finite size study for the hard hexagon model of the zeros of the partition function and of the equimodular curves of the transfer matrix in the complex fugacity plane z. This study reveals that the partition function per site has more structure for complex z than has been seen in previous studies on much smaller systems [246, 248, 250, 251]. In particular our results demonstrate that the conjecture on zeros of the hard hexagon partition function made in [251] is incorrect, and corresponds to a too simple high density equimodular condition of the Hauptmodul being real. This condition has to be replaced by more involved equimodular conditions involving both the low and high density partition functions. Furthermore we have found that the results of [22, 29, 30] on the positive z axis are not sufficient to determine all of the analytic structure of the partition function per site in the complex z plane.

The full significance of our results is to be seen in the comparison with hard squares and with the Ising model in a magnetic field which do not satisfy a Yang-Baxter equation and will not have the global properties of modular functions. In particular we note that in section 5.4.1 it was found that on the negative z axis the zeros of the resultant of the characteristic equation of the transfer matrix have the remarkable property that their multiplicity is two. This is in distinct contrast with hard squares where the multiplicity of the roots of the resultant is one.

Hard squares and hexagons are the limiting case of Ising models in a magnetic field when the field becomes infinite. The results of this paper have extensions to Ising models in a finite magnetic field which will be presented elsewhere.

Acknowledgments

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Appendix

5.A The singularities of $\kappa_\pm(z)$

The partition functions per site $\kappa_\pm(z)$ are singular at z_c, z_d and ∞. At $z = z_c$, and $z = z_d$, the values of the three Ω_i read respectively

$$\Omega_1(z_c) \, = \, 0, \qquad \Omega_2(z_c) \, = \, (5^{5/2} z_c)^2, \qquad \Omega_3(z_c) \, = \, -(5^{5/2} z_c)^3, \qquad (5.51)$$

$$\Omega_1(z_d) \, = \, 0, \qquad \Omega_2(z_d) \, = \, (5^{5/2} z_d)^2, \qquad \Omega_3(z_d) \, = \, (5^{5/2} z_d)^3. \qquad (5.52)$$

5.A.1 High density

As $z \to \infty$ the physical $\kappa_+(z)$, which satisfies the algebraic equation (5.33), diverges. There is only one such real solution and by direct expansion of (5.33) we find that

$$\kappa_+(z) \; = \; z^{1/3} \; + \frac{1}{3}\, z^{-2/3} + \frac{5}{9}\, z^{-5/3} \; + \frac{158}{81}\, z^{-8/3} \; + \frac{2348}{243}\, z^{-11/3} \; + \cdots \tag{5.53}$$

which agrees with eqn. (7.14) in [133]. It follows from (5.53) that $\kappa_+(z)$ has a branch cut on the segment $-\infty < z \le z_d$ and that on this segment the phase is

$$e^{\pm \pi i/3} \qquad \text{for} \qquad \mathrm{Im} z \; = \; \pm \epsilon \; \to \; 0. \tag{5.54}$$

When $z_c \; < \; z \; < \; \infty$ there is one real positive, one real negative, and one complex conjugate pair of solutions to the fourth order equation (5.33) for κ_+^6. The negative solution is larger in magnitude than the positive solution, and, thus, cannot correspond to any eigenvalue of the transfer matrix. However, the magnitude of the complex conjugate pair of solutions is less than the value of the real positive root. At $z \, = \, z_c$ the real positive root collides with the complex conjugate pair.

When $z \, = \, z_c$, introducing the rescaled variable

$$w_{c+} \;\; = \;\; \Omega_3(z_c) \cdot \frac{\kappa_+^6(z_c)}{z_c^6} \;\; = \;\; -(5^{5/2}/z_c)^3 \cdot \kappa_+^6(z_c), \tag{5.55}$$

we find that (5.33) reads $(w_{c+} + 3^9)^3 \; = \; 0$. Thus, using (5.55) and the fact that $\kappa_+(z_c)$ must be positive, we obtain

$$\kappa_+(z_c) \;\; = \;\; (3^3 \cdot 5^{-5/2}\, z_c)^{1/2} \;\; = \;\; 2.3144003 \; \cdots \tag{5.56}$$

which is (7.17) of [133].

For $z \, = \, z_d$, introducing the rescaled variable $w_{d+} \; = \; \Omega_3(z_d) \cdot \kappa_+^6(z_d)/z_d^6 \; = \; (5^{5/2}/z_d)^3 \cdot \kappa_+^6(z_d)$, we find that (5.33) also reads $(w_{d+} + 3^9)^3 \; = \; 0$. Using (5.54), one gets $\kappa_+(z_d)^6 \; = \; 3^9/5^8\,(1525 \, - \, 682 \; 5^{1/2})$ or $\kappa_+(z_d) \; = \; e^{\pm \pi i/3}\; 0.208689 \; \cdots$.

5.A.2 Low density

When $z \, = \, z_c$ equation (5.35) reduces using (5.51) to the eleventh order equation

$$f_-(z_c, w_{c-}) \;\; = \;\; \sum_{k=0}^{11} \tilde{C}_k^- \cdot w_{c-}^k \;\; = \;\; 0 \tag{5.57}$$

with $w_{c-} = 5^{5/2}\,\kappa_-^2(z_c)/z_c$ and

$$\begin{aligned}
\tilde{C}_0^- &= -2^{32}\cdot 3^{27}, \\
\tilde{C}_1^- &= 0, \\
\tilde{C}_2^- &= 2^{26}\cdot 3^{23}\cdot 31, \\
\tilde{C}_3^- &= -2^{26}\cdot 3^{19}\cdot 47, \\
\tilde{C}_4^- &= -2^{17}\cdot 3^{18}\cdot 5701, \\
\tilde{C}_5^- &= 2^{16}\cdot 3^{14}\cdot 7^2\cdot 19\cdot 37, \\
\tilde{C}_6^- &= -2^{10}\cdot 3^{10}\cdot 7\cdot 273001, \\
\tilde{C}_7^- &= 2^{9}\cdot 3^{10}\cdot 11\cdot 13\cdot 139, \\
\tilde{C}_8^- &= -3^{5}\cdot 7\cdot 1028327, \\
\tilde{C}_9^- &= 37\cdot 79087, \\
\tilde{C}_{10}^- &= -19\cdot 139, \\
\tilde{C}_{11}^- &= 1,
\end{aligned} \tag{5.58}$$

which factorizes as

$$f_-(z_c,\, w_{c-}) \;=\; (w_{c-}+2^4)^2\cdot(w_{c-}-3^3)^3\cdot(w_{c-}-2^4\cdot 3^3)^6 \;=\; 0. \tag{5.59}$$

From the second factor in (5.59) we obtain the solution

$$\kappa_-(z_c) \;=\; (3^3\cdot 5^{-5/2}\,z_c)^{1/2} \;=\; \kappa_+(z_c), \tag{5.60}$$

as required by continuity. At $z = z_c$ the solution for $\kappa_-(z_c)$ is three fold degenerate which also agrees with the degeneracy of $\kappa_+(z_c)$.

For $0 < z < z_c$ there is one real positive, one real negative and five complex conjugate solutions of the 12th order equation (5.35). Three of the complex conjugate pairs have a modulus less than the real positive solution. At $z = z_c$ a collision of the real positive root with one of the complex conjugate pairs occurs.

When $z = z_d$ an analogous reduction can be made by use of (5.52) and of the rescaling $w_{d-} = 5^{5/2}\,\kappa_-^2(z_d)/z_d$. We find, in analogy to (5.59), the factorization

$$f_-(z_d, w_{d-}) \;=\; -(w_{d-}-2^4)^2\cdot(w_{d-}+3^3)^3\cdot(w_{d-}+2^4\cdot 3^3)^6 \;=\; 0. \tag{5.61}$$

At $z = z_d$ the last factor in (5.61) vanishes and we find

$$\begin{aligned}
\kappa_-(z_d) &= (-2^4\cdot 3^3\cdot 5^{-5/2}\,z_d)^{1/2} \;=\; (2^4\cdot 3^3\cdot 5^{-5/2}/z_c)^{1/2} \\
&= 4\,|\kappa_+(z_d)| \;=\; 0.83475738\,\cdots\,.
\end{aligned} \tag{5.62}$$

For $z_d < z < 0$ there are three real positive, three real negative, and three complex conjugate solutions of the polynomial relation (5.35) of degree twelve in κ_-^2, and all three of the complex conjugate solutions have a modulus smaller than the largest positive real solution. The largest positive real solution is the dominant eigenvalue, until $z = z_d$, when a collision with the next real largest solution and two complex conjugate pairs occurs.

5.B Expansion of $\rho_-(z)$ at z_c and z_d

The low density function $\rho_-(z)$ satisfies the polynomial equation of degree twelve in ρ_- and degree four in z (see eqn. (12.10) in [133])

$$\begin{aligned} \rho_-^{11} \cdot (\rho_- - 1) \cdot z^4 \quad & - [\rho_-^5 \, z^3 - (\rho_- - 1)^5 \, z] \cdot p_7 \\ & + \rho_-^2 \cdot (\rho_- - 1)^2 \cdot p_8 \cdot z^2 \quad + \rho_- \cdot (\rho_- - 1)^{11} \;=\; 0 \end{aligned} \tag{5.63}$$

where

$$\begin{aligned} p_7 &= 22\rho_-^7 - 77\,\rho_-^6 + 165\rho_-^5 - 220\rho_-^4 + 165\rho_-^3 - 66\rho_-^2 + 13\rho_- - 1, \\ p_8 &= 119\rho_-^8 - 476\rho_-^7 + 689\rho_-^6 - 401\rho_-^5 - 6\rho_-^4 + 125\rho_-^3 - 63\rho_-^2 + 13\rho_- - 1. \end{aligned} \tag{5.64}$$

This equation has the remarkable property that at $z = z_c, \; z_d$ it reduces to a fifth order equation

$$-\frac{275 + 123\sqrt{5}}{8000} \cdot (10\rho_- - 5 + \sqrt{5})^5 \;=\; 0 \qquad \text{for} \quad z = z_c, \tag{5.65}$$

$$-\frac{275 - 123\sqrt{5}}{8000} \cdot (10\rho_- - 5 - \sqrt{5})^5 \;=\; 0 \qquad \text{for} \quad z = z_d. \tag{5.66}$$

There are four distinct Puiseux expansions of ρ_- about z_c which are real for $z < z_c$. The leading exponents of these expansions are -1, $-1/6$, 0, 0. The physical solution must be finite at $z = z_c$ and we see from (5.65) that the two solutions which are constant at $z = z_c$ have the value $\rho_-(z_c) = (1 - 5^{-1/2})/2$. To decide which of these two Puiseux expansions is the correct physical solution we need the independent condition that the leading nonanalytic term has exponent 2/3. The result [133, p. 12.15] follows from this additional condition.

At $z = z_d$ there are also four Puiseux expansions of $\rho_-(z)$ which are real for $z_d < z$. The leading exponents are, again, -1, $-1/6$, 0, 0. Now, unlike $\rho_-(z_c)$, the density is not constant at $z = z_d$, but diverges with exponent $-1/6$. Furthermore, in the cluster expansion of $\rho_-(z)$ about $z = 0$, it follows, from a theorem of Groeneveld [104], that because the sign of the coefficient of z^n is $(-1)^{n-1}$, the density must be negative in the segment $z_d < z < 0$. The leading term of the Puiseux expansion with exponent -1 is positive and is, thus, excluded. There are six conjugate solutions with exponent $-1/6$. The member of this class which has the correct negative behavior $z \to z_d+$ is the result given in (5.45).

5.C The Hauptmodul equations and the $\kappa_\pm$ equimodular curves

The equations (5.33) and (5.35) for $\kappa_\pm$ may be usefully re-expressed in terms of the Hauptmodul H

$$H \;=\; 1728\, z \cdot \frac{\Omega_1^5(z)}{\Omega_3^2(z)}, \qquad (5.67)$$

by making the rescaling

$$W_\pm \;=\; \Omega_3(z) \cdot \Big(\frac{\kappa_\pm}{z}\Big)^6. \qquad (5.68)$$

For high density it is straight forward to use (5.67) and (5.68) in (5.33) to obtain

$$\begin{aligned} P_+(W_+,\, H) \;=\; & H^2 \cdot W_+^4 \;+\; 2^7 \cdot 3^6 \cdot (27\, H - 32) \cdot W_+^3 \\ & + 2^7 \cdot 3^{16} \cdot (45\, H - 32) \cdot W_+^2 \; - 2^{12} \cdot 3^{25}\, W_+ \; - 2^{12} \cdot 3^{33} \;=\; 0. \end{aligned} \qquad (5.69)$$

The algebraic curve $P_+(W_+,\, H) \;=\; 0$ is the union of two genus zero curves.

For low density the polynomial relation (5.35) on κ_- in the z variable can be written in terms of the Hauptmodul (5.67), and of the rescaled variable W_- (5.68), as follows

$$\begin{aligned} P_-(W_-, H) \;=\; & H^6 \cdot W_-^{12} \;+ 2^{12} \cdot 3^7 \cdot P_{11} \cdot W_-^{11} \;+\; 2^{19} \cdot 3^{13} \cdot P_{10} \cdot W_-^{10} \\ & -2^{32} \cdot 3^{18} \cdot P_9 \cdot W_-^9 \; - 2^{36} \cdot 3^{29} \cdot P_8 \cdot W_-^8 \; + 2^{52} \cdot 3^{38} \cdot P_7 \cdot W_-^7 \\ & +2^{62} \cdot 3^{46} \cdot P_6 \cdot W_-^6 \; - 2^{77} \cdot 3^{56} \cdot P_5 \cdot W_-^5 \; - 2^{85} \cdot 3^{65} \cdot P_4 \cdot W_-^4 \\ & +2^{100} \cdot 3^{73} \cdot P_3 \cdot W_-^3 \; - 2^{110} \cdot 3^{83} \cdot P_2 \cdot W_-^2 \; + 47 \cdot 2^{126} \cdot 3^{92} \cdot W_- \\ & -2^{132} \cdot 3^{99} \;=\; 0, \end{aligned} \qquad (5.70)$$

where the polynomials P_n read:

$$
\begin{aligned}
P_{11} \, = \, & \, 85423588659 \, H^5 \, - 1273194070087 \, H^4 \, + 5683675368960 \, H^3 \\
& -3624245 \cdot 2^{12} \cdot 3^6 \, H^2 \, + 901 \cdot 2^{19} \cdot 3^9 \, H \, - 2^{24} \cdot 3^{11}, \\
P_{10} \, = \, & \, 2098366262345322754767 \, H^5 \, - 4991131592299977169590 \, H^4 \\
& +3893219286516719759223 \, H^3 \, - 1056221406812154079936 \, H^2 \\
& +56427952366139092992 \, H \, - 483780265 \cdot 2^{17} \cdot 3^5, \\
P_9 \, = \, & \, 15382723254412673871318753 \, H^4 \, + 26277083153777345473689849 \, H^3 \\
& +4098422120568047655974595 \, H^2 \, + 379212297070602867375 87 \, H \\
& +1560354561975860656, \\
P_8 \, = \, & \, 102093912526673507175090 4401 \, H^4 \, - 116180097399714008352514 3956 \, H^3 \\
& +214393801490313112726470774 \, H^2 - 2006070488338798415238516 \, H \\
& +5919095524632964 8961, \\
P_7 \, = \, & \, 508697400997842959916351 \, H^3 \, - 554351605658908065490725 \, H^2 \\
& -3519280097639420383205 1 \, H \, - 2775596721861024679, \\
P_6 \, = \, & \, 1245962466251450908065 \, H^3 \, - 1525544981578249672864 5 \, H^2 \\
& +845759654345674420717 5 \, H \, - 13332664262978720611, \\
P_5 \, = \, & \, 114630292396020573 \, H^2 \, - 366034684810378734 \, H \, + 92792159042784817, \\
P_4 \, = \, & \, 938107512437391 \, H^2 \, - 1026461977730478 \, H \, + 933965999427127, \\
P_3 \, = \, & \, 121395557277 \, H \, - 59327302513, \\
P_2 \, = \, & \, 11532609 \, H \, - 1281659.
\end{aligned}
\tag{5.71}
$$

Do note that the algebraic curve $P_-(W_-, \, H) \, = \, 0$ is actually a genus zero curve. The algebraic curve (5.70) is the sum of 43 monomials of degree six in H and degree 12 in W_-, as compared to a sum of 157 monomials of degree 22 in z and degree 24 in κ_- for (5.35). At first sight, the polynomial relation (5.70), in the Hauptmodul and the rescaled variable W_-, looks quite different from (5.35). In fact, the two polynomial relations (5.70) and (5.35) are in agreement, as can be seen on the quite remarkable identity

$$
z^{66} \cdot \, P_-(W_-, \, H) \, = \, 12^{18} \cdot \, f_-(z, \kappa_-) \cdot \, f_-(z, e^{2\pi i/3} \, \kappa_-) \cdot \, f_-(z, e^{-2\pi i/3} \, \kappa_-), \tag{5.72}
$$

where the l.h.s. of (5.72) is actually a polynomial expression in terms of κ_- and z.

5.C.1 κ_+ versus κ_-

The functions κ_- and κ_- are not related by analytic continuation. However, because both W_+ and W_- are algebraic functions of the same Hauptmodul we can eliminate H between

(5.69) and (5.70) to obtain the following algebraic relation between W_+ and W_-

$$\begin{aligned} & {W_-}^4 {W_+}^6 \;\; + 32\, {W_-}^3\, W_+^5 \cdot\, (1509\, W_- - 512\, W_+) \\ & -2\; W_-^2\, W_+^3 \cdot\, (W_-^3 \; - 411832512\, W_-^2\, W_+ + 937623552\, W_- W_+^2 \; - 50331648\, W_+^3) \\ & -32\, W_-\, W_+^2 \cdot\, (34791\, W_-^4 - 182579836224\, W_-^3 W_+ \; - 1128985165824\, W_-^2\, W_+^2 \\ & \qquad\qquad -549067948032\, W_-\, W_+^3 + 8589934592\, W_+^4) \\ & + (W_-^4 - 84091500544\, W_-^3\, W_+ - 1482164797440\, W_-^2\, W_+^2 - 8145942347776\, W_-\, W_+^3 \\ & \qquad +68719476736\, W_+^4) \cdot\, (W_-^2 - 172928\, W_-\, W_+ + 4096\, W_+^2) \;\; = \;\; 0. \end{aligned} \tag{5.73}$$

This remarkable algebraic relation for hard hexagons follows from the modular properties of κ_+ and κ_- and is not expected to exist for a generic system.

One verifies easily that eliminating W_+ between (5.69) and (5.73) one recovers (5.70), and that eliminating W_- between (5.70) and (5.73) one recovers (5.69).

The polynomial relation (5.73) of degree six in W_+ and W_-, is actually also a genus zero algebraic curve.

The situations where $\kappa_- \; = \; \kappa_+$ (see (5.60)) correspond to $W_- \; = \; W_+$ in (5.73). It yields the values $0, \, -3^9, \, -57707, \, 22743 \, \pm \, 30268\, i$, corresponding to $W_- \; = \; W_+ \; = \; -3^9$. Note that $\kappa_- \; = \; .83475738 \, \cdots$ in (5.62) corresponds to the integer value $W_- \; = \; -2^{12}\, 3^9$.

5.C.2 The $\kappa_\pm$ equimodular curves

The $\kappa_\pm$ equimodular condition reads $|W_+| \; = \; |W_-|$ in terms of $W_\pm$. Setting the ratio

$$r \; = \; \frac{W_+}{W_-}, \tag{5.74}$$

we can obtain a polynomial relation between this ratio r and the Hauptmodul H, eliminating W_- between $P_-(W_-, \, H) \; = \; 0$ and $P_+(r \cdot W_-, \, H) \; = \; 0$, by performing a resultant. This resultant calculation yields a polynomial condition $P(r, \, H) \;\; = \;\; 0$, where the polynomial, of degree 36 in r and degree 18 in H, is the sum of 577 monomials. When $H \; = \; 0$ this polynomial reduces to

$$P(r, \, 0) \;\; = \;\; 2^{108} \cdot r^3 \cdot \, (4096\, r \; + 19683)^6 \cdot \, (4096\, r \; - 1)^{12} \cdot \, (r \; - 1)^6, \tag{5.75}$$

and when $H \; = \; 1$, it reduces to

$$\begin{aligned} P(r, 1) \;\; = \;\; & (330225942528\, r^3 \; + 216854102016\, r^2 \; + 72695294208\, r \; + 1)^3 \\ & \times (16777216\, r^3 \; - 297467904\, r^2 \; + 2692418304\, r \; - 1)^6 \cdot \, (256\, r \; + 27)^9. \end{aligned} \tag{5.76}$$

The equimodularity condition $|\kappa_+| \;\; = \;\; |\kappa_-|$ corresponds to an algebraic curve in the $(x, \, y)$ complex plane $(z \; = \; x + i\, y)$. This curve can be obtained by writing the Hauptmodul as a function of x and y, namely $H \; = \; X(x, \, y) \, + \, i\, Y(x, \, y)$, where $X(x, \, y)$ and $Y(x, \, y)$ are quite large rational expressions of x and y, and then parametrising the equimodularity condition $|r| = 1$ as $r = (1-t^2)/(1+t^2) + 2\,i\,t/(1+t^2)$, where t is a real variable. This amounts to writing

$$P\Big(\frac{1-t^2}{1+t^2} + i\cdot \frac{2\,t}{1+t^2},\; X(x,\,y) + i\,Y(x,\,y)\Big) \;=\; \mathcal{P}(x,\,y,\,t) + \; i\cdot \mathcal{Q}(x,\,y,\,t) \;=\; 0.$$

where $\mathcal{P}(x,\,y,\,t)$ and $\mathcal{Q}(x,\,y,\,t)$ are quite large rational expressions of the real variables $x,\,y$ and t. Let us denote $\mathcal{N}_1(x,\,y,\,t)$ the numerator of $\mathcal{P}(x,\,y,\,t)$ and $\mathcal{N}_2(x,\,y,\,t)$ the numerator of $\mathcal{Q}(x,\,y,\,t)$. Eliminating t between $\mathcal{N}_1(x,\,y,\,t) = 0$ and $\mathcal{N}_2(x,\,y,\,t) = 0$, performing a resultant, one will get finally a quite large polynomial condition $\mathcal{P}(x,\,y) = 0$, corresponding to the algebraic equation of the equimodularity condition $|\kappa_+| = |\kappa_-|$.

Icosahedral symmetry of the equimodular curve

The polynomial condition is too large to be given explicitly here. It is, however, worth noting that, since the equimodular curve is deduced from polynomial expressions that depend only on the Hauptmodul H, the equimodular curve has the quite non-trivial property that it is compatible with the icosahedral symmetry of the hard hexagon model [134]. This icosahedral symmetry corresponds to the following symmetry of the Hauptmodul (5.67). Let us introduce the complex variable ζ defined by $z = \zeta^5$, the fifth root of unity ω and the golden number τ

$$\omega \;=\; 1/4\sqrt{5} - 1/4 + 1/4\,i\sqrt{2}\sqrt{5+\sqrt{5}}, \qquad \tau \;=\; \frac{1+\sqrt{5}}{2}. \tag{5.77}$$

Let us consider the order-five transformation h_5

$$\zeta \quad\longrightarrow\quad h_5(\zeta) \;=\; \tau\cdot\frac{\omega + (1-\tau)\,\zeta}{\omega + \tau\,\zeta}. \tag{5.78}$$

It is a non-trivial but straightforward calculation to see that the Hauptmodul H, seen as a function of the complex variable ζ, is actually invariant by this order-five transformation h_5, by the involution $\zeta \to -1/\zeta$ as well as the order-five transformation $\zeta \to \omega\cdot\zeta$:

$$H(\zeta) \;=\; H(h_5(\zeta)) \;=\; H\Big(\frac{-1}{\zeta}\Big) \;=\; H(\omega\cdot\zeta). \tag{5.79}$$

A selected point of the equimodular curve

The algebraic equimodular curve $\mathcal{P}(x,\,y) = 0$ intersects the real axis $y = 0$ at the critical value z_c (i.e. $H = 0$, see (5.75)) and at an algebraic value $z = -5.94254104\cdots$ corresponding to the algebraic value of the Hauptmodul $H = 1.2699347\cdots$, a root of the polynomial $P_{12}(H)$ of degree twelve in H:

$$
\begin{aligned}
P_{12}(H) \;=\; & 420659520093064357478960957541^2 \cdot H^{12} \\
& -3035676163450716673183784433435873765727935868148497169025 \cdot 2^9 \cdot H^{11} \\
& +180032218185835528405034756761309783218694171171683152985 \cdot 2^{16} \cdot H^{10} \\
& -963917598568487789731961832547602704647778692096330233 \cdot 2^{25} \cdot H^9 \\
& +4687917985071549790872555988500591318811098924601809 \cdot 2^{33} \cdot H^8 \\
& -11794524087347323954434252908699683281468087505905 \cdot 2^{41} \cdot H^7 \\
& +34111250660390601705930372758400977149413250857 \cdot 2^{48} \cdot H^6 \\
& -16562829715197286592872531393597405351924479 \cdot 2^{57} \cdot H^5 \\
& +10432786705236893496285793791292996147041 \cdot 2^{65} \cdot H^4 \\
& -4452980987936971936196603653288348935 \cdot 2^{73} \cdot H^3 \\
& +2184609189525225289847951233328377 \cdot 2^{80} \cdot H^2 \\
& -14687865423363371951559480967168 \cdot 176160768^3 \cdot H \\
& +956497920^6.
\end{aligned}
\qquad (5.80)
$$

This algebraic point corresponds to the following algebraic values of $W_\pm$, in (5.70) and (5.69), $W_+ = -5404.2605 \cdots$ and $W_- = 2118.9287 \cdots + 971.5363 \cdots i$, the ratio $r = W_+/W_-$ being, as it should, a complex number of unit modulus, namely $-0.3920 \cdots + i\,.9199 \cdots$ This algebraic point is characterized by the fact that W_+ or κ_+^6 (but not κ_-) is a real number: $\kappa_+^6 = 26.6786 \cdots$ but $\kappa_- = 0.864 \cdots - 1.497 \cdots i$.

5.D Cardioid fitting of partition function zeros

Examples of the excellent fit by the cardioid curve (5.43) of the inner boundary of the partition function zero on cylindrical lattices referred to in section 5.5.1 for the cases 33×33, 36×36 and 39×39 are plotted in figure 5.D.15. In figure 5.D.16 we plot the values of $a(L)$ and $c(L)$ the best fitted cardioid of (5.43) versus $1/L$ and observe that they are remarkable well fitted by a straight line which extrapolates as $L \to \infty$ to

$$a \;=\; 7.6302 \cdots \qquad c \;=\; -4.1268 \cdots \qquad (5.81)$$

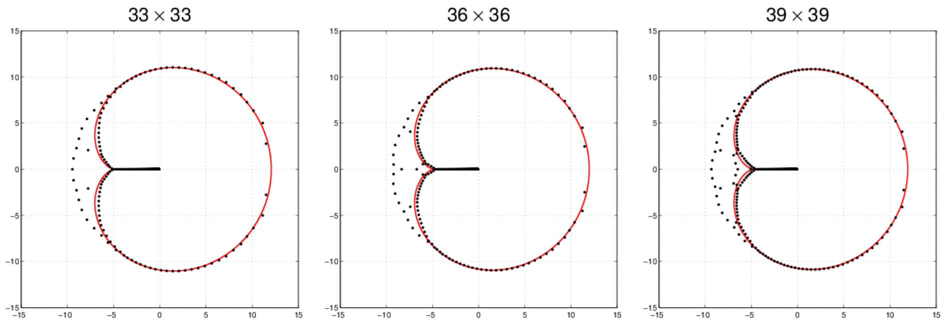

Figure 5.D.15: Fitting of the partition function zeros for cylindrical boundary conditions to the cardioid of (5.43) for the 33×33, 36×36 and 39×39 lattice.

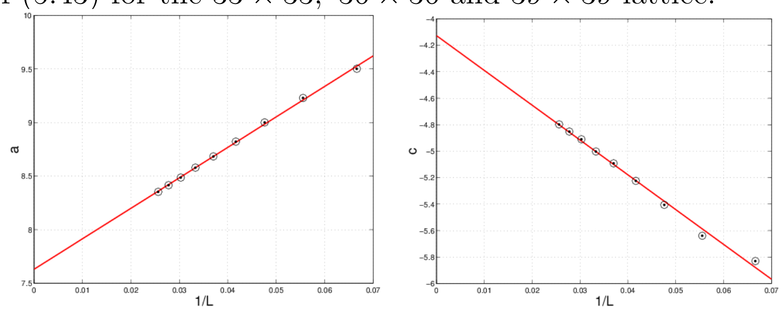

Figure 5.D.16: The fitting parameters a and c for cylindrical boundary conditions of the cardioid (5.43) versus L for the partition zeros of the $L \times L$ lattice.

5.E Transfer-matrix algorithms

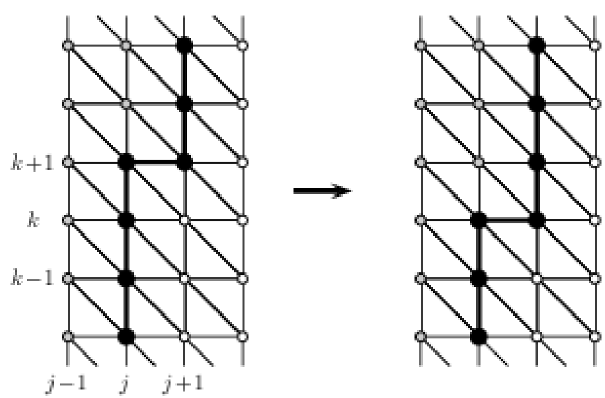

Figure 5.E.17: The movement of the transfer-matrix cut-line in the general case.

To calculate the partition functions $Z_{L_v,L_h}(z)$ we use what are known as 'transfer matrix' techniques. These work by moving a cut-line through the lattice and constructing a partial partition function for each possible configuration/state of sites on the cut-line. The most efficient way of calculating the partition function is to build up the lattice site-by-site as illustrated in figure 5.E.17. Sites on the cut-line are shown as large solid circles. Each of these sites can be either empty or occupied. Because of the hard particle constraint, nearest neighbors cannot be occupied simultaneously. So any configuration can be mapped to a binary integer in an obvious fashion with empty sites mapped to 0 and occupied sites to 1. The distinct configurations along the cut-line are thus circular n-bit strings with no repeated 1's. Their number is given by the Lucas numbers $L(n)$ (sequence A000204 in the OEIS [225]), which have the simple recurrence $L(n) = L(n-1) + L(n-2)$. In fact, $L(n) = (1+\sqrt{5})/2)^n + (1-\sqrt{5})/2)^n$, so the number of allowed configurations has the growth constant $(1+\sqrt{5})/2 = 1.618\ldots$, and are therefore exponentially rare among the integers. Hence as is standard in such a case we use hash tables as our basic data structure to store and access the sparse array representing the state space of the model.

For each configuration we maintain a partial partition function (sum over all states) for the lattice sites already visited with each occupied site given weight z and each empty site given weight 1. The shaded circles in figure 5.E.17 represent sites already fully accounted for, that is, all possible occupancies have been summed over. The open circles are sites that are yet to be visited and hence are not yet accounted for. The black circles are not yet fully accounted for since their possible 'interactions' with the open sites have not yet been included. The movement of the cut-line in figure 5.E.17 consists of a move from the site at position $(j, k+1)$ to the 'new' site at position $(j+1, k)$ with 'interactions' with the neighbor sites at (j, k) and $(j+1, k+1)$. Notice that the update of the partial partition functions does not depend on the state of any other sites on the cut-line. Formally we can view the update as a matrix multiplication $\mathbf{w} = \mathbf{T}\mathbf{v}$, mapping the vector of partition functions $\mathbf{v}$ prior to the move to the vector of partition functions $\mathbf{w}$ after the move. The great advantage of the site-by-site updating is that we need not store the actual transfer matrix $\mathbf{T}$; it is given implicitly by a set of simple updating rules depending only on the 'local' configuration (states) of the sites on the cut-line which are nearest neighbors to the new site.

We shall refer to the configuration of sites prior to the move as a 'source' and denote its integer representation with an S while a configuration after the move is referred to as a 'target' and denoted with a T. In an update we simply have to determine the allowed configuration of the 'new' site, that is, whether the new site is occupied or empty. The 'hard' constraint makes this very simple since the new site can be occupied only when all neighbor sites in the source configuration are empty. Since each site can be either empty (0) or occupied or (1) the four sites around the face have 16 possible configurations but only 6 are allowed because of the hard constraint. The 3 sites along the left and top form the 'local' source configuration and there are 5 (out of 8) allowed configurations. The local target configuration is given by the states of the 3 sites along the bottom and right of the face (2 sites occur in both source and target). By writing down the 6 allowed local configurations one can easily deduce the following simple updating rules

$$
\begin{aligned}
Z(T_{000}) &= Z(S_{000}) + Z(S_{010}), \\
Z(T_{100}) &= Z(S_{100}), \\
Z(T_{010}) &= z \cdot Z(S_{000}), \\
Z(T_{001}) &= Z(S_{001}), \\
Z(T_{101}) &= Z(S_{101}),
\end{aligned}
\tag{5.82}
$$

where the subscript triplets represent the states of the 'local' source sites at positions (j,k), $(j,k+1)$, $(j+1,k+1)$ and target sites at positions (j,k), $(j+1,k)$, $(j+1,k+1)$, respectively.

The transfer matrix algorithm described above takes care of the summation over sites in the interior of the lattice. Special rules apply at the top and bottom of a column. When adding a site at the top of a new column we include interactions between the site left of the new site and the site in the previous column on the bottom row (this interaction along a diagonal edge implements part of the periodic boundary condition in the L_h direction). Finally after we have completed a new column the site 'left over' in the previous column is superfluous to requirements and we can 'contract' the state space by summing over the states of this site. The number of distinct configurations for a column of height L_h sites is then $L(L_h+1)$ for a partially completed column, and $L(L_h)$ when the column has been completed.

The transfer matrix algorithm described above is the same whether used in the calculation of partition function zeroes or eigenvalue crossings. Below we briefly outline how it is used in the two cases.

5.E.1 Partition function zeros

To calculate partition function zeros we need the exact partition function on an $L_v \times L_h$ lattice. This is simply a polynomial in z of degree $L_v \cdot L_h/3$ with integer coefficients. So for each state along the cut-line the partial partition function is maintained as an array of integers of size $L_v \cdot L_h/3 + 1$. The coefficients become very large and in order to deal with this the calculations were performed using modular arithmetic. So the calculation for a given size lattice was performed several times modulo different prime numbers with the full integer coefficients reconstructed from the calculated remainders using the Chinese remainder theorem. Utilizing the standard 32-bit integers we used primes of the form $p_i = 2^{30} - d_i$, that is we used the set of largest primes smaller than 2^{30}. Depending on the L_v and L_h the number of primes required to reconstruct the exact integer coefficients can exceed 100. The zeros of the partition function can then be calculated numerically (to any desired accuracy) using root finders such as `MPSolve` [37] or `Eigensolve` [94]. We used `MPSolve` with a few calculations checked by using `Eigensolve`.

The transfer-matrix algorithm can readily be parallelised. One of the main ways of achieving a good parallel algorithm using data decomposition is to identify an invariant under the operation of the updating rules. That is, we seek to find some property of the configurations along the cut-line which does not alter in a single iteration. As mentioned above only the 'new' site can change occupation status. Thus, any site not directly involved in the update cannot change from being empty to being occupied and vice versa. This invariant allows us to parallelise the algorithm in such a way that we can do the calculation completely independently on each processor with just two redistributions of the data set each time an extra column is added to the lattice. This method for achieving a parallel algorithm has been used extensively for other combinatorial problems and the interested reader can look at [126] or [107, Ch 7] for details.

Cylindrical boundary conditions are simply implemented by starting the transfer matrix calculation with the all empty state having weight one (all other states having weight zero), iterating the algorithm to add L_h columns and then summing over all states.

Toroidal boundary conditions are fairly easy to implement but they are computationally expensive. The problem is that in order to include the interactions between sites in the first and last columns we have to 'remember' the state of the first column. Here we did this by simply specifying the initial state of the first column S_I, starting with the initial weights $Z(S) = 0$ when $S \neq S_\mathrm{I}$ and $Z(S_\mathrm{I}) = z^m$, where m is number of occupied sites in S_I. For each value of S_I we then perform the transfer matrix calculation as described above until the final column has been completed. Finally we put in the interactions between the occupation numbers in the last column with state S and those in the first column, sum over all states S, and repeat for all S_I. The saving grace is that one does not have to do this calculation for all values of S_I. Indeed, any S_I related by translational and reflection symmetry give rise to the same result. In table 5.E.6 we have listed the number of distinct initial states N_I one needs to consider in a calculation of the partition function with toroidal boundary conditions on a lattice of width L_h. The numbers N_I are given by sequence A129526 in the OEIS [225]. Note that for large L_h states which are invariant under the generators of the dihedral group D_{L_h} are exponentially rare. Therefore $L(L_h)/N_I \sim 2L_h$ for $L_h \gg 1$, and this is nicely brought out by the entries in table 5.E.6. Naturally the calculations for different initial states can be done completely independently making it trivial to parallelise over S_I (one can also fairly easily combine this with the parallel algorithm over state space should this be required).

L_h	N_I	$L(L_h)$	$L(L_h)/N_I$	L_h	N_I	$L(L_h)$	$L(L_h)/N_I$
3	2	4	2.00	6	5	18	3.60
9	9	76	8.44	12	26	18	12.38
15	64	1364	21.31	18	209	5778	27.64
21	657	24476	37.25	24	2359	103682	43.95
27	8442	439204	52.02	30	31836	1860498	58.44

Table 5.E.6: The number N_I of distinct initial states required to calculate the partition function with toroidal boundary conditions compared to the total number of states given by the Lucas numbers.

The bulk of the large scale calculations for this part of the project were performed on the cluster of the NCI National Facility at ANU. The NCI peak facility is a Sun Constellation Cluster with 1492 nodes in Sun X6275 blades, each containing two quad-core 2.93GHz Intel Nehalem CPUs with most nodes having 3GB of memory per core (24GB per node). The largest size calculation we performed was for cylindrical boundaries where we went up to 39×39. This required the use of 256 processors (cores to be precise) taking around 140 CPU hours per prime with the calculation being repeated for 25 primes. The largest calculation for toroidal boundaries was the 27×27 lattice. This is sufficiently small memory wise to fit on a single core so we only used a parallelisation over initial states. The calculation took around 550 CPU hours per prime with the calculation repeated for 14 primes.

5.E.2 Transfer matrix eigenvalues

The equimodular curves on $L_h \times \infty$ strips where eigenvalues of largest modulus cross can be obtained from numerical studies using the transfer matrix algorithm outlined above. As we have seen, the dimension $\dim \mathbf{T}$ of the transfer matrix $\mathbf{T}$ for hard hexagons confined to a strip of height L_h grows exponentially fast with L_h. Hence the calculation of the eigenvalues of $\mathbf{T}$ and the resulting equimodular curves quickly becomes a very demanding task. We have however seen that the updating rules (5.82) do not require us to manipulate or store all the $(\dim \mathbf{T})^2$ entries of $\mathbf{T}$, but rather operate on two vectors of size $\dim \mathbf{T}$, namely $\mathbf{v}$ and $\mathbf{Tv}$, representing the set of conditional probabilities before and after a move of the cut-line. In other words, the trick of adding the sites to the system one at a time has produced a sparse-matrix factorization of $\mathbf{T}$.

It is possible to take further advantage of this gain to extract also the leading eigenvalues of $\mathbf{T}$. Namely, we use a set of iterative diagonalisation methods in which the object being manipulated is not $\mathbf{T}$ itself but rather its repeated action on a suitable set of vectors. An iterative scheme that works well even in the presence of complex and degenerate eigenvalues is known as Arnoldi's method [8]. This forms part of a class of algorithms called Krylov subspace projection methods [203, 204]. These methods take full advantage of the intricate structure of the sequence of vectors $\mathbf{T^n v}$ naturally produced by the power method. If one hopes to obtain additional information through various linear combinations of the power sequence, it is natural to formally consider the Krylov subspace

$$\mathcal{K}_n(\mathbf{T}, \mathbf{v}) = \mathrm{Span}\{\mathbf{v}, \mathbf{Tv}, \mathbf{T^2 v}, ..., \mathbf{T^{n-1} v}\}$$

and to attempt to formulate the best possible approximations to eigenvectors from this subspace. We make use of the public domain software package ARPACK [152] implementing Arnoldi's method with suitable subtle stopping criteria. The ARPACK package allows one to extract eigenvalues (and eigenvectors) based on various criteria, including the one relevant to our calculations, namely the eigenvalues of largest modulus.

The problem specific input for this type of calculation only consists in a user supplied subroutine providing the action of $\mathbf{T}$ on an arbitrary complex vector $\mathbf{v}$. In our case this amounts to iterating the update rules (5.82) until a complete column has been added to the lattice. In particular, the sparse-matrix factorization and the subtleties having to do with the 'inflation' of the state space before the addition of the first site in a new row, as well as the 'contraction' after the addition of the last site in a completed row, are all hidden inside this subroutine and not visible to Arnoldi's method. The iterations of $\mathbf{T}$ are thus computed for a fixed complex value of the fugacity z until the ARPACK routines have converged.

Very briefly, we trace the equimodular curve as follows. First we find a point on the equimodular curve; we can choose a point on the negative real axis, say $z_0 = -1$, that we know is on the curve. To find a new point z on the curve we start at the previous point and look for a new point on a circle of radius ϵ (in general we use $\epsilon = 10^{-2}$) at an angle θ_0 from the previous point. In general this trial point will not lie on the equimodular curve. Our algorithm then finds a new point by using the Newton-Raphson method to converge in the angle θ towards a zero in the distance between leading eigenvalues. The pair (z, θ) is then used as the starting values (z_0, θ_0) for a new iteration of the search algorithm. This procedure in then iterated until the equimodular curve has been traced. Points where the curve branches are detected by noting that the third leading eigenvalue becomes equal in modulus to the leading eigenvalue. End points are detected by noting that the procedure cannot find a new point (in fact it turns around and converges towards a point on the part of the curve already traced). Many aspects of this search algorithm involve subtleties, in particular automatizing the procedure in the case where the equimodular curve has a complicated topology with many branchings; this will be described fully in a separate publication [120].

As for the partition function zeroes, we are interested in tracing the equimodular curves for both toroidal and cylindrical boundary conditions. Since in both cases we use the same transfer matrix $\mathbf{T}$ (i.e., with periodic boundary conditions in the L_h direction) it might seem that the curves would be identical. This is not the case. Indeed, in the cylindrical case the initial condition imposed on the first column of the lattice is that all sites in the preceding column are empty. In particular, this initial state is translational invariant and thus has momentum $P = 0$. This momentum constraint can be imposed by rewriting $\mathbf{T}$ in the translational and reflection symmetric subspace of dimension N_I. Once again, an appropriate 'inflation' and 'contraction' of the state space has to be performed at the beginning and the end of the user supplied subroutine, as the kink on the cut-line describing the intermediate states breaks the dihedral symmetries explicitly. But since these intermediate steps are hidden from Arnoldi's method, the end result amounts to diagonalising a transfer matrix of smaller dimension, $\dim \mathbf{T} = N_I$. Meanwhile, the equimodular curve for toroidal boundary conditions is obtained by diagonalising the original transfer matrix without the $P = 0$ constraint, i.e., with dimension $\dim \mathbf{T} = L(L_h)$.

The memory requirements of the algorithm up to the largest size $L_h = 30$ that we attempted is quite modest and the calculation can be performed on a basic desktop or laptop computer. As an example the calculation of the equimodular curve for $L_h = 30$ with cylindrical boundary conditions took about 10 days on a MacBook Pro with a quad core I7 2.3GHZ processor.

5.F Finite-size scaling analysis of $z_c(L)$ and $z_d(L)$

According to the theory of finite-size scaling (FSS) [67], the free energy per site corresponding to the j-th eigenvalue of the transfer matrix has the scaling form

$$\frac{1}{L} f_j \left(|z - z_c| L^y, u L^{-|y'|} \right) , \tag{5.83}$$

where z_c is the critical point, y is the leading relevant eigenvalue under the renormalization group (RG), and u is the coupling to an RG irrelevant operator with eigenvalue $y' < 0$. If more than one RG irrelevant coupling is present there will be further arguments to the function, which we here omit for clarity. The equimodularity condition $|f_1| = |f_2|$ can obviously be written in the same scaling form as can the partition function zeros. Moreover, FSS assumes that the functions f_j are analytic in their arguments for $z \neq z_c$, which implies at leading order that

$$|z - z_c| = A L^{-y} + B u L^{-y-|y'|} + \dots , \tag{5.84}$$

where A and B are non-universal constants. To higher orders, the terms appearing on the right-hand side involve powers of L^{-1} that can be any non-zero linear combination of y and $|y'|$ with non-negative integer coefficients. There is obviously no guarantee that all such terms will appear, since some of the multiplying constants $(A, B, \dots)$ may be zero.

When it is known that $z \to z_c$ as $L \to \infty$, with z_c real, one can similarly analyze distances other than $|z - z_c|$ to the critical point that vanish linearly with $z - z_c$. Examples include $||z| - z_c|$, $\mathrm{Re}(z) - z_c$, $\mathrm{Im}(z)$, and $\mathrm{Arg}(z)$.[1] According to the general principles of FSS [67] these variables can be developed on $|z - z_c|$ and the irrelevant RG couplings, and (5.84) will follow, albeit necessarily with different values of the non-universal constants $(A, B, \dots)$.

The critical point $z_c > 0$ in the hard hexagon model is known to be in the same universality class as the three-state ferromagnetic Potts model [252]. The energy operator of the latter [87] provides the RG eigenvalue $y = 2 - 2h_{2,1} = 6/5$, where we have used the Kac table notation $h_{r,s}$, familiar from conformal field theory (CFT), for the conformal weight of a primary operator $\phi_{(r,s)}$. Subdominant energy operators, $\phi_{(3,1)}$ and $\phi_{(4,1)}$, follow from CFT fusion rules and lead to RG eigenvalues $y' = -4/5$ and $y'' = -4$ respectively. Our numerical analysis of $|z_c(L)| - z_c$ for L up to 39 (see table 5.5) gives good evidence for the FSS form

$$|z_c(L)| - z_c = a_0 L^{-6/5} + a_1 L^{-2} + a_2 L^{-14/5} + \dots . \tag{5.85}$$

The powers of L^{-1} appearing on the right-hand side can be identified with y, $y + |y'|$ and $y + 2|y'|$. This is compatible with the above general result; note however that the power $2y = 12/5$, which is a priori possible, is not observed numerically.

The CFT of the Lee-Yang point $z_d < 0$ is much simpler [68], since there is only one non-trivial primary operator $\phi_{(2,1)}$. It provides the RG eigenvalue $y = 12/5$. Our numerical

[1] Obviously we here exclude cases where the variable is identically zero, such as when $\mathrm{Im}(z) = 0$, or when $||z| - z_c| = 0$ because of a circle theorem.

analysis of $|z_d(L) - z_d|$ (see table 5.5) gives strong evidence for the FSS form

$$|z_d(L) - z_d| = b_0 L^{-12/5} + b_1 L^{-17/5} + b_2 L^{-22/5} + \dots \,. \tag{5.86}$$

The powers of L^{-1} on the right-hand side can be identified with y, $y+1$ and $y+2$. The integer shifts in (5.86) can be related to descendent operators in the CFT, since $|y'|$ is a positive integer for descendents of the identity operator; note that some descendents are ruled out by symmetry arguments, as in section 5.5.3. Another source of corrections in powers of L^{-1} is that the data of table 5.5 are computed for $L \times L$ systems with cylindrical boundary conditions. Indeed, while the length L along the periodic direction is unambiguous, the one along the free direction should possibly be interpreted as $L+a$ in the continuum limit, where a is a constant of order unity. In any case, it is remarkable that $y+1 = 11/5$ does not occur in (5.86).

To probe the finite-size scaling form, i.e., determine which terms actually occur in the asymptotic expansion, we carry out a careful numerical analysis of how the endpoints $z_d(L)$ and $z_c(L)$ approach z_d and z_c in the thermodynamic limit. Since our data for end-point positions is most extensive in the case of partition function zeros with cylindrical boundary conditions we analyse the data of table 5.5. We also tried to analyse the data in table 5.3 obtained from equimodular calculations, but we found that this data set suffers from numerical instability presumably because our determination of the end-point position is not sufficiently accurate. Note that the data in table 5.5 can be calculated to any desired numerical accuracy since it is obtained from the zeros of polynomials. Obviously the data for $z_d(L)$ is much closer to the thermodynamic limit z_d than is the corresponding data for $z_c(L)$ so it is no surprise that the analysis of $z_d(L)$ is 'cleaner' than that for $z_c(L)$ and hence we start our exposition with the former.

Firstly, plotting $\ln|z_d(L) - z_d|$ versus $\ln L$ confirms a power-law relationship (see left panel of figure 5.F.18). To estimate the exponent we take a pair of points at L and $L-3$, calculate the resulting slope of a straight line through the data-points, and in figure 5.F.18 we plot the slope versus $1/L$. Clearly, the slope can be extrapolated to the predicted value, 12/5, for the exponent. We next look for sub-dominant exponents. Accepting the 12/5 exponent as exact we form the scaled sequence, $s(L) = L^{12/5}|z_d(L) - z_d| \simeq a + b/L^{\alpha}$, and look at the sequence of differences, $d(L) = s(L) - s(L-3) \propto 1/L^{\alpha+1}$, thus eliminating the constant term. As before we calculate the slope of $\ln d(L)$ versus $\ln L$ and plot against $1/L$. From figure 5.F.18 the slope is seem to extrapolate to a value of -2, so $\alpha = 1$ and hence the sub-dominant exponent is 17/5. We then repeat the analysis starting with the $d(L)$ sequence which we scale by L^2. The estimates for the local slopes are shown in figure 5.F.18 and are again consistent with a slope of -2, indicating that the third exponent in the asymptotic expansion is 22/5.

From the above analysis we conclude that the correct asymptotic form is (5.86). It is tempting to conjecture that the sequence of integer spaced corrections $L^{-12/5-k}$ will continue indefinitely. However, we cannot completely rule out the presence of extra terms such as $L^{-n\cdot 12/5}$ for $n \geq 2$. This is borne out by a further analysis using five terms in the asymptotic expansion namely the three exponents firmly established above and a further two terms with exponents $2y = 24/5$, $y+3 = 27/5$, and $y+3 = 27/5$, $y+4 = 32/5$, respectively. The

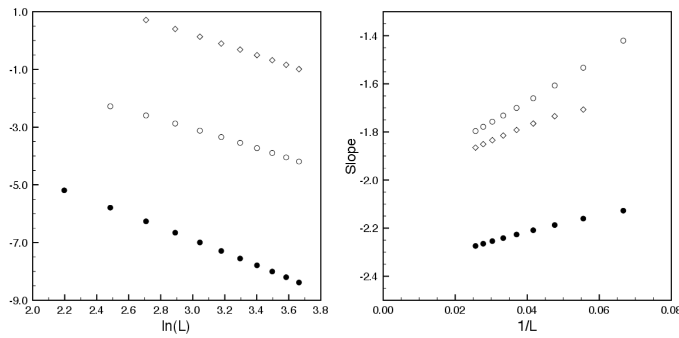

Figure 5.F.18: The left panel are log-log plots of the data for $|z_d(L) - z_d|$ (filled circles), $d(L)$ (open circles) and $L^2 d(L) - (L-3)^2 d(L-3)$ (diamonds). In the right panel we plot the corresponding local slopes versus $1/L$.

resulting amplitude estimates are shown in figure 5.F.19. Clearly, the fits using only terms of the form $y+k$ display much less variation against $1/L$ and this could be an indication that only these types of terms are present in the asymptotic expansion. However, the amplitude b_3 when fitting using an exponent 24/5 does not appear to vanish and hence we are not willing to claim with certainty that this term is absent. If we assume only terms of the form $y+k$, we can obtain refined amplitude estimates by truncating the expansion after a fixed number of terms and fitting using sub-sequences of consecutive data points. Results for the leading amplitude b_0 are displayed in figure 5.F.20. Note that the estimates are quite accurate and that as more terms from the asymptotic expansion are included the estimates have less variation. We estimate that

$$b_0 = 1.7147(1), \quad b_1 = -9.30(2), \quad b_2 = 48(2), \quad b_3 = -180(30). \tag{5.87}$$

We now turn to $z_c(L)$ where we start by analysing the data for $|z_c(L)| - z_c$. Note that the modulus $|z_c(L)|$ can be viewed as a crude approximation to where the zeros intercept the real axis since it amounts to saying that the zeros approach the real axis along a circle. Many other measures of the distance/approach to z_c could be used but this one happens to be particularly well-behaved so we start our exposition with this quantity. As above we first look at the local log-log slope for this data shown in the left panel of figure 5.F.21. In this case the data displays pronounced curvature but nevertheless it seems reasonable that the slope can be extrapolated to the predicted value $-6/5$. We next look for sub-dominant exponents. Accepting the 6/5 exponent as exact we form the scaled sequence, $s(L) = L^{6/5}(|z_c(L)| - z_c) \simeq a + b/L^{\alpha}$. We again look at the sequence $d(L)$ of differences and plot the local slopes in the right panel of figure 5.F.21 using open circles. In this case the results are not as clear cut. The data can be extrapolated to a value > -2 and it is consistent with the predicted exponent $y + |y'| = 2$, which would yield a slope of -1.8. We then repeated the analysis scaling $d(L)$ by $L^{9/5}$ and looking at the differences. The local slopes are shown as diamonds in the right panel of figure 5.F.21. Clearly no meaningful extrapolation can be performed on this data other than to say that a value of -1.8 cannot

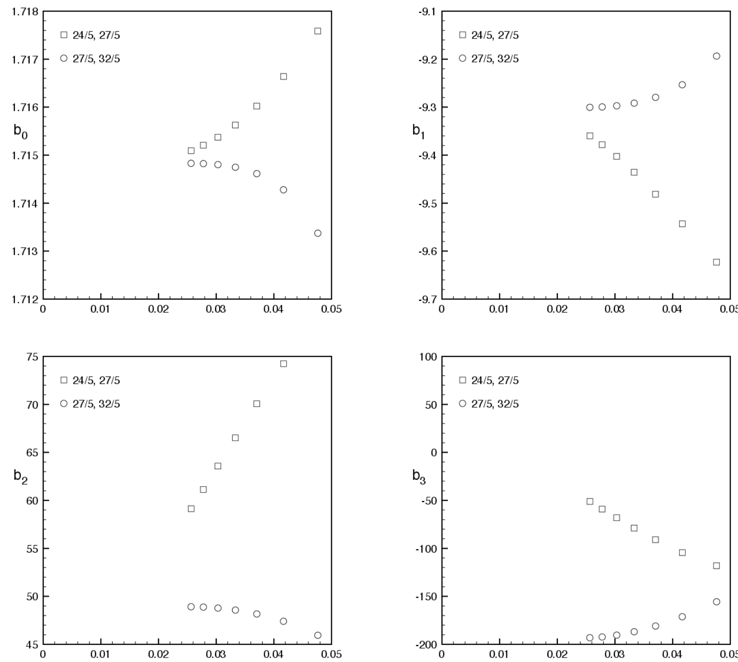

Figure 5.F.19: Amplitude estimates versus $1/L$ when fitting to a five-term asymptotic form akin to (5.86), but with two additional exponents as indicated on the plots.

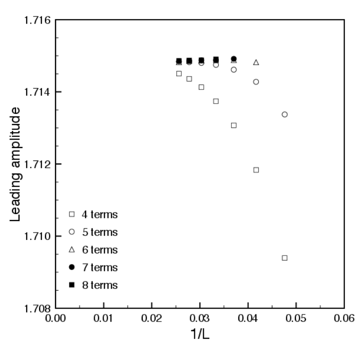

Figure 5.F.20: Estimates for the leading amplitude b_0, plotted versus $1/L$ in the asymptotic expansion (5.86) when truncating after 4 to 8 terms and using only exponents $24/5 + k$.

be ruled out.

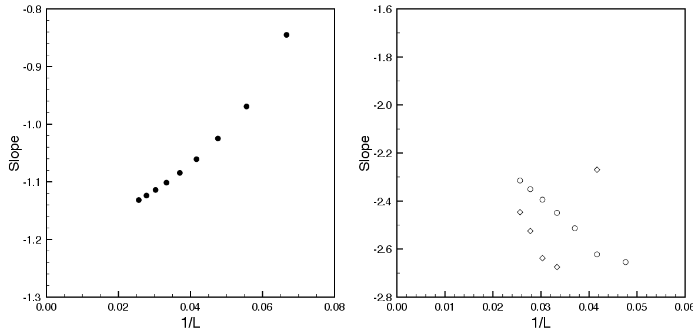

Figure 5.F.21: Local slopes versus $1/L$ for $||z_c(L)| - z_c|$ in the left panel and in the right panel the sequences $d(L)$ (open circles) and $L^{9/5}d(L) - (L-3)^{9/5}d(L-3)$ (diamonds).

To further investigate the asymptotic scaling form we turn to amplitude fitting using

$$|z_c(L)| - z_c = a_0/L^{6/5} + a_1/L^{10/5} + a_2/L^{\Delta}. \tag{5.88}$$

We look at three possible values for the third exponent Δ, namely $y+1 = 11/5$, $2y = 12/5$, or $y + 2|y'| = 14/5$. The results are displayed in figure 5.F.22 where we plot the estimated values of the three amplitudes for the three different values of Δ. Firstly, we note that the estimates for the amplitude a_0 (left panel) are quite stable though the estimates become more stable as the value of Δ is increased. Secondly, the data for the amplitude a_1 (middle panel) is very striking; for a Δ of 11/5 or 12/5 the estimates vary greatly with L and even have the wrong sign from the extrapolated value; in sharp contrast for $\Delta = 14/5$ the estimates are quite well converged with only a mild dependence on L. Finally, for the amplitude a_2 (right panel) we see that the amplitude estimates for $\Delta = 11/5$ or 12/5 may well extrapolate to a value of 0 while the estimates for $\Delta = 14/5$ clearly extrapolate to a non-zero values around -200 or so. Taken together this is quite clear evidence that the correct value of the third exponent is $\Delta = y + 2|y'| = 14/5$. We estimate roughly that

$$a_0 = 53.0(1), \quad a_1 = -50(5), \quad a_2 = -200(50). \tag{5.89}$$

In figure 5.F.23 we plot the data for $|z_c(L)| - z_c$ (left panel) and $|z_d(L) - z_d|$ (right panel) and the asymptotic fits obtained above.

It is universally expected that the end-point $z_c(L)$ converges towards z_c, as can be confirmed by analyzing the behavior of $\mathrm{Re}(z_c(L))$ and $\mathrm{Im}(z_c(L))$ against $1/L$. This obviously means that the imaginary part must vanish as $L \to \infty$. To examine this we repeat the above analysis for $\arg(z_c(L))$. The 'local-slope' analysis is not as clear-cut in this case but it is consistent with the two leading terms in (5.88). The amplitude analysis is again very clean as can be seen in figure 5.F.24 and from this we obtain the amplitude estimates

$$a_0 = 15.83(2), \quad a_1 = -3.0(5), \quad a_2 = 8(2). \tag{5.90}$$

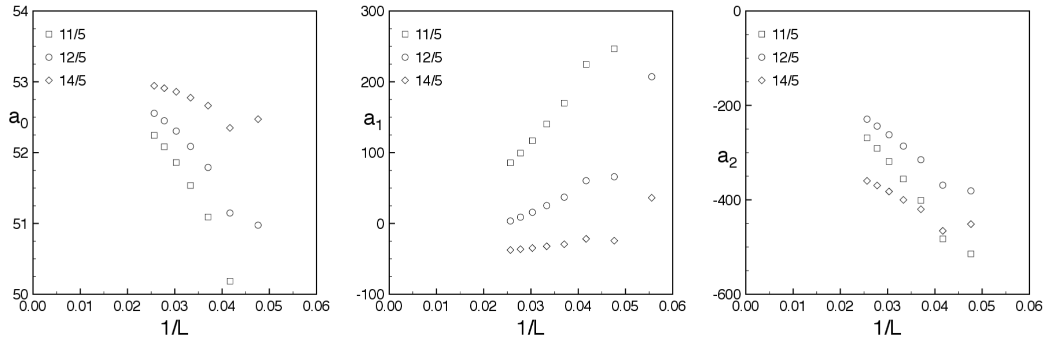

Figure 5.F.22: Amplitude estimates versus $1/L$. The panels (from left to right) shows the estimates for the amplitudes a_0, a_1 and a_2 when fitting to the asymptotic form (5.88) while using three different values for the third exponent Δ.

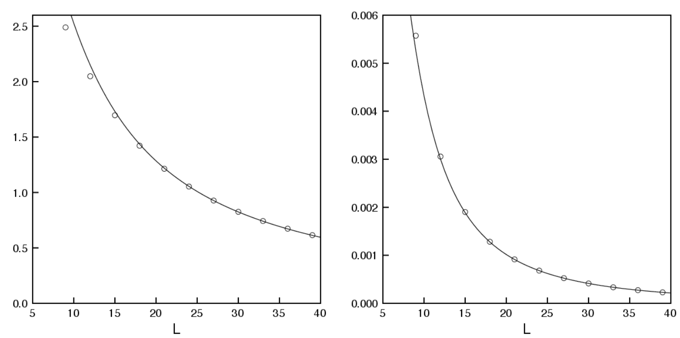

Figure 5.F.23: Data for $|z_c(L)| - z_c$ (left panel) and $|z_d(L) - z_d|$ (right panel) and fitted curves to the asymptotic forms (F.3) and (5.86) using the listed amplitude estimates (5.89) and (5.87).

These values of course differ from those in (5.89) since we are analyzing a different quantity.

Finally we carried out a similar analysis for the quantity $|z_c(L) - z_c|$. Again the evidence for the leading amplitude being $-6/5$ was firm. However, the local-slope analysis for the sub-dominant term was inconclusive. In figure 5.F.25 we plot the amplitude estimates obtained when fitting to (F.3). We observe a very strong variation in a_1 and a_2, but on the other hand the amplitude estimates are nice and monotonic, suggesting that the data might just be really hard to fit. In particular we note that a_1 could extrapolate to 0. We then tried a new fit using an additional fourth term with exponent $-18/5$, thus assuming exponents of the form $y + k|y'| = 6/5 + k \cdot 4/5$ In this case we found much more stable amplitude estimates with $a_0 = 183.5(5)$. The other amplitudes displayed quite a bit of scatter so we will not quote error-bars, but we found $a_1 \simeq 6.5$, $a_2 \simeq 930$ and $a_3 \simeq -5200$. Remarkably a_1 is quite small compared to the other quantities which may well explain the numerical difficulties we had with the analysis. Note that we make no claim that $y + k|y'|$ exhausts the exponents and it is quite likely that other exponents, such as $2y + |y'| = 16/5$, could occur, but our data sets are too limited to answer such questions beyond the terms explicitly included in (F.3).

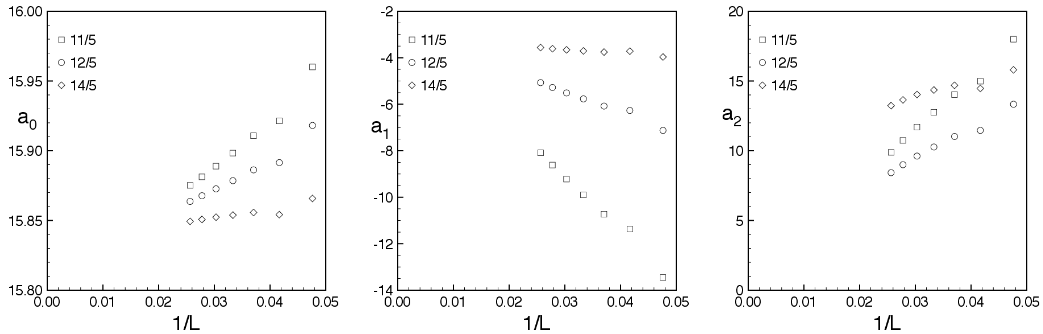

Figure 5.F.24: Amplitude estimates versus $1/L$. The panels (from left to right) shows the estimates for the amplitudes a_0, a_1 and a_2 when fitting $\arg(z_c(L))$ to the asymptotic form (5.88) while using three different values for the third exponent Δ.

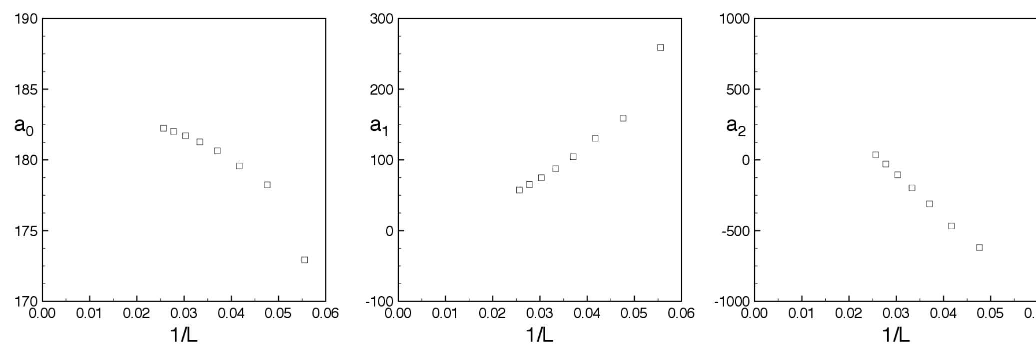

Figure 5.F.25: Amplitude estimates versus $1/L$. The panels (from left to right) shows the estimates for the amplitudes a_0, a_1 and a_2 when fitting to the asymptotic form (F.3) while using the data for $|z_c(L) - z_c|$.

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Chapter 6

Paper 4

Integrability vs non-integrability Hard hexagons and hard squares compared

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Abstract

In this paper we compare the integrable hard hexagon model with the non-integrable hard squares model by means of partition function roots and transfer matrix eigenvalues. We consider partition functions for toroidal, cylindrical, and free-free boundary conditions up to sizes 40×40 and transfer matrices up to 30 sites. For all boundary conditions the hard squares roots are seen to lie in a bounded area of the complex fugacity plane along with the universal hard core line segment on the negative real fugacity axis. The density of roots on this line segment matches the derivative of the phase difference between the eigenvalues of largest (and equal) moduli and exhibits much greater structure than the corresponding density of hard hexagons. We also study the special point $z = -1$ of hard squares where all eigenvalues have unit modulus, and we give several conjectures for the value at $z = -1$ of the partition functions.

6.1 Introduction

There is a fundamental paradox in the practice of theoretical physics. We do exact computations on integrable systems which have very special properties and then apply the intuition gained to generic systems which have none of the special properties which allowed the exact computations to be carried out. The ability to do exact computations relies on the existence of sufficient symmetries which allow the system to be solved by algebraic methods. Generic systems do not possess such an algebra and the distinction between integrable and non-integrable may be thought of as the distinction of algebra versus analysis.

This paradox is vividly illustrated by the two dimensional Ising model. In zero magnetic field Onsager [176] computed the free energy by means of exploiting the algebra which now bears his name. On the other hand in 1999 Nickel [171, 172] analyzed the expansion of the susceptibility at zero magnetic field for the isotropic Ising model on the square lattice and discovered that as a function of the variable $s = \sinh 2E/k_B T$ the susceptibility has a dense set of singularities on the circle $|s| = 1$ which is the same location as the thermodynamic limit of the locus of zeros of the finite lattice partition function. From this Nickel concluded that the curve of zeros is a natural boundary of the susceptibility in the complex s plane. This is a phenomenon of analysis not seen in any previously solved statistical system. Further study of this new phenomenon has been made by Orrick, Nickel, Guttmann and Perk [177] and in [69] the phenomenon of the natural boundary was studied on the triangular lattice. However the implication of these results for other models has not been investigated.

The hard square and hard hexagon models can be obtained from the Ising model in a magnetic field H in the limit $H \to \infty$ for the square and triangular lattices respectively, and thus it is natural to study the question of analyticity in these two models. However, unlike the Ising model at $H = 0$ where both the square and triangular lattices have been exactly solved, the hard hexagon model is exactly solved [22, 29, 30, 27] whereas the hard square model is not. Thus, the comparison of these two models is the ideal place to study the relation of integrability to the analyticity properties of the free energy in the complex plane.

Three different methods may be used to study the non-integrable hard square model: Series expansions of the free energy in the thermodynamic limit, transfer matrix eigenvalues for chains of finite size L_h and zeros of partition functions on the $L_v \times L_h$ lattices of finite size and arbitrary aspect ratio L_v/L_h.

Series expansions of the partition function per site $\kappa(z)$ of the hard square model [98, 200, 26, 188, 70, 136] of up to 92 terms [70] and analysis of transfer matrix eigenvalues [188] for chains of up to 34 sites [105] show that $\kappa(z)$ has a singularity on the positive z-axis [105]

$$z_c = 3.79625517391234(4) \tag{6.1}$$

and a singularity on the negative z-axis [106, 127]

$$z_d = -0.119338886(5) \tag{6.2}$$

The hard hexagon model has two singular points at [22, 29, 30, 27]

$$z_{c;hh} = \frac{11+5\sqrt{5}}{2} = 11.09016\cdots$$
$$z_{d;hh} = \frac{11-5\sqrt{5}}{2} = -0.09016\cdots \tag{6.3}$$

For hard squares, series expansions [98, 200, 26, 188, 70, 136] have been used to estimate the leading critical exponents at z_c and z_d, and correction to scaling exponents have been estimated as well. For hard hexagons there are no singular points of the free energy other than $z_{c;hh}$, $z_{d;hh}$, ∞. It is not known if there are any further singular points for hard squares. In [105] the singularity at z_c is determined to be in the Ising universality class and in [127] the first two exponents at z_d are shown to agree with those of the Lee-Yang edge and hard hexagons. However these long series expansions have not given information about additional higher order singularities at z_c and z_d or singularities which may occur at other values of z.

In 2005 a very remarkable property of hard squares, which is not shared by hard hexagons, was discovered [90] by means of studying the eigenvalues of the transfer matrix for finite size systems [90, 130, 131, 132, 4, 25]. These studies discovered that at the value of the fugacity $z = -1$ all eigenvalues of the transfer matrix with cylindrical boundary conditions have unit modulus and the partition function of the $L_h \times L_v$ lattice with toroidal boundary conditions depends on divisibility properties of L_v and L_h. However, the free energy for these boundary conditions in the thermodynamic limit is zero. For the lattice oriented at 45^o, on the other hand, for cylindrical boundary conditions of the transfer matrix, there are some eigenvalues which do not have unit modulus [131] and for free boundary conditions of the transfer matrix with $L_h \equiv 1 \pmod 3$ all roots of the characteristic equation are zero and thus the partition function vanishes.

In [10] we computed for hard hexagons the zeros of the partition function for $L\times L$ lattices with cylindrical and toroidal boundary conditions as large as 39×39 and the eigenvalues of the transfer matrix with cylindrical boundary conditions. For these cylindrical transfer matrices both momentum and parity are conserved, and for physical (positive) values of z the maximum eigenvector is in the sector of zero momentum positive parity $P = 0^+$. From these cylindrical transfer matrices we computed the equimodular curves where there are two eigenvalues of the row transfer matrix of (equal) maximum modulus both in the sector $P = 0^+$ and for the full transfer matrix.

In this paper we extend our study of partition function zeros and transfer matrix equimodular curves to hard squares for systems as large as 40×40 and compare them with corresponding results for hard hexagons [10]. There are many differences between these two systems which we analyze in detail. In addition to the transfer matrix with cylindrical boundary conditions we also introduce the transfer matrix with free boundary conditions. Thus we are able to give two different transfer matrix descriptions for the partition function zeros of the cylindrical lattice. For hard hexagons there is strong evidence that this boundary condition preserves integrability.

In section 6.2 we recall the relation between finite size computations in the complex plane of zeros of $L \times L$ lattices and eigenvalues of the L site transfer matrix. In section 6.3 we make a global comparison in the complex z plane of the equimodular curves and partition function zeros of hard squares with hard hexagons. In section 6.4 we make a more refined comparison on the negative z axis.

The comparisons presented in sections 6.3 and 6.4 reveal many significant differences between hard squares and hard hexagons which we discuss in detail in section 6.5. We conclude in section 6.6 with a presentation of potential analyticity properties of hard squares which can be different from hard hexagons.

In 6.A we tabulate the factored characteristic polynomials of the transfer matrix at the point $z = -1$ and the multiplicity of the eigenvalue $+1$. We also give formulas for the growth of the orders of the transfer matrices, where such a formula is known, and for all cases the asymptotic growth is given by $N_G^{L_h}$ where N_G is the golden ratio.

In 6.B we consider the partition function values at $z = -1$ on $L_v \times L_h$ lattices for the torus, cylinder, free-free rectangle, Möbius band and Klein bottle boundary conditions. We give generating functions for the sequences of values of the partition function of the $L_v \times L_h$ lattice as a function of L_v and find that almost all sequences of values are repeating. We conjecture that along the periodic L_v direction (including twists for the Möbius band and Klein bottle cases) the sequences will always be repeating. Furthermore, for the torus and the cylinder (along the periodic L_v direction), we conjecture that the generating functions are given by the negative of the logarithmic derivative of the characteristic polynomial of their transfer matrices at $z = -1$. This allows us to conjecture the periods of their repeating sequences. Finally, for the Möbius band (along the periodic L_v direction) and Klein bottle we conjecture that their generating functions are the logarithmic derivative of products of factors $(1 - x^{n_i})^{m_j}$, where $n_i,\ m_j$ are integers.

6.2 Formulation

The hard square lattice gas is defined by a (occupation) variable $\sigma = 0, 1$ at each site of a square lattice with the restriction that no two adjacent sites can have the values $\sigma = 1$ (i.e. the gas has nearest neighbor exclusion). The grand partition function on the finite $L_v \times L_h$ lattice is defined as the polynomial

$$Z_{L_v,L_h}(z) = \sum_{n=0} z^n g(n; L_v, L_h). \tag{6.4}$$

where $g(n; L_v, L_h)$ is the number of hard square configurations which have n occupied sites. These polynomials can be characterized by their zeros z_j as

$$Z_{L_v,L_h}(z) = \prod_j (1 - z/z_j), \tag{6.5}$$

where z_j and the degree of the polynomial will depend on the boundary condition imposed on the lattice. This formulation of the partition function as a polynomial is completely general for lattice models with arbitrary interactions.

The partition function for hard squares may also be expressed in terms of the transfer matrix formalism. For the cylindrical transfer matrix with periodic boundary conditions in the horizontal direction, the transfer matrix for hard squares is defined as

$$T_{C\{b_1,\cdots b_{L_h}\},\{a_1,\cdots .a_{L_h}\}}(z;L_h) \;=\; \prod_{j=1}^{L_h} W(a_j,\, a_{j+1};\, b_j,\, b_{j+1}), \tag{6.6}$$

where the local Boltzmann weights $W(a_j, a_{j+1}; b_j, b_{j+1})$ for hard squares of figure 6.1 may be written as

$$W(a_j, a_{j+1}; b_j, b_{j+1}) = 0 \;\text{ for }\; a_j a_{j+1} = a_{j+1} b_{j+1} = b_j b_{j+1} = a_j b_j = 1 \tag{6.7}$$

with $a_{L_h+1} \equiv a_1,\; b_{L_h+1} \equiv b_1$ and otherwise

$$W(a_j, a_{j+1}; b_j, b_{j+1}) = z^{b_j}. \tag{6.8}$$

For the transfer matrix with free boundary conditions

$$T_{F\{b_1,\cdots b_{L_h}\},\{a_1,\cdots .a_{L_h}\}}(z;L_h) = \left(\prod_{j=1}^{L_h-2} W(a_j,\, a_{j+1};\, b_j,\, b_{j+1})\right) W_F(a_{L_h-1}, a_{L_h}; b_{L_h-1}, b_{L_h}), \tag{6.9}$$

where

$$W_F(a_{L_h-1}, a_{L_h}; b_{L_h-1}, b_{L_h}) = z^{b_{L_h-1}+b_{L_h}}. \tag{6.10}$$

The corresponding transfer matrices for hard hexagons are obtained by supplementing (6.7) with

$$W(a_j, a_{j+1}; b_j, b_{j+1}) = 0 \;\text{ for }\; a_{j+1} b_j = 1. \tag{6.11}$$

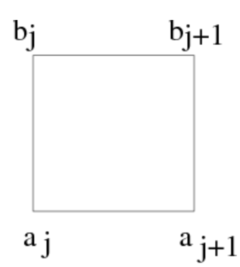

Figure 6.1: Boltzmann weights for the transfer matrix of hard squares

We will consider four types of boundary conditions.

The grand partition function for $L_v \times L_h$ lattices with periodic boundary conditions in both the L_v and L_h directions is given in terms of T_C as

$$Z^{CC}_{L_v,L_h}(z) \quad = \quad \mathrm{Tr}\ T_C^{L_v}(z; L_h). \tag{6.12}$$

For free boundary conditions in the horizontal direction and periodic boundary conditions the vertical direction the partition function is obtained from T_F as

$$Z^{CF}_{L_v,L_h}(z) \quad = \quad \mathrm{Tr}\ T_F^{L_v}(z; L_h). \tag{6.13}$$

For periodic boundary conditions in the horizontal direction and free boundary conditions the vertical direction the partition function is obtained from T_C as

$$Z^{FC}_{L_v,L_h}(z) = \langle \mathbf{v}_B | T_C^{L_v-1}(z; L_h) | \mathbf{v}'_B \rangle, \tag{6.14}$$

where $\mathbf{v}_B$ and $\mathbf{v}'_B$ are suitable vectors for the boundary conditions on rows 1 and L_v. For the transfer matrix (6.6) with Boltzmann weights given by the asymmetrical form (6.7), (6.8) the components of the vectors $\mathbf{v}_B$ and $\mathbf{v}'_B$ for free boundary conditions are

$$\mathbf{v}_B(a_1, a_2, \cdots, a_{L_h}) = \prod_{j=1}^{L_h} z^{a_j}, \qquad \mathbf{v}'_B(b_1, b_2, \cdots, b_{L_h}) = 1. \tag{6.15}$$

These vectors are invariant under translation and reflection.

For free boundary conditions in both directions

$$Z^{FF}_{L_v,L_h}(z) = \langle \mathbf{v}_B | T_F^{L_v-1}(z; L_h) | \mathbf{v}'_B \rangle, \tag{6.16}$$

When the transfer matrix is diagonalizable (6.12)-(6.16) may be written in terms of the eigenvalues λ_k and eigenvectors $\mathbf{v}_k$ of the transfer matrix

$$Z^{CC}_{L_v,L_h}(z) = \sum_k \lambda^{L_v}_{k;C}(z; L_h), \tag{6.17}$$

$$Z^{CF}_{L_v,L_h}(z) = \sum_k \lambda^{L_v}_{k:F}(z; L_h), \tag{6.18}$$

$$Z^{FC}_{L_v,L_h}(z) = \sum_k \lambda^{L_v-1}_{k;C}(z; L_h) \cdot d_{C,k} \ \text{ where } \ d_{C,k} = (\mathbf{v_B} \cdot \mathbf{v_{C,k}})(\mathbf{v_{C,k}} \cdot \mathbf{v'_B}), \tag{6.19}$$

$$Z^{FF}_{L_v,L_h}(z) = \sum_k \lambda^{L_v-1}_{k;F}(z; L_h) \cdot d_{F,k} \ \text{ where } \ d_{F,k} = (\mathbf{v_B} \cdot \mathbf{v_{F,k}})(\mathbf{v_{F,k}} \cdot \mathbf{v'_B}). \tag{6.20}$$

For hard squares and hard hexagons the transfer matrices $T_C(z; L_h)$ are invariant under translations and reflections and thus momentum P and parity $\pm$ are good quantum numbers. Furthermore the boundary vectors $\mathbf{v}_B$ and $\mathbf{v}'{}_B$ of (6.15) are invariant under translation and reflection, and consequently $d_{C,k} = 0$ unless the eigenvectors $\mathbf{v}_k$ lie in the positive parity sector $P = 0^+$.

For hard squares the matrix $T_F(z; L_h)$ is invariant under reflection so the eigenvectors in the scalar products are restricted to positive parity states. However for hard hexagons $T_F(z; L_h)$ is not invariant under reflection and all eigenvectors will contribute to (6.20).

Note that partition function zeros for all four boundary conditions have previously been studied for antiferromagnetic Potts models [220, 194, 36, 216, 222, 221, 217, 223, 76, 78, 74, 75, 77, 79, 210, 122, 125, 123, 124]. In that case the relations to transfer matrix eigenvalues were similar to (6.19),(6.20). However, with periodic boundary conditions along the transfer direction the partition function was defined as a Markov trace, and (6.17),(6.18) were replaced by expressions involving non-trivial eigenvalue multiplicities [189, 190].

6.2.1 Integrability

To compare integrable with non-integrable systems a definition of integrability is required.

The notion of integrability originates in the discovery by Baxter that the Ising model and the 6 and 8 vertex models, which have transfer matrices that depend on several variables, have a one parameter subspace for which the transfer matrices with different parameters will commute if cyclic boundary conditions are imposed [29, 30]. This global property of the transfer matrix follows from a local property of the Boltzmann weights used to construct the transfer matrix, known as the star-triangle or the Yang-Baxter equation.

The hard hexagon model has only one parameter, the fugacity, but is also referred to as integrable because Baxter [22, 29, 30] found that it may be realized as a special case of the model of hard squares with diagonal interactions which does have a one parameter family of commuting transfer matrices with cylindrical boundary conditions.

This concept of integrability has been generalized to transfer matrices with boundary conditions which are not cylindrical if special boundary conditions are imposed which satisfy a generalization of the Yang-Baxter equation [82, 83, 224] known as the boundary Yang-Baxter equation. This has been investigated for models closely related to hard hexagons [31, 5] but the specialization to hard hexagons with free boundary conditions has apparently not been made.

6.2.2 The physical free energy

For thermodynamics we are concerned with the limit $L_v,\ L_h \to \infty$, and in the physical region where z is real and positive the partition function per site $\kappa(z)$, the physical free energy $F(z)$ and the density $\rho(z)$ are defined as limits of the finite size grand partition function as

$$\kappa(z) = \lim_{L_v, L_h \to \infty} Z_{L_v,L_h}(z)^{1/L_v L_h}, \tag{6.21}$$

$$-F(z)/k_B T = \lim_{L_v, L_h \to \infty} (L_v L_h)^{-1} \cdot \ln Z_{L_v,L_h}(z) \tag{6.22}$$

and

$$\rho(z) = -z\frac{d}{dz}F(z). \tag{6.23}$$

This limit must be independent of the boundary conditions and aspect ratio $0 < L_v/L_h < \infty$ for thermodynamics to be valid. The free energy vanishes and is analytic at $z = 0$. For hard hexagons as $z \to \infty$

$$F(z)/k_BT = \frac{1}{3}\ln z + \tilde{F}_{HH}(z) \;\; \text{and} \;\; \rho(z) \to \frac{1}{3} \tag{6.24}$$

and for hard squares

$$F(z)/k_BT = \frac{1}{2}\ln z + \tilde{F}_{HS}(z) \;\; \text{and} \;\; \rho \to \frac{1}{2}, \tag{6.25}$$

where $\tilde{F}_{HH}(z)$ and $\tilde{F}_{HS}(z)$ are analytic at $z \to \infty$. From this formulation series expansions of the free energy about both $z = 0$ and $1/z = 0$ are derived. The partition function per site, physical free energy and density for $0 \leq z \leq z_c$ and $z_c \leq z \leq \infty$ are different functions which are not related to each other by analytic continuation around the singularity at z_c. For hard hexagons the density for both the low and the high density regime may be continued to the full z plane which for low density is cut from $-\infty \leq z \leq z_{d;hh}$ and $z_{c;hh} \leq z \leq \infty$ and for high density cut from $z_{d;hh} \leq z \leq z_{c;hh}$. Indeed, both the low and high density partition functions per site and the density for hard hexagons are algebraic functions [133, 10] and thus have analytic continuations even beyond the cuts in the z plane.

To study the possibility of analytic continuation for hard squares of the physical partition function per site and density from the positive z axis into the complex z plane we consider both the formulation in terms of the transfer matrix and the zeros of the partition function.

6.2.3 Analyticity and transfer matrix eigenvalues

For $0 < z < \infty$ all matrix elements of the transfer matrices are positive so the Perron-Frobenious theorem guarantees that the largest eigenvalue $\lambda_{\max}$ is positive and the corresponding eigenvector has all positive entries. Thus for all cases

$$\lim_{L_v \to \infty} L_v^{-1} \cdot \ln Z_{L_v,L_h}(z) \;\; = \;\; \ln \lambda_{\max}(z; L_h) \tag{6.26}$$

and thus the free energy is

$$-F/k_BT = \lim_{L_h \to \infty} L_h^{-1} \ln \lambda_{\max}(z; L_h). \tag{6.27}$$

Furthermore the cylindrical transfer matrices for both squares and hexagons have translation and reflection invariance. Therefore the eigenvalues of the lattice translation operator are e^{iP} where P, the total momentum, has the values $2\pi n/L_h$, and the eigenvalues of the reflection operator are ± 1. Each transfer matrix eigenvalue has a definite value of P and parity and $\lambda_{\max}$ has $P = 0^+$ (where + indicates the reflection eigenvalue). Therefore for $0 \leq z \leq \infty$ the eigenvalue $\lambda_{\max}$ of the transfer matrix T_C is the eigenvalue of an eigenvector in the sector $P = 0^+$.

To obtain the analytic continuation of the density from the positive z axis into the complex z plane we need to continue the limit as $L_h \to \infty$ of the eigenvalue with $P = 0^+$ which is maximum on the positive axis. However, the analytic continuation of $\lambda_{\max}$ off of the segment $0 \leq z \leq \infty$ will not, of course, have the largest modulus in the entire complex z plane. The analytic continuation of $\lambda_{\max}$ will be maximum only as long as it has the largest modulus of all the eigenvalues and ceases to be maximum when z crosses an equimodular curve where the moduli of two (or more) eigenvalues are the same. It is thus of importance to determine the thermodynamic limit of the equimodular curves of the largest eigenvalues of the transfer matrix. In the thermodynamic limit the regions of $0 \leq z \leq z_c$ and $z_c \leq z \leq \infty$ are separated by one or more of these equimodular curves. In [10] it was seen that for hard hexagons with finite L_h the equimodular curves separate the z plane into several regions. However, because the eigenvectors with different momentum and parity lie in different subspaces only the eigenvalues corresponding to eigenvectors with $P = 0^+$ can affect the analytic continuation of the density.

For the hard square transfer matrix with free boundary conditions, $T_F(z; L_h)$, the eigenvalue $\lambda_{\max}$ will lie in the positive parity sector for positive z and the analytic continuation off the positive real axis will be constrained to eigenvalues in the positive parity sector. For hard hexagons, where $T_F(z; L_h)$ is not reflection symmetric, $\lambda_{\max}$ is not constrained to lie in a restricted sub-space.

It is thus clear from the formulation of the physical free energy and the density in terms of the transfer matrix that the process of analytic continuation off of the positive z axis and the taking of the thermodynamic limit do not commute. In the thermodynamic limit it is not even obvious that for a non-integrable model an analytic continuation through the limiting position of the equimodular curves is possible.

6.2.4 Analyticity and partition function zeros

The considerations of analytic continuation in terms of partition function zeros is slightly different because by definition polynomials are single valued. However, once the thermodynamic limit is taken the limiting locations of the zeros will in general divide the complex z plane into disconnected zero free regions. For hard squares and hard hexagons the physical segments $0 \leq z < z_c$ and $z_c < z < \infty$ lie in two separate zero free regions. The density is uniquely continuable into the zero free region and in these regions the free energy will be independent of boundary conditions and aspect ratio. For hard hexagons the density for both the low and high density cases are further continuable beyond the zero free region into the respective cut planes of section 6.2.2. However, for hard squares there is no guarantee that further continuation outside the zero free regions is possible.

6.2.5 Relation of zeros to equimodular curves

For finite lattices the partition function zeros can be obtained for $Z^{CC}_{L_v,L_h}(z)$ and $Z^{CF}_{L_v,L_h}(z)$ from (6.17) and (6.18) if all eigenvalues are known. For $Z^{FC}_{L_v,L_h}(z)$ and $Z^{FF}_{L_v,L_h}(z)$ both the eigenvalues and eigenvectors are needed to obtain the zeros from (6.19) and (6.20).

The limiting case where

$$L_v \;\to\; \infty \qquad \text{with fixed} \qquad L_h, \tag{6.28}$$

is presented in [210, 122, 125, 123, 124],[246, 248, 23] with various boundary conditions extending the work of [34, 35, 32]. In this limit (6.28) the partition function will have zeros when two or more maximum eigenvalues of $T(z; L_h)$ have equal moduli

$$|\lambda_1(z; L_h)| \;=\; |\lambda_2(z; L_h)|. \tag{6.29}$$

Consider first $Z^{CC}_{L_v,L_h}(z)$ and $Z^{CF}_{L_v.L_h}(z)$ where we see from (6.17) and (6.18) that only eigenvalues are needed. Thus, for these two cases, when only two largest eigenvalues $\lambda_{1,2}$ need to be considered we may write

$$Z_{L_v,L_h}(z) = \lambda_1^{L_v}\left[1 + \left(\frac{\lambda_2}{\lambda_1}\right)^{L_v} + \cdots\right]. \tag{6.30}$$

Then at values of z where $|\lambda_1| = |\lambda_2|$ with $\lambda_2/\lambda_1 = e^{i\theta}$ we have for large L_v

$$Z_{L_v,L_h}(z) = \lambda_1^{L_v}[1 + e^{i\theta L_v} + \cdots] \tag{6.31}$$

and hence $Z_{L_v,L_h}(z)$ will have a zero close to this z when

$$e^{i\theta L_v} = -1, \tag{6.32}$$

that is when

$$\theta L_v = (2n + 1)\pi \tag{6.33}$$

with n an integer. This relation becomes exact in the limit $L_v \to \infty$. Calling z_i and z_{i+1} the values of z at two neighboring zeros on the equimodular curve we thus obtain from (6.33)

$$\theta(z_{i+1}) - \theta(z_i) = 2\pi/L_v. \tag{6.34}$$

Let $s(z)$ be the arclength along an equimodular curve. Then the derivative of $\theta(s(z))$ with respect to s is defined as the limit of

$$\frac{\Delta\theta}{\Delta s} \equiv \frac{\theta(s(z_{i+1})) - \theta(s(z_i))}{s(z_{i+1}) - s(z_i)}, \tag{6.35}$$

Thus, defining the density of roots on the equimodular curve as

$$D(s) = \lim_{L_v \to \infty} \frac{1}{L_v[s(z_{i+1}) - s(z_i)]}, \tag{6.36}$$

we find from (6.34) and (6.35) that for $L_v \to \infty$ with L_h fixed that the density of zeros on an equimodular curve is

$$\frac{d\theta(s)}{ds} = 2\pi D(s). \tag{6.37}$$

For $Z^{FC}_{L_v,L_h}(z)$ and $Z^{FF}_{L_v,L_h}(z)$ from (6.19) and (6.20) we have instead of (6.30)

$$Z_{L_v,L_h}(z) = \lambda_1^{L_v} d_1 \left[1 + \left(\frac{\lambda_2}{\lambda_1} \right)^{L_v} \frac{d_2}{d_1} + \cdots \right], \tag{6.38}$$

with

$$\frac{d_2}{d_1} = re^{i\psi}, \tag{6.39}$$

where in general $r \neq 1$. Thus writing

$$\frac{\lambda_2}{\lambda_1} = \epsilon e^{i\theta}, \tag{6.40}$$

the condition for a zero in the limit $L_v \to \infty$ which generalizes (6.32) is

$$\epsilon^{L_v} e^{i\theta L_v} re^{i\psi} = -1, \tag{6.41}$$

from which we obtain

$$\epsilon = r^{-1/L_v} = e^{-\ln r/L_v} \sim 1 - \frac{\ln r}{L_v}, \tag{6.42}$$

$$\theta L_v + \psi = (2n+1)\pi. \tag{6.43}$$

Thus as $L_v \to \infty$ the locus of zeros approaches the equimodular curve as $\ln r/L_v$ and the limiting density is still given by (6.37).

These considerations, however, are in general not sufficient for the study of the thermodynamic limit where instead of (6.28) we are interested in the limit

$$L_v \to \infty, \quad L_h \to \infty, \quad \text{with fixed } L_v/L_h \tag{6.44}$$

and the physical free energy must be independent of the aspect ratio L_v/L_h.

To study the limit (6.44) there are several properties of the dependence of the equimodular curves on L_h which need to be considered:

1. The derivative of the phase $\theta(s)$ on a curve can vanish as $L_h \to \infty$ on some portions of the curve;

2. The number of equimodular curves can diverge as $L_h \to \infty$ and there can be regions in the z plane where they become dense;

3. The length of an equimodular curve can vanish as $L_h \to \infty$.

The first of these properties is illustrated for hard hexagons in [10]. The second and third properties have been observed for antiferromagnetic Potts models in [73].

We will see that all three phenomena are present for hard squares. The roots of the $L \times L$ partition function in the limit $L \to \infty$ converge to lie on the $L_h \to \infty$ limit of the equimodular curves.

6.3 Global comparisons of squares and hexagons

In [10] we computed for hard hexagons the zeros for $L \times L$ lattices of $Z^{CC}_{L,L}(z)$ for toroidal boundary conditions, and for cylindrical boundary conditions where

$$Z^{FC}_{L,L}(z) = Z^{CF}_{L,L}(z). \tag{6.45}$$

We also computed the equimodular curves for both the full transfer matrix $T_C(z; L_h)$ relevant to $Z^{CC}_{L_v,L_h}(z)$ and the restriction to the subspace $P = 0^+$ relevant for $Z^{FC}_{L_v,L_h}(z)$. In this paper we compute the same quantities for hard squares and compare them with the results of [10]. We also compute the equimodular curves for $T_F(z; L_h)$ relevant for $Z^{CF}_{L_v,L_h}(z)$ and $Z^{FF}_{L_v,L_h}(z)$. For hard hexagons we restricted attention to $L_v,\ L_h$ multiples of three which is commensurate with hexagonal ordering. Similarly for hard squares we restrict attention here to $L_v,\ L_h$ even to be commensurate with square ordering.

6.3.1 Comparisons of partition function zeros

We have computed zeros of the hard square partition function in the complex fugacity z plane for $L \times L$ lattices with cylindrical and free boundary conditions for $L \leq 40$ and for toroidal boundary conditions for $L \leq 26$ using the methods of [10]. In figure 6.2 we compare partition function zeros for cylindrical boundary conditions of hard squares on the 40×40 lattice with hard hexagons on the 39×39 lattice and in figure 6.4 the comparison is made for free boundary conditions. In figure 6.3 we compare for toroidal boundary conditions hard squares on the 26×26 lattice with hard hexagons on the 27×27 lattice.

For both hard squares and hard hexagons there is a line of zeros on the negative real axis ending at z_d and $z_{d;hh}$, respectively. The ratio of real roots to complex roots for hard squares is roughly 1/2:1/2 while for hard hexagons the ratio is roughly 2/3:1/3.

The most obvious difference between hard squares and hard hexagons in figures 6.2-6.4 is that the zeros of hard squares are seen to lie in an area instead of being confined to a few well defined curves as is seen for hard hexagons.

For cylindrical boundary conditions the filling up of this area proceeds in a remarkably regular fashion.

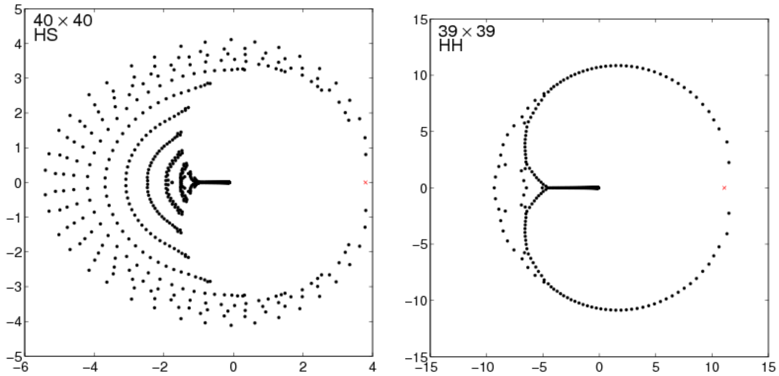

Figure 6.2: Comparison in the complex fugacity plane z of the zeros of the partition function $Z^{FC}_{L,L}(z) = Z^{CF}_{L,L}(z)$ with cylindrical boundary conditions of hard squares on the 40×40 lattice on the left to hard hexagons on the 39×39 lattice on the right. The location of z_c and $z_{c;hh}$ is indicated by a cross.

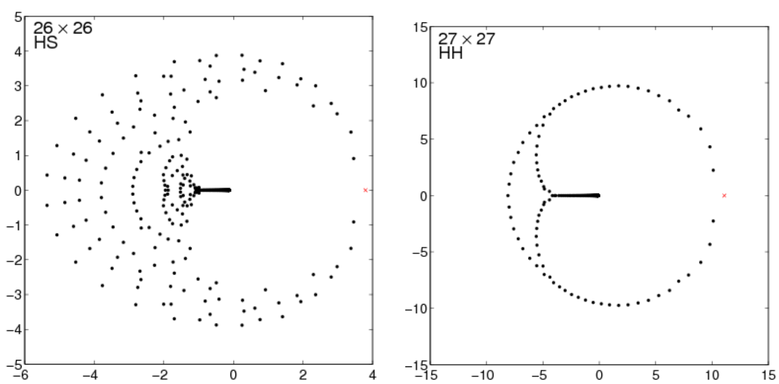

Figure 6.3: Comparison in the complex fugacity plane z of the zeros of the partition function $Z^{CC}_{L,L}(z)$ with toroidal boundary conditions of hard squares on the 26×26 lattice on the left to hard hexagons on the 27×27 lattice on the right.The location of z_c and $z_{c;hh}$ is indicated by a cross.

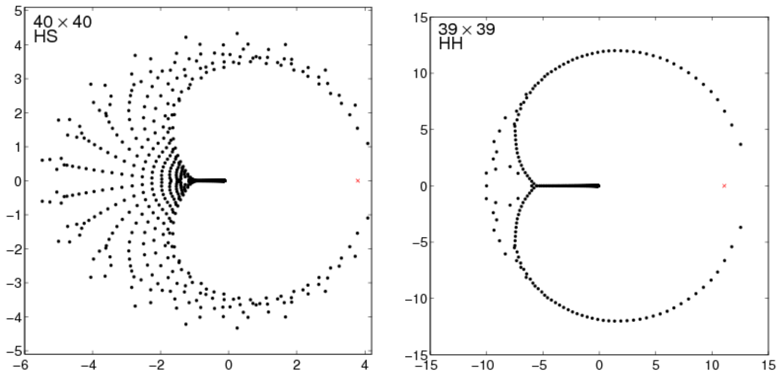

Figure 6.4: Comparison in the complex fugacity plane z of the zeros of the partition function $Z^{FF}_{L,L}(z)$ with free boundary conditions of hard squares on the 40×40 lattice on the left to hard hexagons on the 39×39 lattice on the right. The location of z_c and $z_{c;hh}$ is indicated by a cross.

For the lattices $4N \times 4N$ there are $N-1$ outer arcs each of $4N$ points, then there is a narrow arclike area with close to $4N$ zeros and finally there is an inner structure that is connected to $z = -1$. For the innermost of the $N-1$ arcs the zeros appear in well defined pairs.

For lattices $(4N+2) \times (4N+2)$ there are $N-1$ outer arcs each of $4N+2$ points, then a narrow arclike area which has close to $4N+2$ zeros and finally an inner structure that is connected to $z = -1$.

For all boundary conditions the zeros of hard squares appear to converge in the $L \to \infty$ limit to a wedge which hits the positive z axis at z_c. This is distinctly different from the behavior of hard hexagons where the zeros appear to approach $z_{c;hh}$ on a well defined one dimensional arc.

In figure 6.5 we illustrate the dependence on L of the hard square zeros of $Z^{FC}_{L,L}(z) = Z^{CF}_{L,L}(z)$ of the $L \times L$ lattice by giving a combined plot of all the zeros for $12 \leq L \leq 40$. This reveals that the three cases of $L = 6n+4,\ 6n+2$ and $6n$ approach the common limit in three separate ways. There is one well defined curve whose position does not depend on L which consists only of the points of $L = 6n+4$ lattices.

In table 6.1 we list the value of the zero closest to the three endpoints $z_c,\ z_d$ and -1 for the $L \times L$ cylindrical lattices with $24 \leq L \leq 40$. We also list the number N_L of zeroes in $-1 \leq z \leq z_d$ plus the number of zeroes $z < -1$. For $L = 40$ we note that $\mathrm{Re}[z_c(40)] > z_c$ whereas for $L \leq 38$ we have $\mathrm{Re}[z_c(L)] < z_c$. This behavior of $z_c(L)$ in relation to z_c is similar to what is seen for hard hexagons in table 5 of [10] where $\mathrm{Re}[z_c(L)] > z_c$ for $L \geq 21$ and only starts to approach z_c from the right for $L = 36$.

L	$z_c(L)$	$z_d(L)$	$z_{-1}(L)$	N_L
24	$3.690334 \pm i1.324109$	-0.119976	-0.956723	$128 + 0$
26	$3.718433 \pm i1.226238$	-0.119871	-0.979835	$153 + 5$
28	$3.739986 \pm i1.141529$	-0.119788	-0.986589	$176 + 0$
30	$3.756751 \pm i1.067554$	-0.119723	-0.991656	$201 + 5$
32	$3.769947 \pm i1.002431$	-0.119671	-0.992168	$231 + 1$
34	$3.780438 \pm i0.944686$	-0.119628	-0.989045	$259 + 9$
36	$3.788852 \pm i0.893150$	-0.119592	-0.976523	$288 + 0$
38	$3.795647 \pm i0.846884$	-0.119563	-0.994325	$325 + 9$
40	$3.801169 \pm i0.805129$	-0.119538	-0.991673	$358 + 0$
∞	3.796255	-0.119338	-1	

Table 6.1: The endpoints $z_c(L)$, $z_d(L)$ and $z_{-1}(L)$ for the $L \times L$ cylindrical lattices with $24 \leq L \leq 40$. The number of zeros N_L on the segment $-1 \leq z \leq z_d$ as well as the very small number of points $z \leq -1$ which do not contribute to the density.

6.3.2 Comparisons of equimodular curves with partition zeros

We have computed equimodular curves for the hard square transfer matrix $T_C(z; L_h)$ in the sector $P = 0^+$ for even $L_h \leq 26$ and for the full transfer matrix for $L_h \leq 18$. For hard squares we have computed the equimodular curves for the full $T_F(z; L_h)$ and the restriction to the positive parity sector for $L_h \leq 16$. For hard hexagons the equimodular curves of $T_C(z; L_h)$ were computed in [10] for $L_h \leq 21$ and in the sector $P = 0^+$ for $L_h \leq 30$. Equimodular curves for the hard hexagon transfer matrix $T_F(z; L_h)$ are computed here for $L_h \leq 21$.

In figure 6.6 we plot the equimodular curves and zeros for hard squares. This is to be compared with the similar plot for hard hexagons in figure 6.7. In both cases we note that the zeros for $Z^{FC}_{L,L}(z)$ and $Z^{CF}_{L,L}$ are identical while the corresponding equimodular curves are different.

The equimodular curves of hard squares are strikingly different from those of hard hexagons for all cases considered. The hard hexagon plots consist of a few well defined sets of curves which, with the exception that the curves for $P = 0^+$ do not have rays extending to infinity, are qualitatively very similar for all four cases. For hard squares, on the other hand, the four different plots are qualitatively different from each other and are far more complicated than those for hard hexagons.

The cylinder partition function $Z^{FC}_{L,L}(z) = Z^{CF}_{L,L}(z)$ allows a direct comparison between the equimodular curves of $T_F(z)$ and $T_{C0^+}(z)$ in figures 6.6 and 6.7, since both transfer matrices can be used to construct the same partition function. For both hard squares and hard hexagons these figures show that the zeros of the $L \times L$ cylindrical partition function lie much closer to the equimodular curves of $T_F(z)$ rather than T_{C0^+}. It is only for much larger aspect ratios that the cylinder zeros lie close to the T_{C0^+} equimodular curves, as can be seen, for example, in figure 6.8, where we plot the hard square $Z^{FC}_{26n,26}(z)$ roots for

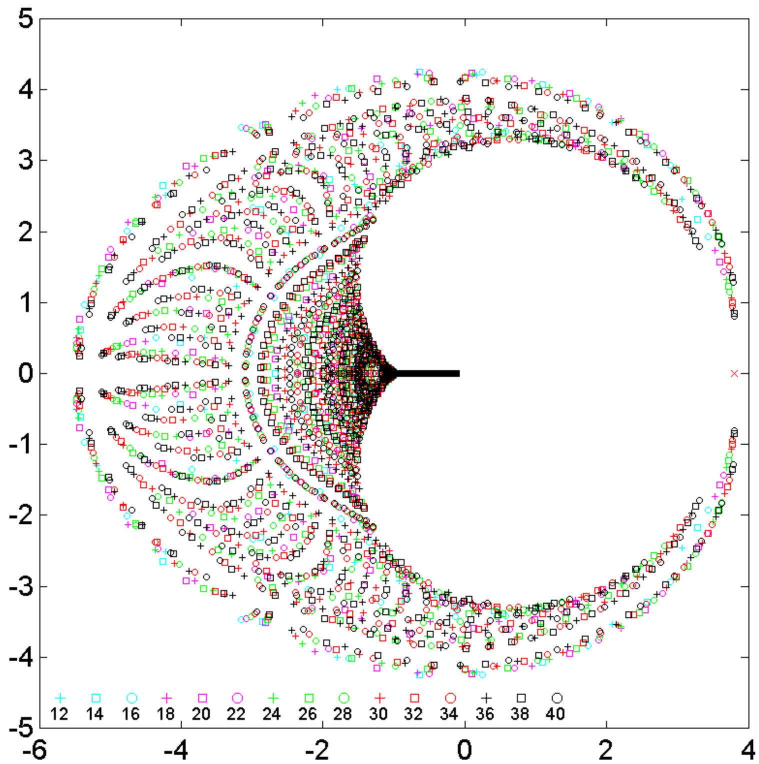

Figure 6.5: Combined plot of hard square zeros of $Z^{CF}_{L,L}(z) = Z^{FC}_{L,L}(z)$ for the $L \times L$ lattice with cylindrical boundary conditions for $12 \leq L \leq 40$. We exhibit a mod six effect by plotting $L = 6n + 4$ as circles, $L = 6n + 2$ as boxes and $L = 6n$ as crosses, The values of L_h are shown in the different colors indicated in the legend. It is to be noticed that there is a distinguished curve where only points $L = 6n + 4$ lie. The location of z_c is indicated by a cross.

$n = 1,\ 2,\ 3,\ 4,\ 5,\ 10$ along with the $L_h = 26$ equimodular curves of $T_{C0^+}(z)$.

For hard squares, the arclike structures noted above for figure 6.2 are in remarkable agreement with the $T_F(z)$ curves which originate near $z = -1$ and extend to infinity. There are L_h such equimodular curves which is exactly the number of points seen above to lie on each of the arclike structures of zeros.

For hard squares both $T_C(z; L_h)$ and $T_F(z; L_h)$ shown in figure 6.6 have equimodular curves which extend out to $|z| = \infty$. In 6.C we present an analytical argument that both the $T_C(z; L_h)$ and $T_F(z; L_h)$ curves have L_h branches going out to infinity at asymptotic angles $\arg z = \frac{(1+2k)\pi}{L_h}$ with $k = 0, 1, \ldots, L_h - 1$.

For hard hexagons it was seen in [10] that when $L_h \equiv 0 \pmod 3$ the curves for $T_C(z; L_h)$ as illustrated in figure 6.7 have $2L_h/3$ rays extending to infinity which separate regions with $P = 0^+$ from regions with $\pm 2\pi/3$. However, for the hard hexagon matrix $T_F(z; L_h)$ it is evident in figure 6.7 there is much more structure in the curves which extend to infinity.

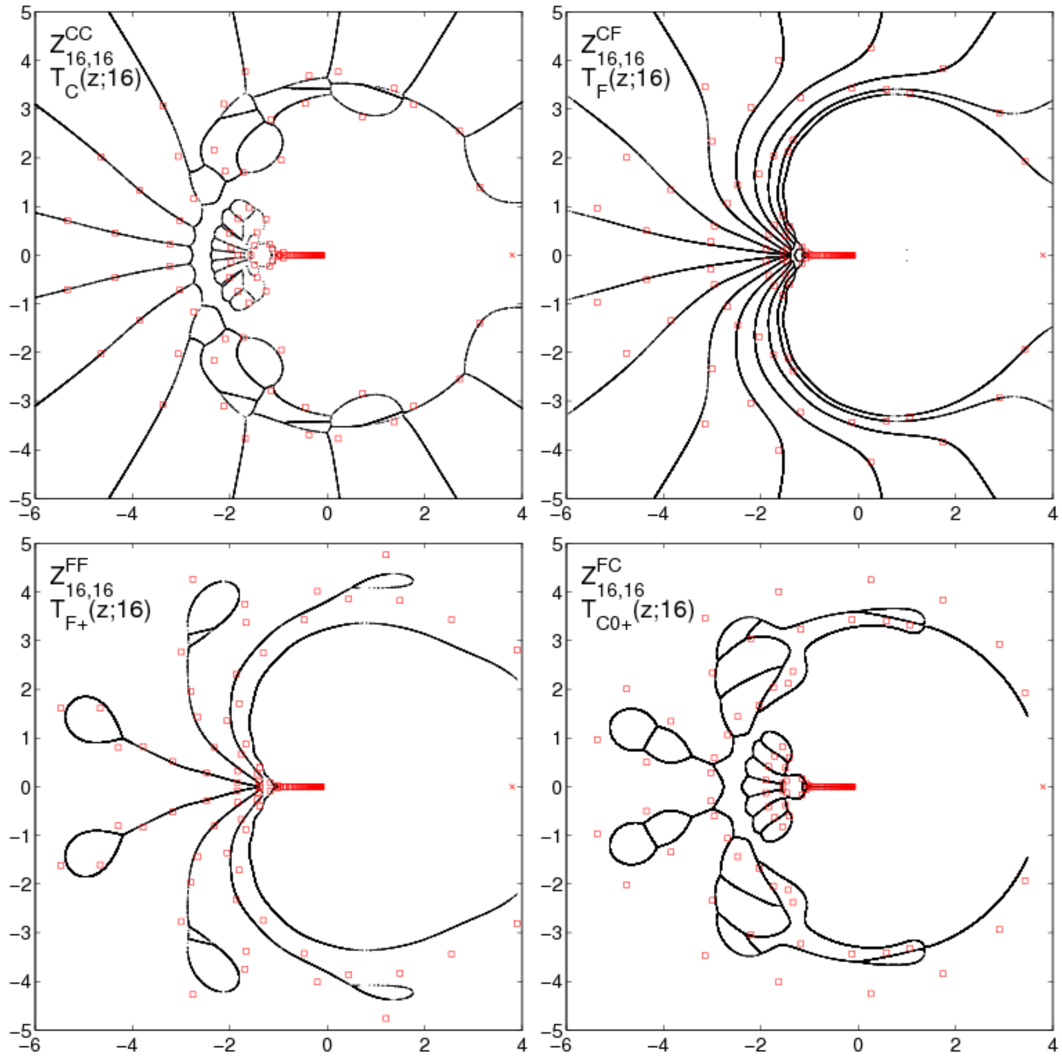

Figure 6.6: Comparison for hard squares of the three types of zeros and the 4 types of equimodular curves. Clockwise from the upper left we have for $L = 16$: $Z^{CC}_{L,L}(z)$ with $T_C(z; L)$, $Z^{CF}_{L,L}(z)$ with $T_F(z; L)$, $Z^{FC}_{L,L}(z)$ with $T_C(z; L)$ restricted to $P = 0^+$ and $Z^{FF}_{L,L}(z)$ with $T_F(z; L)$ restricted to positive parity. We note that the zeros of $Z^{FC}_{L,L}(z)$ and $Z^{CF}_{L,L}(z)$ are identical even though the equimodular curves are very different. The location of z_c is indicated by a cross.

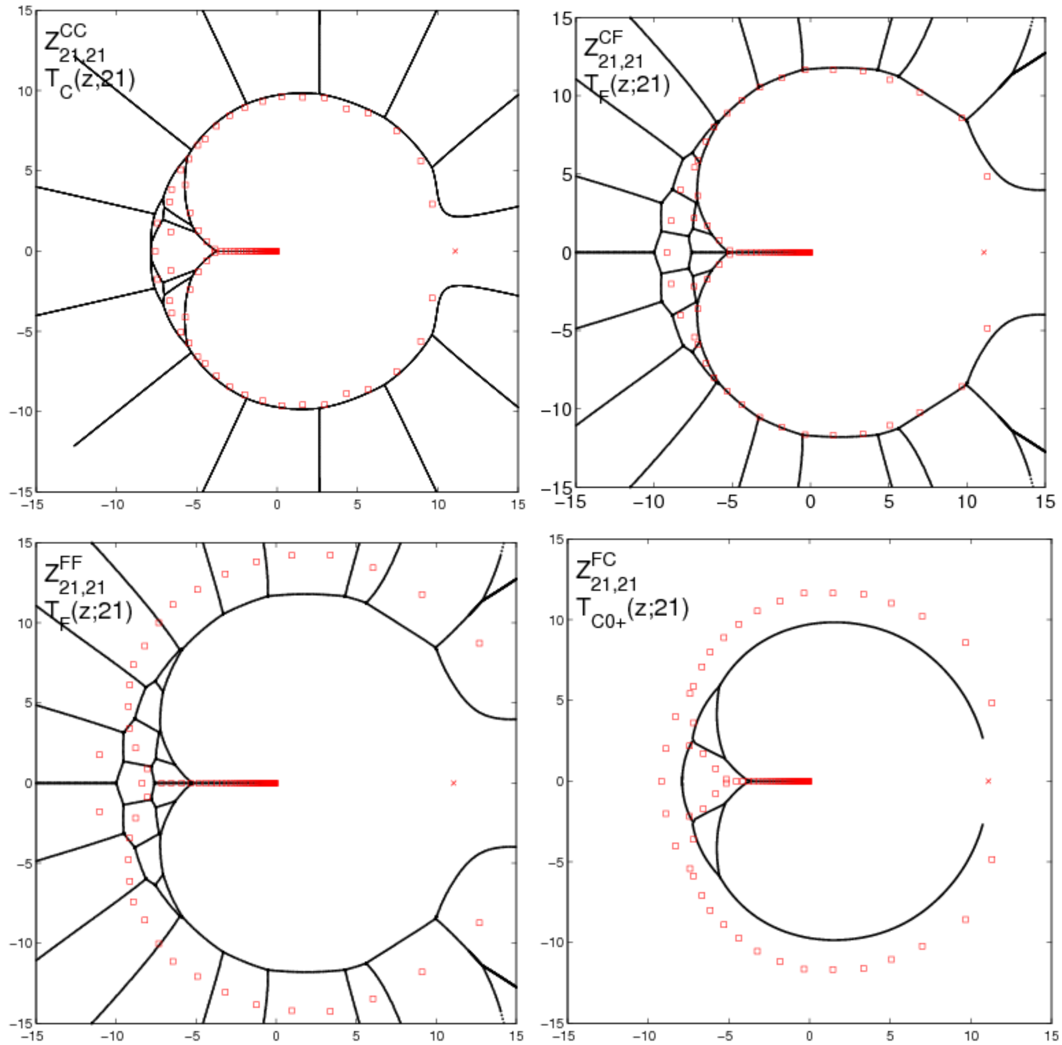

Figure 6.7: Comparison for hard hexagons of the three types of zeros and the 3 types of equimodular curves. Clockwise from the upper left we have for $L = 21$: $Z_{L,L}^{CC}(z)$ with $T_C(z; L)$, $Z_{L,L}^{CF}(z)$ with $T_F(z; L)$, $Z_{L,L}^{FC}(z)$ with $T_C(z; L)$ restricted to $P = 0^+$ and $Z_{L,L}^{FF}(z)$ with $T_F(z; L)$. We note that the zeros of $Z_{L,L}^{FC}(z)$ and $Z_{L,L}^{CF}(z)$ are identical even though the equimodular curves are very different. The location of $z_{c;hh}$ is indicated by a cross.

This is shown on a much larger scale in figure 6.9. This more complicated structure for the equimodular curves of $T_F(z;L_h)$ presumably results from the fact that for hard hexagons $T_F(z;L_h)$ is neither translation nor reflection invariant.

Just as for hard hexagons it is only possible for hard squares to identify an endpoint of an equimodular curve approaching z_c for the transfer matrix $T_C(z;L_h)$ in the $P=0^+$ sector. We give the location of the $z_c(L_h)$ and $z_d(L_h)$ endpoints for $P=0^+$ in table 6.2.

For hard squares the transfer matrix $T_F(z;L_h)$ with free boundary conditions is invariant under parity in contrast with hard hexagons where there is no parity invariance. The maximum eigenvalue for hard squares has positive parity and in figure 6.10 we compare for $L_h=16$ the equimodular curves of $T_F(z;L_h)$ with the restriction to positive parity. We also compare the equimodular curves for $L_h=16$ of $T_C(z;L_h)$ and its restriction to $P=0^+$.

L_h	$z_c(L_h)$ endpoint	$z_d(L_h)$ endpoint
4	$-0.8806 \pm i3.4734$	-0.1259
6	$1.6406 \pm i3.2293$	-0.1216
8	$2.5571 \pm i2.6694$	-0.1204
10	$2.9955 \pm i2.2264$	-0.1200
12	$3.2374 \pm i1.8961$	-0.1197
14	$3.3845 \pm i1.6461$	-0.1196
16	$3.479 \pm i1.4547$	
18	$3.544 \pm i1.3032$	
20	$3.591 \pm i1.1780$	
22	$3.627 \pm i1.0722$	
24	$3.654 \pm i0.9841$	
26	$3.675 \pm i0.9117$	
∞	3.796255	-0.119338

Table 6.2: The endpoints of the equimodular curves of $T_C(z;L_h)$ with $P=0^+$ which approach z_c and z_d as L_h increases. For $L_h \leq 14$ the endpoints are computed from the vanishing of the discriminant of the characteristic polynomial and have been computed to 50 decimal places. For $L_h \geq 16$ they are determined numerically to 3 decimal places and consequently the deviation from z_d is too small to be accurately determined.

6.4 Comparisons on $-1 \leq z \leq z_d$

A much more quantitative comparison of hard squares and hard hexagons can be given on the interval $-1 \leq z \leq z_d$. We treat both transfer matrix eigenvalues and partition function zeros.

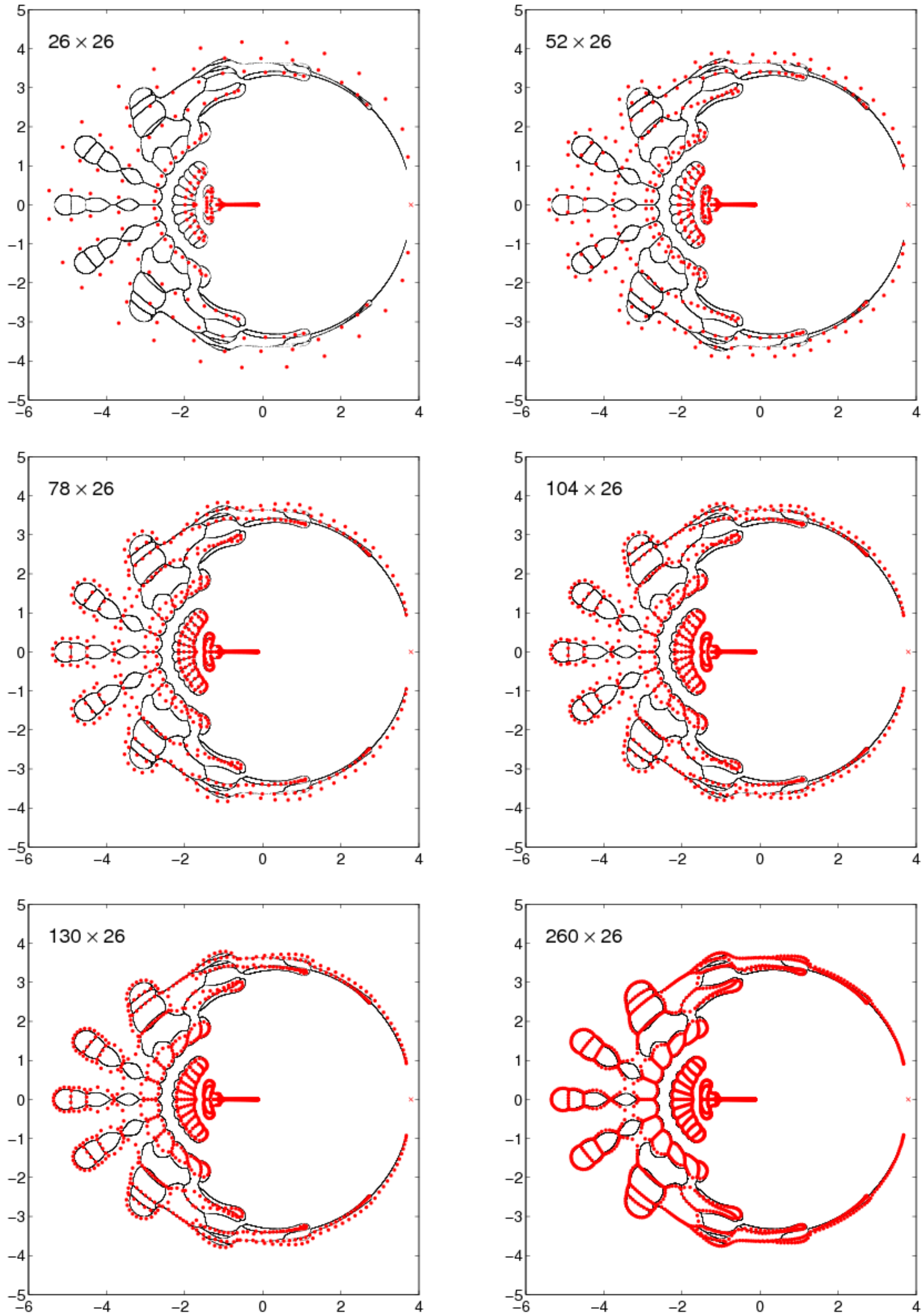

Figure 6.8: Plots in the complex fugacity z-plane of the zeros of the partition function $Z^{FC}_{L_v,L_h}(z)$ of hard squares for $L_v \times 26$ lattices with cylindrical boundary conditions (in red) compared with the $P = 0^+$ equimodular curves of $T_C(z; 26)$ (in black). The location of z_c is indicated by a cross.

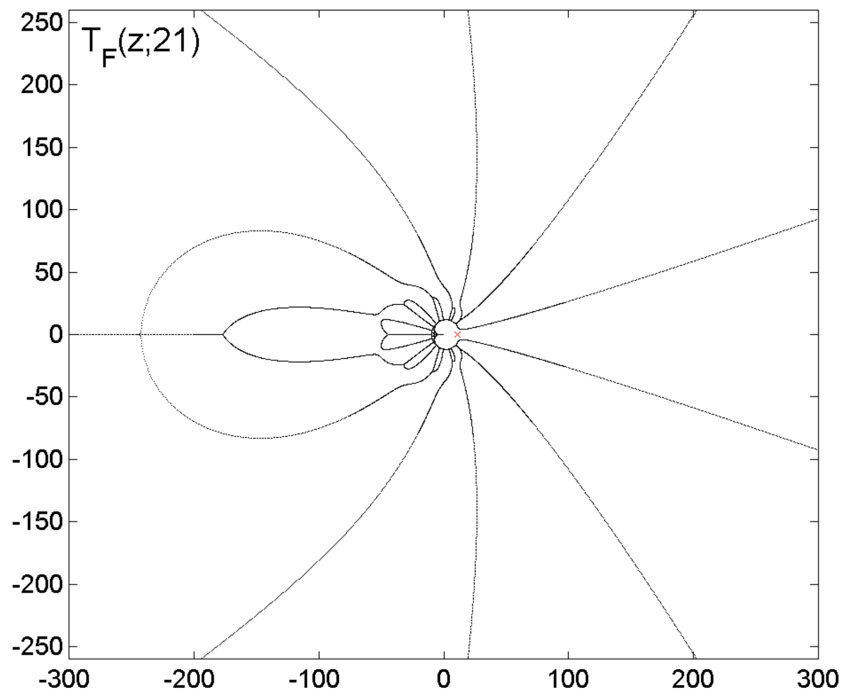

Figure 6.9: Equimodular curves for the hard hexagon transfer matrix $T_F(z; L_h)$ for $L_h = 21$ showing the complex structure which exists for $|z| \geq 12$. The location of z_c is indicated by a cross.

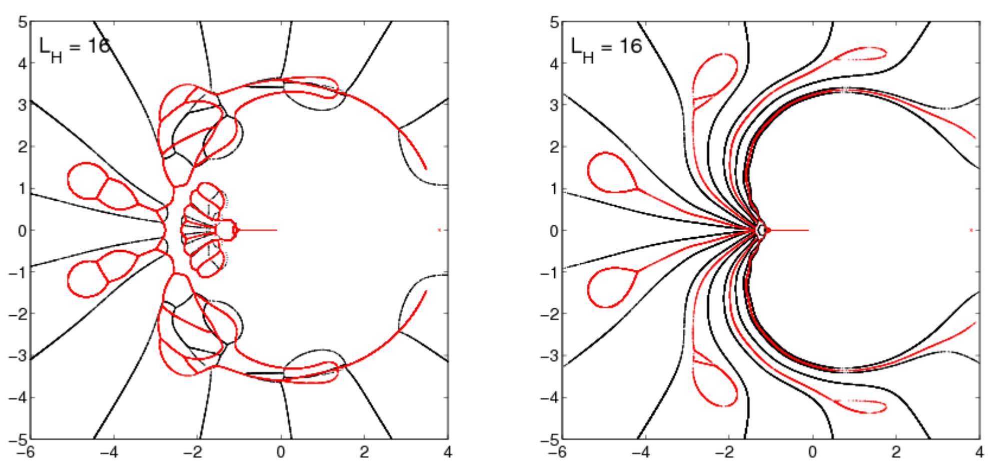

Figure 6.10: On the left the comparison for hard squares with $L_h = 16$ of the equimodular curves of $T_C(z; L_h)$ in black with the restriction to $P = 0^+$ in red. On the right the comparison for hard squares with $L_h = 16$ of the equimodular curves of $T_F(z; L_h)$ in black with the restriction to the positive parity sector in red. The location of z_c is indicated by a cross.

6.4.1 Transfer matrix eigenvalue gaps

The eigenvalues of the transfer matrix $T_C(z; L_h)$ for hard hexagons for $P = 0^+$ have two very remarkable properties discovered in [10]

1. The characteristic polynomial of $T_C(z)$ in the sector $P = 0^+$ for $L_h = 9,\ 12,\ 15,\ 18$ factorizes into the product of two irreducible polynomials with integer coefficients.

2. The roots of the discriminant of the characteristic polynomial which lie on the real axis for $z < z_{d;hh}(L)$ all have multiplicity two for $L_h \leq 18$. In particular on the negative real axis the maximum eigenvalue is real only at isolated points. We conjecture this is valid for all L_h.

The hard hexagon transfer matrix $T_F(z; L_h)$ for $L_h = 3,\ 6,\ 9$ also has the remarkable property that all the roots of the resultant on the interval $-1 < z < z_d$ have multiplicity two. This is very strong evidence to support the conjecture that hard hexagons with free boundary conditions in one direction and cyclic in the other direction is obtained as a limit from a model which obeys the boundary Yang-Baxter equation of [82, 83, 224].

Neither property i) nor ii) can be considered as being generic and neither property holds for hard squares where there are small gaps in the equimodular curves where the maximum eigenvalues of both $T_c(z; L_h)$ and $T_F(z; L_h)$ are real and non-degenerate. These gaps are caused by the collision of a complex conjugate pair of eigenvalues at the boundaries of the gaps. On $-1 \leq z \leq z_d$ the maximum eigenvalue of $T_C(z; L_h)$ is in the sector $P = 0^+$. We have computed these gaps numerically for $L_h \leq 20$ and more accurately from the discriminant of the characteristic polynomial for $L_h \leq 14$. We give these gaps in table 6.3 for $L_h \leq 20$. For $L_h \geq 22$ most of the gaps are too small to actually observe their width, but their locations can still be determined numerically and are given in table 6.4 for $22 \leq L_h \leq 30$.

The gaps of $T_F(z; L_h)$ are not the same as those of $T_C(z; L_h)$. The gaps of $T_F(z; L_h)$ are given in table 6.5 where we see that with increasing L_h they approach the gaps of $T_C(z; L_h)$ of table 6.3.

The location of gaps for larger values of L_h may be extrapolated by observing that when the maximum eigenvalues $\lambda_{\max}$ are complex they may be written as $|\lambda_{\max}|e^{\pm i\theta/2}$ where θ is defined in section 6.2.5. The eigenvalues collide and become real when θ/π is an integer. In principle each of the separate equimodular curves on $-1 \leq z \leq z_d$ could be independent of each other, but as long as we are to the right of any equimodular curve which intersects the z axis, we define by convention the eigenvalue phase at the right of a gap to be the same as the phase at the left of the gap. We then choose θ not to be restricted to the interval 0 to π but to continuously increase as z decreases from z_d to the first crossing of an equimodular curve. This convention preserves the alternation of the signs of the real eigenvalues seen in table 6.3. For $L_h = 6$ we illustrate the behavior of this phase in figure 6.11. At the boundaries of the gaps the derivative of the phase diverges as a square root, and for $L_h = 6$ this derivative is also plotted in figure 6.11.

L_h	$z_l(L_h)$	$z_r(L_h)$	gap	eigenvalue sign
6	-0.52385422	-0.47481121	4.904301×10^{-2}	$-$
8	-0.30605227	-0.30360084	2.35243×10^{-3}	$-$
10	-0.23737268	-0.23720002	1.7266×10^{-4}	$-$
	-0.77929238	-0.73645527	4.283711×10^{-2}	$+$
12	-0.20401756	-0.20400239	1.517×10^{-5}	$-$
	-0.49539291	-0.49352002	1.87289×10^{-3}	$+$
14	-0.18464415	-0.18464265	1.50×10^{-6}	$-$
	-0.37193269	-0.37180394	1.2875×10^{-4}	$+$
	-0.92551046	-0.91949326	6.01721×10^{-3}	$-$
16	-0.17211444	-0.1721143	1.4×10^{-7}	$-$
	-0.305086	-0.305078	8×10^{-6}	$+$
	-0.64336	-0.64204	1.32×10^{-3}	$-$
18	-0.163389012	-0.163388998	1.4×10^{-8}	$-$
	-0.2643054	-0.2643045	9×10^{-7}	$+$
	-0.494482	-0.494388	9.4×10^{-5}	$-$
20	-0.156991031	-0.156991029	2×10^{-9}	$-$
	-0.23723539	-0.23723530	9×10^{-8}	$+$
	-0.404127	-0.494120	7×10^{-6}	$-$
	-0.7537	-0.7523	1.4×10^{-3}	$+$

Table 6.3: The gaps on the segment $-1 \leq z \leq z_d$ where the maximum eigenvalue of the transfer matrix $T_C(z; L_h)$ for hard squares on cylindrical chains of length L_h is real for $6 \leq L_h \leq 20$.

L_h	1	2	3	4	5	6	7	8
22	-0.152	-0.218	-0.346	-0.598				
24	-0.148	-0.204	-0.305	-0.494	-0.844			
26	-0.145	-0.193	-0.276	-0.423	-0.683			
28	-0.143	-0.184	-0.254	-0.371	-0.574	-0.93		
30	-0.140	-0.178	-0.237	-0.334	-0.495	-0.75		
32	-0.1388	-0.172	-0.223	-0.305	-0.435	-0.642	-0.972	
34	-0.1373	-0.167	-0.213	-0.282	-0.390	-0.558	-0.815	
36	-0.1360	-0.163	-0.204	-0.264	-0.355	-0.494	-0.701	
38	-0.1348	-0.160	-0.196	-0.249	-0.327	-0.444	-0.616	-0.871
40	-0.1338	-0.157	-0.190	-0.237	-0.305	-0.405	-0.548	-0.752

Table 6.4: The location of the very small gaps on the segments $-1 \leq z \leq z_d$ where the maximum eigenvalue of the transfer matrix $T_C(z; L_h)$ for hard squares is real. For $L_h =$ 22, 24, 26, 28, 30 the values are obtained from the data; for $L_h \geq 32$ the values are obtained from extrapolation using figure 6.12.

L_h	$z_l(L_h)$	$z_r(L_h)$	gap	eigenvalue sign
6	-0.4517	-0.4439	7.8×10^{-3}	$-$
8	-0.3004	-0.2999	5×10^{-4}	$-$
10	-0.23987	-0.23983	4×10^{-5}	$-$
	-0.6933	-0.6868	6.6×10^{-3}	$+$
12	-0.2079551	-0.2079504	4.6×19^{-6}	$-$
	-0.46977	-0.46908	6.9×10^{-4}	$+$
14	-0.18864888	-0.8864835	5.3×10^{-7}	$-$
	-0.362749	-0.362722	2.7×10^{-5}	$+$
	-0.85376	-0.85315	6.1×10^{-4}	$-$
16	-0.175819604	-0.175819540	6.4×10^{-8}	$-$
	-0.3024077	-0.3024052	2.5×10^{-6}	$+$
	-0.61069	-0.61049	2.0×10^{-4}	$-$

Table 6.5: The gaps on the segment $-1 \leq z \leq z_d$ where the maximum eigenvalue of the transfer matrix $T_F(z; L_h)$ for hard squares on the free chain of length L_h is real for $6 \leq L_h \leq 16$.

For any given value of z this unrestricted phase grows linearly with L_h and thus we define a normalized phase

$$\phi = \frac{\theta}{2\pi L_h}. \tag{6.46}$$

The gaps occur when $L_h\phi = 1$. In figure 6.12 we plot the normalized phases ϕ_C of $T_C(z; L_h)$ for $4 \leq L_h \leq 26$ and observe that they fall remarkably close to a common limiting curve. We may thus use this curve to extrapolate the locations of the gaps for $L_h \geq 32$. These values are given in table 6.4 for $32 \leq L_h \leq 40$. We also plot in figure 6.12 the normalized phase ϕ_F for $T_F(z; L_h)$ and note that $\phi_F \to \phi_C$ as L_h becomes large.

6.4.2 The density of partition zeros of $L \times L$ lattices on the negative z axis

For both hard squares and hard hexagons the zeros on the negative real axis are sufficiently dense that a quantitative comparison in terms of a density is possible.

The density of partition function zeros on $L_v \times L_h$ lattices with L_v/L_h fixed and $L_v,\ L_h \to \infty$ is defined here as the limit of the finite lattice quantity

$$\tilde{D}_{L_v,L_h}(z_j) = \frac{1}{L_v L_h (z_{j+1} - z_j)} > 0 \tag{6.47}$$

and the positions of the zeros z_j increase monotonically with j. To analyze this density we

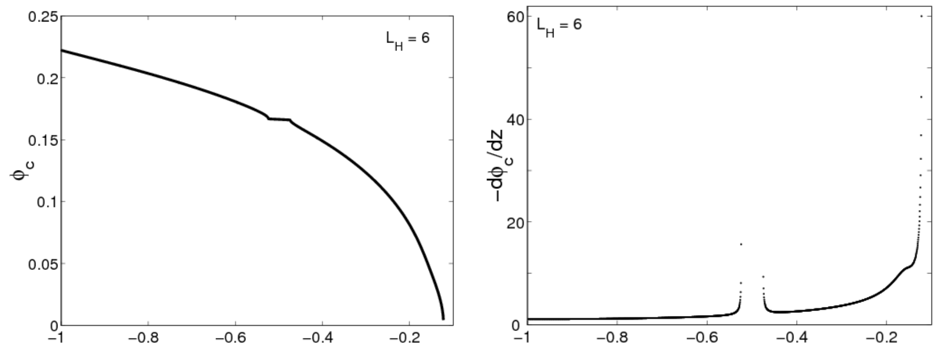

Figure 6.11: The normalized phase $\phi_C(z)$ of the equimodular curve of $T_C(z; L_h)$ and the derivative $-d\phi_C(z)/dz$ for $L_h = 6$ which has one gap on $-1 \le z \le z_d$ where $\lambda_{\max}$ is real.

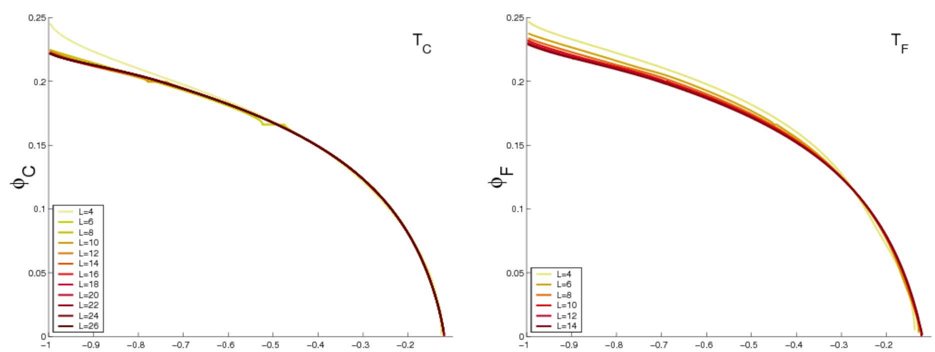

Figure 6.12: The normalized phase angles ϕ_C of $T_C(z; L_h)$ (on the left) and ϕ_F of $T_F(z; L_h)$ (on the right) on the segment $-1 \le z \le z_d$ as a function of z.

will also need the n^{th} order lattice derivative

$$\tilde{D}^{(n)}_{L_v,L_h}(z_j) = \frac{\tilde{D}^{(n-1)}_{L_v,L_h}(z_{j+1}) - \tilde{D}^{(n-1)}_{L_v,L_h}(z_j)}{z_{j+1} - z_j}. \tag{6.48}$$

As long as the density on $-1 \le z \le z_d$ is the boundary of the zero free region which includes the positive real axis (and where the thermodynamic limiting free energy is independent of the aspect ratio L_v/L_h), the limiting density computed directly for the $L_v \times L_h$ lattice is given in terms of the normalized phase angle (6.46) $\phi(z)$ on the interval $-1 \le z \le z_d$ by use of (6.37) as

$$\lim_{L_h,L_v \to \infty} \tilde{D}_{L_v,L_h}(z) = -\lim_{L_h \to \infty} \frac{d\phi(z)}{dz}. \tag{6.49}$$

Partition function zeros have been computed for systems much larger than it has been possible to compute eigenvalues and the largest lattices are for the $L \times L$ cylinders. In figure 6.13 we plot the density and the first three lattice derivatives for hard squares for the 40×40 cylindrical lattice on $-1 \leq z \leq z_d$. On this scale the density appears to be quite smooth and a local maximum is seen in the first derivative.

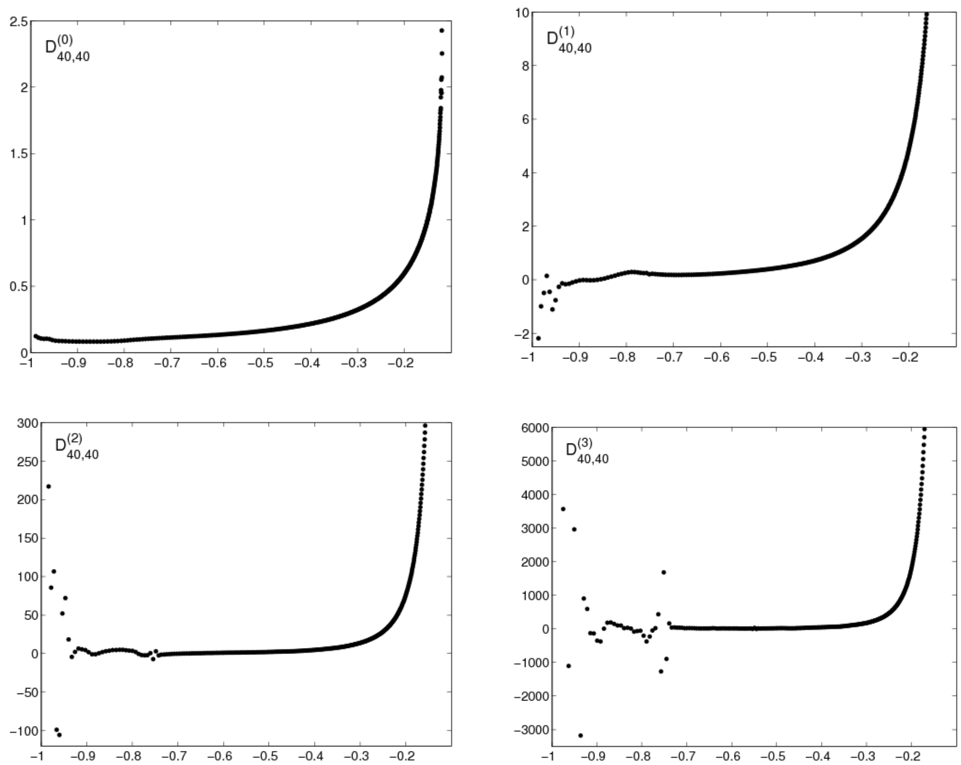

Figure 6.13: The density of zeros and the first three lattice derivatives for hard squares for the 40×40 lattice with cylindrical boundary conditions in the region $-1 \leq z \leq z_d$. The glitch, defined in section 6.4.4, caused by the gap given in table 6.4 at $z = -0.752$ is clearly visible in the second and third derivatives.

6.4.3 Partition zeros versus phase derivatives

For hard hexagons the density of partition function zeros on the negative z axis lie very close to the density computed from the derivative of the phase angle (6.49). Moreover all the lattice derivatives are smooth and featureless except very near $z_{d;hh}$ and also agree remarkably well with the derivatives computed from the phase angle. This is in significant contrast to hard squares.

In figure 6.14 we compare the density of zeros and its first two lattice derivatives with the same quantities computed from the normalized phase derivative curves of the corresponding transfer matrix for the 22×22 toroidal lattice and the 14×14 cylindrical lattice. For the density almost all zeros are seen to fall remarkably close to the normalized phase derivative curves. In the first derivative of the normalized phase derivative curve we see the divergences due to the gaps at -0.60 for $T_C(z;22)$ and at -0.85 and -0.36 for $T_F(z;14)$. In the second derivative, the divergences become more pronounced and the gap at -0.35 of $T_C(z;22)$ becomes noticeable.

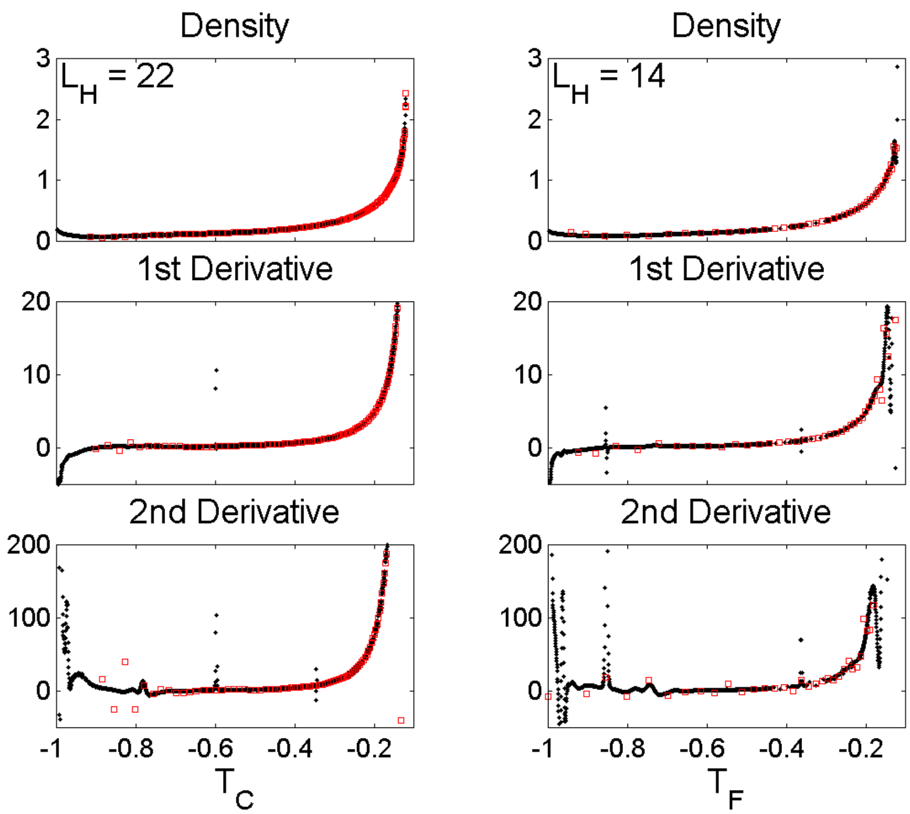

Figure 6.14: The density and the first two derivatives of the partition function zeros (in red) compared with the derivatives of the normalized phase derivative curves (in black) of the toroidal lattice $Z^{CC}_{22,22}(z)$ for the $T_C(z;22)$ on the left and the zeros of $Z^{CF}_{14,14}(z) = Z^{FC}_{14,14}(z)$ cylinder and the $T_F(z;14)$ transfer matrices (on the right). The divergences due to the gaps at $z = -0.598,\ -0.346$ for $T_C(z;22)$ and at $z = -0.853,\ -0.3627$ for $T_F(z;14)$ can be seen.

The derivatives of the normalized phase derivative curves all exhibit oscillations in the vicinity of $z = -1$ which become larger and cover an increasing segment of the z axis as the order of the derivative increases. In these oscillatory regions noticeable discrepancies between the lattice derivative of the zeros and the derivatives of the normalized phase are apparent.

6.4.4 Glitches in the density of zeros

The gaps in the equimodular curves of hard squares on $-1 \leq z \leq z_d$ which caused the divergences in the normalized phase curves in figure 6.14 lead to irregularities in the density of the $L \times L$ partition function zeros which we refer to as "glitches". These glitches upset the smoothness of the density of zeros on the finite lattice and become increasingly apparent in the higher derivatives of the density. The glitch at $z = -0.752$ is quite visible in the second and third derivatives in figure 6.13.

To illustrate further the relation of gaps to glitches in the density of zeros we plot the third derivatives of the density of cylindrical $L \times L$ lattices on an expanded scale in figure 6.15 where we indicate with solid arrows the positions of the corresponding gaps in the $T_C(z; L_h)$ equimodular curves of table 6.4. On these expanded scales we observe that as the size of the $L \times L$ lattice increases the number of glitches increases, they move to the right and their amplitude decreases. These properties follow from the properties of the gaps of table 6.4 and the normalized phase curve of figure 6.12.

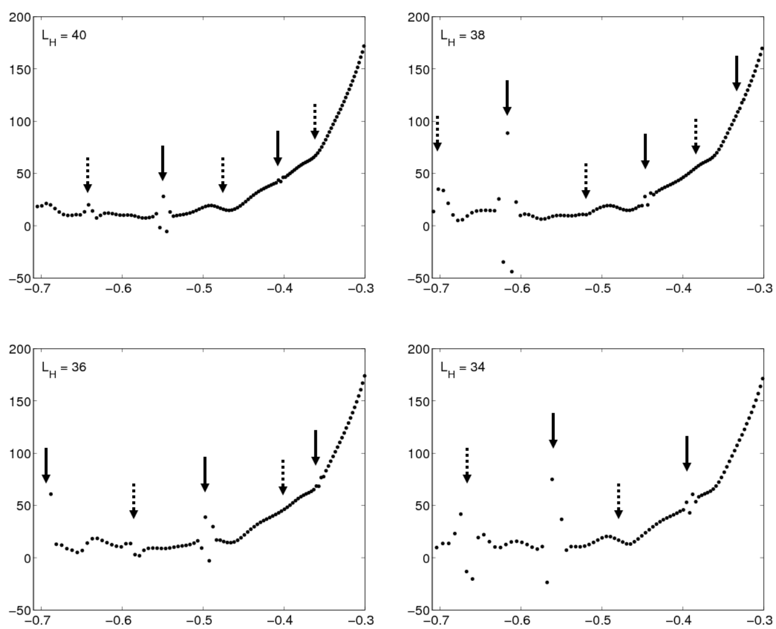

Figure 6.15: The third derivative of the density of hard squares for $40 \times 40,\ 38 \times 38,\ 36 \times 36,\ 34 \times 34$ lattices with cylindrical boundary conditions in the region $-0.7 \leq z \leq -0.25$. The gaps of table 6.4 are indicated by solid arrows

There also appear to be deviations of the zeros from a smooth curve at values of z where the phases of the complex conjugate pair of maximum modulus eigenvalues are $\pm\pi/2$. These deviations have no relation to gaps in the equimodular curves and are indicate with dashed arrows in figure 6.15.

6.4.5 Hard square density of zeros for $z \to z_d$.

As $z \to z_d$ the density diverges as

$$D(z) \sim (z_d - z)^{-\alpha}, \tag{6.50}$$

where from the universality of the point z_d with the Lee-Yang edge it is expected that $\alpha = 1/6$, which was also found to be the case for hard hexagons. We investigate the exponent α using the method used in [10] by plotting in figure 6.16 the quantity $D_L(z)/D_L^{(1)}(z)$ for $L = 40$ and compare this with

$$D(z)/D'(z) \sim (z_d - z)/\alpha \quad \text{with} \quad \alpha = 1/6, \tag{6.51}$$

which is expected to hold for $z \to z_d$.

As was the case for hard hexagons this limiting form is seen to hold only for z very close to z_d and for comparison we also plot a fitting function

$$f(z) = (z_f - z)/\alpha_f \quad \text{with} \quad z_f = -0.058, \quad \alpha_f = 1/0.88, \tag{6.52}$$

which well approximates the curve in the range $-0.30 \le z \le -0.16$. This same phenomenon has been seen in [121, equation (4.8) and figure 41] for Hamiltonian chains.

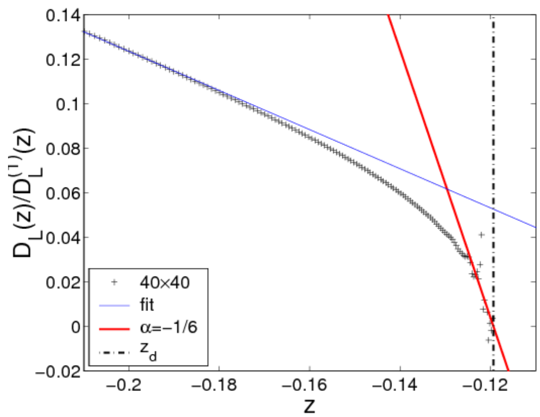

Figure 6.16: The plot of density/derivative for the partition function zeros of hard squares for 40×40 cylindrical lattice. The red line has $\alpha = 1/6$ and $z_d = -0.119$. The blue line has $\alpha_f = 1/0.88 = 1.14$ and $z_f = -0.058$.

6.4.6 The point $z = -1$

Hard squares have the remarkable property, which has no counterpart for hard hexagons, that at $z = -1$ all roots of the characteristic equation are either roots of one, or minus one, with various multiplicities. These roots have been computed for the full transfer matrix

$T_C(-1; L_h)$ either directly [90], [25] to size 15 or using a mapping to rhombus tilings [130] to size $L_h = 50$. In 6.A we present factorizations of the characteristic polynomial $T_C(-1; L_h)$ for the reduced sector $P = 0^+$ for $L_h \leq 29$, and of $T_F(-1; L_h)$ for $L_h \leq 20$ both for the unrestricted and positive parity sectors. In 6.B we give the partition function values at $z = -1$.

6.4.7 Behavior near $z = -1$

The density of zeros of figure 6.13 for the 40×40 cylinder is finite as $z \to -1$. However the first derivative is sufficiently scattered for $z \leq -0.95$ that an estimate of the slope is impracticable.

Furthermore there is a great amount of structure in the equimodular curves near the point $z = -1$ where all eigenvalues are equimodular and which is not apparent on the scale of the plots in figure 6.6. We illustrate this complexity for $L_h = 12$ for $P = 0^+$ in figure 6.17 where we see that there are equimodular curves which intersect the z axis for $z \geq -1$. These level crossings are a feature also for $T_C(z)$ without the restriction to $P = 0^+$ and for $T_F(z)$ and $T_F(z)$ with + parity as well. In general there are several such crossings for a given L_h. We give the values of the crossing furthest to the right in table 6.6. It is not clear whether these level crossings will persist to the right of $z = -1$ as $L_h \to \infty$. We also note that often there are more than one such level crossing, as illustrated in figure 6.17 for $T_F(z; 12)$.

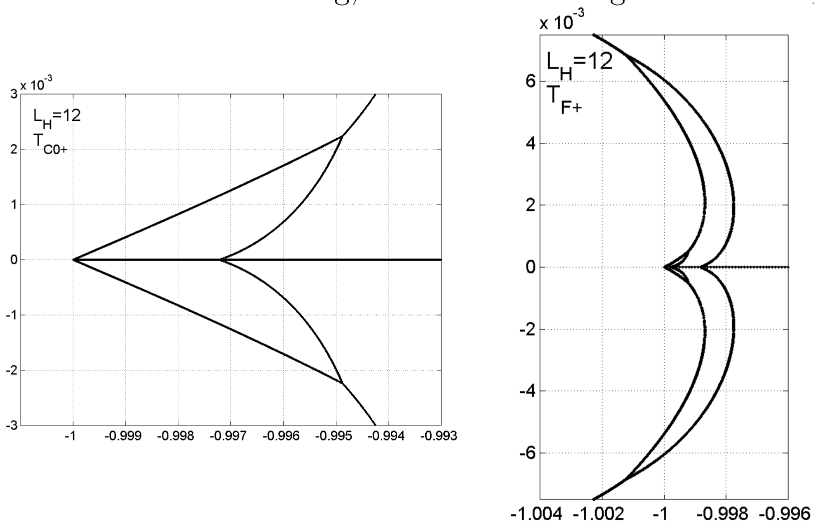

Figure 6.17: Plots in the complex fugacity z plane near $z = -1$ for $L_h = 12$ of the equimodular curves of hard square transfer matrix $T_C(z; L_h)$ with $P = 0^+$ (on the left) and $T_F(z, L_h)$ with + parity (on the right) on a scale which shows the level crossings on the z-axis to the right of $z = -1$.

L	$P = 0^+$	T_C		parity = +	T_F
12	-0.9973	-0.91295		-0.9988	same
14	none	-0.9195		-0.999296	-0.999092
16	none	-0.96		none	none
18	-0.99994			-0.9990	
20	-0.9995				
22	-0.9999				
24	-0.9974				
26	-0.9990				
28	-0.9996				

Table 6.6: Positions of the right-most equimodular curve crossings of the negative z-axis for hard squares of $T_C(z)$ in the sector $P = 0^+$ and unrestricted and of $T_F(z)$ in the plus parity sector and unrestricted.

6.5 Discussion

The three different techniques of series expansions, transfer matrix eigenvalues and partition function zeros give three quite different perspectives on the difference between the integrable hard hexagon model and non-integrable hard squares.

6.5.1 Series expansions

Consider first the series expansion of the physical free energy of hard squares [70, 127], which is analyzed by means of differential approximants, as compared with the exact solution of hard hexagons [22].

The hard hexagon free energy for both the high and low density regimes satisfies Fuchsian differential equations which can be obtained from a finite number of terms in a series expansion [10].

For an non-integrable model like hard squares, the best kind of differential approximant analysis to be introduced is not clear. For integrable models, even if one has a small number of series coefficients, restricting to Fuchsian ODEs has been seen to be an extremely efficient constraint. However for a (probably non-integrable) model like hard squares, there is no reason to restrict the linear differential equations annihilating the hard square series to be Fuchsian. In [127] the existing 92 term series are analyzed by means of differential approximants but the series is too short to determine whether $z = -1$ is, or is not, a singular point.

The method of series expansions and differential approximants are not well adapted to analyze qualitative differences between hard squares and hard hexagons. This is to be compared with the transfer matrix eigenvalues and partition function zeros presented above which show dramatic differences between the two systems.

6.5.2 Transfer matrices

The clearest distinction between integrable hard hexagons and non-integrable hard squares is seen in the factorization properties of the discriminant of the characteristic polynomials of the transfer matrices $T_C(z; L_h)$ and $T_F(z; L_h)$. At the zeros of the discriminant the transfer matrix in general fails to be diagonalizable and the eigenvalues may have singularities.

For hard hexagons these discriminants contain square factors which exclude the existence of gaps in the equimodular curves and singularities of the maximum eigenvalue on the negative z-axis. This was observed for $T_C(z; L_h)$ in [10]. In the present paper these square factors and lack of gaps has been observed for the transfer matrix $T_F(z; L_h)$ of hard hexagons for all value of L_h studied and supports the conjecture that integrability can be established by extending the methods of [82, 83, 224, 31, 5]. For hard squares there are no such factorizations, so that its equimodular curves have gaps and the maximum eigenvalue has singularities on the negative real z-axis.

6.5.3 Partition function zeros

In [10] we qualitatively characterized the partition function zeros as either being on curves or being part of a necklace, and in the present paper we have characterized the zeros as filling up areas. However, further investigation is required to determine if these characterizations of the qualitative appearance of zeros of the finite system characterize the thermodynamic limit. In [10] we initiated such a study by examining the dependence of the right-hand endpoints of the necklace on the size of the lattice and observed that the endpoints move to the right as the lattice size increases. However, there is not sufficient data to reliably determine the limiting behavior. Thus, if in the thermodynamic limit the endpoint moved to $z_{c;hh}$ the notion of zeros being on a curve might not persist. Similarly, it needs further investigation to determine if the zeros of hard squares, which we have characterized as filling up an area, will fill the area in the thermodynamic limit or whether further structure develops.

On the negative z-axis both hard hexagons and hard squares have a line of zeros which has been investigated in detail in section 6.4. The density of zeros for $z < z_{d:hh}$ for hard hexagons is mostly featureless and smooth, which is quite consistent with the low density free energy having a branch cut starting at $z_{d;hh}$. Hard squares zeros, on the other hand, have a series of "glitches" whose number increases as z approaches z_d and which correspond to the locations of the gaps in the equimodular curves. A rigorous analysis of behavior of these glitches needs to be made.

6.5.4 Behavior near z_c

The equimodular curves of hard hexagons were extensively studied in [10]. The equimodular curves, as illustrated for $L_h = 21$ in figure 6.7, consist of the curve where the low and high density physical free energy are equimodular and a necklace region which surrounds this equimodular curve in part of the left half-plane.

For hard hexagons there is only one unique curve of zeros of the $L \times L$ partition function which is converging towards $z_{c;hh}$ as $L \to \infty$. However, for hard squares the partition function zeros in figures 6.2-6.4 do not lie on a single unique curve near z_c. This is clearly seen in the plots of figure 6.5 where the zeros appear to be converging to a wedge behavior as $L \to \infty$ which is analogous to the behavior of the equimodular curves of figure 6.18.

The behavior of the equimodular curves of hard squares near z_c in figure 6.6 is qualitatively different from the behavior of hard hexagons in figure 6.7. This is vividly illustrated in figure 6.18 where we plot the equimodular curves for $T_c(z; L_h)$ with $P = 0^+$ for all values $4 \leq L_h \leq 26$. We see in this figure that there is an ever increasing set of loops in the equimodular curves which approach z_c as $L_h \to \infty$.

It needs to be investigated if this behavior of both the zeros and the equimodular curves for hard squares will have an effect on the singularity at z_c beyond what is obtained from the analysis of the series expansion of [70, 127].

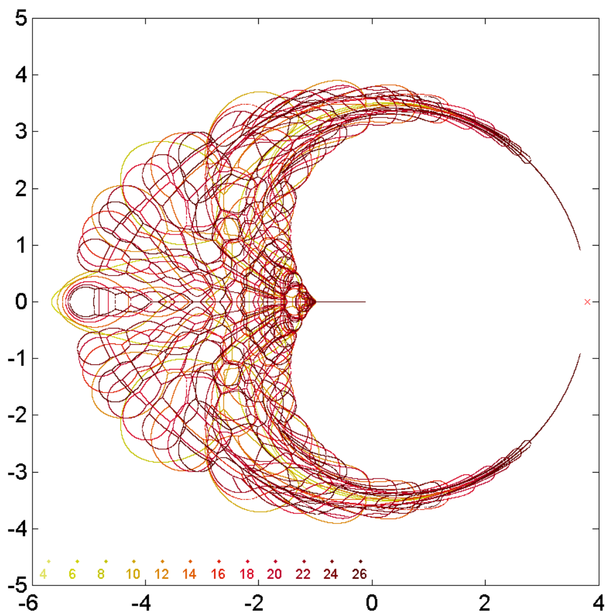

Figure 6.18: The equimodular curves in the complex z plane of the $T_C(z; L_h)$ transfer matrix in the 0^+ sector for $4 \leq L_h \leq 26$ plotted together. The different values of L_h are given different shadings as indicated on the plot. The location of z_c is indicated by a cross.

6.5.5 Behavior near $z = -1$

Finally we note that the relation of the equimodularity of all eigenvalues at $z = -1$ to the analytic behavior of the physical free energy is completely unknown, as is the curious observation for $12 \leq L_h \leq 28$ found in table 6.6 that there are equimodular curves of

$T_C(z; L_h)$ and for $T_F(z; L_h)$ which cross the negative z-axis to the right of $z = -1$. There are many values of L_h for which there are more than one such curve. It would be of interest to know if this feature persists for $L_h > 28$ and if it does, does the point of rightmost crossing move to the right. If such a phenomenon does exist it would cause a re-evaluation of the role of zeros on the negative z-axis.

6.6 Conclusions

The techniques of series expansions, universality and the renormalization group apply equally well to describe the dominant behavior at z_c and z_d of hard hexagons and hard squares. However the results of this paper reveal many differences between integrable hard hexagons and non-integrable hard squares which have the potential to create further analytic properties in hard squares which are not present in hard hexagons.

The renormalization group combined with conformal field theory predicts that both z_c and z_d will be isolated regular singularities where the free energy will have a finite number of algebraic or logarithmic singularities, each multiplied by a convergent infinite series. This scenario is, of course, far beyond what can be confirmed by numerical methods. Indeed hard squares are predicted to have the same set of 5 exponents at z_d which hard hexagons have [133],[10] even though only two such exponents can be obtained from the 92 terms series expansion [127].

The emergence of the critical singularities predicted by the renormalization group at either z_c or z_d is a phenomenon which relies upon the thermodynamic limit and we have seen that hard squares approach this limit in a more complicated manner than do hard hexagons.

Near z_c the limiting position of the zeros for hard squares appears to be a wedge. This is far more complex than the behavior of hard hexagons.

Near z_d the zeros of both hard hexagons and hard squares are observed to lie on a segment of the negative z-axis. If this indeed holds in the thermodynamic limit it would be satisfying if a genuine proof could be found which incorporates the fact that some level crossings have been observed to the right of $z = -1$.

On the negative z-axis hard squares have glitches in the density of zeros and gaps in the equimodular curves which hard hexagons do not have. In the thermodynamic limit the glitches and gaps may become a dense set of measure zero by the analysis leading to table 6.4 . Does this give a hint of the analytical structure of non-integrable models?

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Appendix

6.A Characteristic polynomials at $z = -1$

In [130] it was proven that all of the eigenvalues of the $T_C(-1; L_h)$ transfer matrix at $z = -1$ are roots of unity and the characteristic polynomials were given in that paper up to $L_h = 50$. Below we give the factorized characteristic polynomials $P^{C0+}_{L_h}$ in the 0^+ sector at $z = -1$ up to $L_h = 29$. The transfer matrix $T_F(z; L_h)$ has not been considered before in the literature, and below we give the factorized characteristic polynomials $P^F_{L_h}$ and $P^{F+}_{L_h}$ of the full $T_F(-1; L_h)$ and the restricted positive parity sector, respectively, at $z = -1$ up to $L_h = 20$. In all cases divisions are exact.

6.A.1 Characteristic polynomials $P^F_{L_h}$

The degree of $P^F_{L_h}$ is exactly the Fibonacci number $F(n)$ defined by the recursion relation

$$F(L_h + 2) = F(L_h + 1) + F(L_h) \tag{6.53}$$

with the initial conditions $F(-1) = 0$, $F(0) = 1$, so that its generating function is

$$G^F = \frac{(2 + t)}{(1 - t - t^2)} \tag{6.54}$$

and thus as $L_h \to \infty$ the degree of the polynomial $P^F_{L_h}$ grows as $N_G^{L_h}$, where $N_G = (1 + \sqrt{5})/2 \sim 1.618\cdots$ is the golden ratio.

The first 20 polynomials are

$$
\begin{aligned}
P_1^F &= (x^6-1)(x^3-1)^{-1}(x^2-1)^{-1}(x-1)\\
P_2^F &= (x^4-1)(x^2-1)^{-1}(x-1)\\
P_3^F &= (x^8-1)(x^4-1)^{-1}(x-1)\\
P_4^F &= (x^6-1)(x^4-1)(x^3-1)^{-1}(x-1)\\
P_5^F &= (x^{10}-1)(x^8-1)(x^4-1)^{-1}(x^2-1)^{-1}(x-1)\\
P_6^F &= (x^{14}-1)(x^4-1)^2(x^2-1)^{-1}(x-1)\\
P_7^F &= (x^{18}-1)(x^{12}-1)(x^8-1)(x^6-1)(x^4-1)^{-2}(x^3-1)^{-1}(x-1)\\
P_8^F &= (x^{22}-1)(x^{16}-1)^2(x^8-1)^{-1}(x^4-1)^2(x-1)\\
P_9^F &= (x^{26}-1)(x^{20}-1)^3(x^{14}-1)(x^{10}-1)^{-1}(x^8-1)(x^4-1)^{-2}(x^2-1)^{-1}(x-1)\\
P_{10}^F &= (x^{30}-1)(x^{24}-1)^3(x^{18}-1)^2(x^8-1)^{-1}(x^6-1)(x^4-1)^3(x^3-1)^{-1}\\
&\qquad (x^2-1)^{-1}(x-1)\\
P_{11}^F &= (x^{34}-1)(x^{28}-1)^3(x^{22}-1)^4(x^{16}-1)(x^{14}-1)(x^8-1)(x^4-1)^{-3}(x-1)\\
P_{12}^F &= (x^{38}-1)(x^{32}-1)^4(x^{26}-1)^6(x^{20}-1)^2(x^{10}-1)(x^8-1)^{-1}(x^4-1)^3(x-1)\\
P_{13}^F &= (x^{42}-1)(x^{36}-1)^5(x^{30}-1)^8(x^{24}-1)^5(x^{12}-1)(x^{10}-1)(x^8-1)^2(x^6-1)\\
&\qquad (x^4-1)^{-3}(x^3-1)^{-1}(x^2-1)^{-1}(x-1)\\
P_{14}^F &= (x^{46}-1)(x^{40}-1)^5(x^{34}-1)^{11}(x^{28}-1)^{11}(x^{22}-1)^3(x^{14}-1)^{-1}(x^8-1)^{-1}\\
&\qquad (x^4-1)^4(x^2-1)^{-1}(x-1)\\
P_{15}^F &= (x^{50}-1)(x^{44}-1)^5(x^{38}-1)^{14}(x^{32}-1)^{18}(x^{26}-1)^8(x^{22}-1)(x^{20}-1)\\
&\qquad (x^{16}-1)^{-2}(x^8-1)^2(x^4-1)^{-4}(x-1)\\
P_{16}^F &= (x^{54}-1)(x^{48}-1)^6(x^{42}-1)^{17}(x^{36}-1)^{25}(x^{30}-1)^{17}(x^{24}-1)^4(x^{18}-1)(x^{14}-1)\\
&\qquad (x^{12}-1)^{-1}(x^{10}-1)^{-1}(x^8-1)^{-1}(x^6-1)(x^4-1)^4(x^3-1)^{-1}(x-1)\\
P_{17}^F &= (x^{58}-1)(x^{52}-1)^7(x^{46}-1)^{21}(x^{40}-1)^{35}(x^{34}-1)^{31}(x^{28}-1)^{11}(x^{26}-1)^{-1}\\
&\qquad (x^{22}-1)(x^{20}-1)^3(x^{14}-1)^{-1}(x^{10}-1)^{-1}(x^8-1)^2(x^4-1)^{-4}(x^2-1)^{-1}\\
&\qquad (x-1)\\
P_{18}^F &= (x^{62}-1)(x^{56}-1)^7(x^{50}-1)^{25}(x^{44}-1)^{50}(x^{38}-1)^{52}(x^{32}-1)^{24}(x^{26}-1)^4\\
&\qquad (x^{22}-1)^{-1}(x^{16}-1)^2(x^8-1)^{-2}(x^4-1)^5(x^2-1)^{-1}(x-1)\\
P_{19}^F &= (x^{66}-1)(x^{60}-1)^7(x^{54}-1)^{29}(x^{48}-1)^{67}(x^{42}-1)^{82}(x^{36}-1)^{50}(x^{30}-1)^{14}\\
&\qquad (x^{24}-1)^{-2}(x^{18}-1)^3(x^{14}-1)^{-1}(x^{12}-1)(x^{10}-1)(x^8-1)^2(x^6-1)\\
&\qquad (x^4-1)^{-5}(x^3-1)^{-1}(x-1)\\
P_{20}^F &= (x^{70}-1)(x^{64}-1)^8(x^{58}-1)^{34}(x^{52}-1)^{84}(x^{46}-1)^{122}(x^{40}-1)^{97}(x^{34}-1)^{35}\\
&\qquad (x^{28}-1)^4(x^{26}-1)(x^{20}-1)^{-3}(x^{14}-1)(x^{10}-1)(x^8-1)^{-2}(x^4-1)^5\\
&\qquad (x-1)
\end{aligned}
\tag{6.55}
$$

and from these we see that the degrees of the multiplicity of the eigenvalue +1 are

$$0, 1, 1, 2, 1, 3, 2, 5, 3, 8, 9, 17, 20, 33, 45, 74, 105, 167, 250, 389, \dots \tag{6.56}$$

where we find a "mod 4" effect.

6.A.2 Characteristic polynomials $P^{F+}_{L_h}$

The degrees of $P^{F+}_{L_h}$ follow the sequence A001224 in the OEIS [225] and they are related to the Fibonacci sequence $F(n)$ as follows:

$$\frac{F(L_h+1)+F(\frac{L_h+1}{2}+1)}{2}, \qquad L_h = \text{odd} \tag{6.57}$$

$$\frac{F(L_h+1)+F(\frac{L_h}{2})}{2}, \qquad L_h = \text{even} \tag{6.58}$$

This sequence has the following generating function

$$G^{F+} = \frac{G^F}{2} + \frac{t^3+t^2+t+2}{2(1-t^2-t^4)} \tag{6.59}$$

so that the degree of the polynomials $P^{F+}_{L_h}$ grow as $N_G^{L_h}$ with a sub-dominant growth of $N_G^{L_h/2}$.

The first 20 polynomials are

$$
\begin{aligned}
P_1^{F+} &= (x^6-1)(x^3-1)^{-1}(x^2-1)^{-1}(x-1) \\
P_2^{F+} &= (x^4-1)(x^2-1)^{-1} \\
P_3^{F+} &= (x^8-1)(x^4-1)^{-1} \\
P_4^{F+} &= (x^6-1)(x^3-1)^{-1}(x^2-1) \\
P_5^{F+} &= (x^8-1)(x^5-1)(x^4-1)^{-1} \\
P_6^{F+} &= (x^7-1)(x^4-1)^2(x^2-1)^{-2}(x-1) \\
P_7^{F+} &= (x^{18}-1)(x^9-1)^{-1}(x^8-1)(x^6-1)^2(x^4-1)^{-1}(x^3-1)^{-1}(x^2-1)^{-1} \\
&\qquad (x-1) \\
P_8^{F+} &= (x^{22}-1)(x^{16}-1)^2(x^{11}-1)^{-1}(x^8-1)^{-2}(x^2-1)(x-1) \\
P_9^{F+} &= (x^{20}-1)^3(x^{14}-1)(x^{13}-1)(x^{10}-1)^{-3}(x^8-1)(x^7-1)^{-1}(x^4-1)^{-2} \\
&\qquad (x-1) \\
P_{10}^{F+} &= (x^{18}-1)^2(x^{15}-1)(x^{12}-1)^3(x^9-1)^{-2}(x^6-1)(x^4-1)^2(x^3-1)^{-1} \\
&\qquad (x^2-1)^{-2} \\
P_{11}^{F+} &= (x^{34}-1)(x^{17}-1)^{-1}(x^{16}-1)(x^{14}-1)^4(x^{11}-1)^4(x^4-1)^{-1}(x^2-1)^{-1} \\
P_{12}^{F+} &= (x^{38}-1)(x^{32}-1)^4(x^{19}-1)^{-1}(x^{16}-1)^{-4}(x^{13}-1)^6(x^{10}-1)^3(x^2-1)^2 \\
P_{13}^{F+} &= (x^{36}-1)^5(x^{30}-1)^8(x^{21}-1)(x^{18}-1)^{-5}(x^{15}-1)^{-8}(x^{12}-1)^6(x^{10}-1)(x^9-1) \\
&\qquad (x^8-1)(x^6-1)(x^5-1)^{-1}(x^4-1)^{-2}(x^3-1)^{-1}(x^2-1) \\
P_{14}^{F+} &= (x^{34}-1)^{11}(x^{28}-1)^{11}(x^{23}-1)(x^{20}-1)^5(x^{17}-1)^{-11}(x^{14}-1)^{-11}(x^{11}-1)^3 \\
&\qquad (x^4-1)^3(x^2-1)^{-3}(x-1) \\
P_{15}^{F+} &= (x^{50}-1)(x^{32}-1)^{18}(x^{26}-1)^8(x^{22}-1)^6(x^{25}-1)^{-1}(x^{19}-1)^{14}(x^{16}-1)^{-18} \\
&\qquad (x^{13}-1)^{-8}(x^{10}-1)(x^8-1)(x^4-1)^{-1}(x^2-1)^{-2}(x-1) \\
P_{16}^{F+} &= (x^{54}-1)(x^{48}-1)^6(x^{30}-1)^{17}(x^{27}-1)^{-1}(x^{24}-1)^{-2}(x^{21}-1)^{17}(x^{18}-1)^{26} \\
&\qquad (x^{15}-1)^{-17}(x^{12}-1)^{-4}(x^{10}-1)^{-1}(x^7-1)(x^6-1)(x^5-1)(x^3-1)^{-1} \\
&\qquad (x^2-1)^2(x-1) \\
P_{17}^{F+} &= (x^{52}-1)^7(x^{46}-1)^{21}(x^{29}-1)(x^{28}-1)^{11}(x^{26}-1)^{-7}(x^{23}-1)^{-21}(x^{22}-1) \\
&\qquad (x^{20}-1)^{38}(x^{17}-1)^{31}(x^{14}-1)^{-11}(x^{11}-1)^{-1}(x^{10}-1)^{-1}(x^8-1) \\
&\qquad (x^4-1)^{-3}(x^2-1)(x-1) \\
P_{18}^{F+} &= (x^{50}-1)^{25}(x^{44}-1)^{50}(x^{31}-1)(x^{28}-1)^7(x^{26}-1)^4(x^{25}-1)^{-25}(x^{22}-1)^{-50} \\
&\qquad (x^{19}-1)^{52}(x^{16}-1)^{26}(x^{13}-1)^{-4}(x^8-1)^{-1}(x^4-1)^4(x^2-1)^{-3} \\
P_{19}^{F+} &= (x^{66}-1)(x^{48}-1)^{67}(x^{42}-1)^{82}(x^{33}-1)^{-1}(x^{30}-1)^8(x^{27}-1)^{29}(x^{24}-1)^{-66} \\
&\qquad (x^{21}-1)^{-82}(x^{18}-1)^{52}(x^{15}-1)^{13}(x^{14}-1)^{-1}(x^{12}-1)^{-1}(x^9-1) \\
&\qquad (x^8-1)(x^7-1)(x^6-1)^2(x^5-1)(x^4-1)^{-1}(x^3-1)^{-1}(x^2-1)^{-2} \\
P_{20}^{F+} &= (x^{70}-1)(x^{64}-1)^8(x^{46}-1)^{122}(x^{40}-1)^{97}(x^{35}-1)^{-1}(x^{32}-1)^{-8}(x^{29}-1)^{34} \\
&\qquad (x^{26}-1)^{85}(x^{23}-1)^{-122}(x^{20}-1)^{-97}(x^{17}-1)^{35}(x^{14}-1)^5(x^8-1)^{-1} \\
&\qquad (x^4-1)(x^2-1)^3
\end{aligned}
\tag{6.60}
$$

and from these we find that the degrees of the multiplicity of the eigenvalue +1 are

$$0, 0, 0, 1, 1, 2, 1, 2, 1, 4, 7, 11, 8, 10, 20, 47, 69, 86, 103, 162, \dots \tag{6.61}$$

where again there is a "mod 4" effect.

6.A.3 Characteristic polynomials $P^{C}_{L_h}$

The characteristic polynomials $P^{C}_{L_h}$ for $T_C(-1; L_h)$ have been well analyzed in [130] and are listed in appendix A of that paper to $L_h = 50$. The degree of the polynomials are the Lucas numbers which satisfy the recursion relation (6.53) with initial conditions $L(0) = 2,\ L(1) = 1$ and which have the generating function

$$G^C = \frac{1 + 2t}{(1 - t - t^2)} \tag{6.62}$$

From the long list of [130] we find that the degrees of the multiplicity of the eigenvalue +1 are

$$\begin{aligned}&1, 1, 2, 3, 0, 4, 1, 7, 8, 13, 2, 26, 9, 49, 38, 107, 28, 228, 49, 501, 324, 1101, 258, 2766, 469,\\ &5845, 3790, 13555, 2376, 35624, 5813, 75807, 38036, 180213, 30482, 480782, 69593,\\ &1047429, 485658, 2542453, 385020, 6794812, 914105, 15114481, 9570844, 36794329,\\ &5212354, 101089306, 12602653, 222317557, \dots\end{aligned} \tag{6.63}$$

where we find a "mod 6" effect.

6.A.4 Characteristic polynomials $P^{C0+}_{L_h}$

The degrees of the polynomials $P^{C0+}_{L_h}$ are discussed in appendix B of [188] and are the series A129526 in the OEIS [225]. However, an explicit form is not known.

We have computed the characteristic polynomials in the less restrictive case of the momentum $P = 0$ sector. The degrees of the polynomials follow the series A000358 in the OEIS [225], which is given by the formula

$$\frac{1}{L_h} \sum_{n|L_h} \phi\left(\frac{L_h}{n}\right) [F(n-2) + F(n)] \tag{6.64}$$

where $\phi(n)$ is Euler's totient function (the number of positive integers $< n$ which are relatively prime with n). In particular when L_h is prime (6.64) specializes to

$$1 + \frac{F(L_h - 2) + F(L_h) - 1}{L_h} \tag{6.65}$$

which grows as $N_G^{L_h}$.

The order of the restricted positive parity polynomial P^{C0+} is greater than the negative parity polynomial P^{C0-} and thus P^{C0+} also grows as $N_G^{L_h}$.

The first 29 polynomials are

$$
\begin{aligned}
P_1^{C0+} &= (x-1) \\
P_2^{C0+} &= (x^4-1)(x^2-1)^{-1} \\
P_3^{C0+} &= (x^3-1)(x-1)^{-1} \\
P_4^{C0+} &= (x^2-1)^2(x-1)^{-1} \\
P_5^{C0+} &= (x^2-1)^2(x-1)^{-1} \\
P_6^{C0+} &= (x^4-1)(x^3-1)(x^2-1)^{-1} \\
P_7^{C0+} &= (x^4-1)^2(x^2-1)^{-2}(x-1) \\
P_8^{C0+} &= (x^{10}-1)(x^5-1)^{-1}(x-1)(x^2-1) \\
P_9^{C0+} &= (x^3-1)(x-1)^2(x^2-1)^2 \\
P_{10}^{C0+} &= (x^8-1)(x^7-1)(x^2-1)^{-1}(x-1) \\
P_{11}^{C0+} &= (x^5-1)^2(x^4-1)^3(x^2-1)^{-3} \\
P_{12}^{C0+} &= (x^{18}-1)(x^9-1)^{-1}(x^6-1)(x^4-1)(x^3-1)^2(x^2-1)(x-1)^{-1} \\
P_{13}^{C0+} &= (x^7-1)^3(x^2-1)^6(x-1)^{-2} \\
P_{14}^{C0+} &= (x^{16}-1)^3(x^{11}-1)(x^8-1)^{-3}(x^5-1)(x^4-1)(x^2-1)^3(x-1)^{-1} \\
P_{15}^{C0+} &= (x^9-1)^4(x^6-1)^2(x^4-1)^4(x^3-1)^3(x^2-1)^{-4}(x-1)^{-1} \\
P_{16}^{C0+} &= (x^{26}-1)(x^{14}-1)^3(x^{13}-1)^{-1}(x^{10}-1)^3(x^7-1)^{-2}(x^5-1)^3(x^4-1)^5 \\
&\qquad (x^2-1)^{-4}(x-1) \\
P_{17}^{C0+} &= (x^{11}-1)^6(x^8-1)^8(x^4-1)^{-2}(x^2-1)^4(x-1)^3 \\
P_{18}^{C0+} &= (x^{24}-1)^6(x^{18}-1)^3(x^{15}-1)(x^{12}-1)^{-5}(x^9-1)^3(x^6-1)^{-1}(x^4-1) \\
&\qquad (x^3-1)^4(x^2-1)^8(x-1)^3 \\
P_{19}^{C0+} &= (x^{13}-1)^8(x^{10}-1)^{18}(x^7-1)^3(x^5-1)^{-6}(x^4-1)^5(x^2-1)^{-3}(x-1)^2 \\
P_{20}^{C0+} &= (x^{34}-1)(x^{22}-1)^{15}(x^{17}-1)^{-1}(x^{16}-1)^2(x^{14}-1)^6(x^{11}-1)^{-8}(x^8-1) \\
&\qquad (x^7-1)^4(x^4-1)^{17}(x^2-1)^{-12} \\
P_{21}^{C0+} &= (x^{15}-1)^{10}(x^{12}-1)^{27}(x^9-1)^{12}(x^6-1)^3(x^5-1)(x^4-1)^9(x^3-1)^7 \\
&\qquad (x^2-1)^{-1}(x-1)^{-3} \\
P_{22}^{C0+} &= (x^{32}-1)^{10}(x^{26}-1)^{14}(x^{20}-1)^{15}(x^{19}-1)(x^{16}-1)^{-10}(x^{13}-1)^{14} \\
&\qquad (x^{10}-1)^{-9}(x^7-1)(x^5-1)^6(x^4-1)^2(x^2-1)^{22}(x-1)^{-2} \\
P_{23}^{C0+} &= (x^{17}-1)^{13}(x^{14}-1)^{45}(x^{11}-1)^{43}(x^8-1)^4(x^7-1)^{15}(x^4-1)^5 \\
&\qquad (x^2-1)^{16}(x-1)^{-3}
\end{aligned}
$$

$$
\begin{aligned}
P_{24}^{C0+} &= (x^{42}-1)(x^{30}-1)^{45}(x^{24}-1)^{27}(x^{21}-1)^{-1}(x^{18}-1)^{16}(x^{15}-1)^{-20}\\
&\quad (x^{12}-1)^{9}(x^{10}-1)^{10}(x^{9}-1)^{2}(x^{8}-1)^{3}(x^{6}-1)^{9}(x^{5}-1)^{-10}\\
&\quad (x^{4}-1)^{27}(x^{3}-1)^{12}(x^{2}-1)^{-23}\\
P_{25}^{C0+} &= (x^{19}-1)^{16}(x^{16}-1)^{92}(x^{13}-1)^{116}(x^{10}-1)^{20}(x^{8}-1)^{-8}(x^{5}-1)^{5}\\
&\quad (x^{4}-1)^{41}(x^{2}-1)^{-33}(x-1)^{2}\\
P_{26}^{C0+} &= (x^{40}-1)^{15}(x^{34}-1)^{42}(x^{28}-1)^{105}(x^{23}-1)(x^{22}-1)^{20}(x^{20}-1)^{-15}\\
&\quad (x^{17}-1)^{36}(x^{16}-1)(x^{14}-1)^{-45}(x^{11}-1)^{9}(x^{8}-1)^{-1}\\
&\quad (x^{7}-1)^{28}(x^{4}-1)^{16}(x^{2}-1)^{26}(x-1)^{4}\\
P_{27}^{C0+} &= (x^{21}-1)^{19}(x^{18}-1)^{155}(x^{15}-1)^{263}(x^{12}-1)^{92}(x^{9}-1)^{-27}(x^{7}-1)\\
&\quad (x^{5}-1)^{26}(x^{4}-1)^{17}(x^{3}-1)^{19}(x^{6}-1)^{7}(x-1)^{9}(x^{2}-1)^{67}\\
P_{28}^{C0+} &= (x^{50}-1)(x^{38}-1)^{120}(x^{32}-1)^{168}(x^{26}-1)^{110}(x^{25}-1)^{-1}(x^{22}-1)^{15}\\
&\quad (x^{20}-1)^{5}(x^{19}-1)^{-54}(x^{16}-1)^{42}(x^{13}-1)^{-26}(x^{11}-1)^{6}\\
&\quad (x^{10}-1)(x^{8}-1)^{43}(x^{5}-1)^{4}(x^{4}-1)^{55}(x^{2}-1)^{-10}(x-1)^{2}\\
P_{29}^{C0+} &= (x^{23}-1)^{23}(x^{20}-1)^{205}(x^{17}-1)^{581}(x^{14}-1)^{364}(x^{11}-1)^{36}(x^{7}-1)^{-14}\\
&\quad (x^{10}-1)^{15}(x^{5}-1)^{-5}(x^{4}-1)^{131}(x^{2}-1)^{-115}
\end{aligned}
\tag{6.66}
$$

and from these we find that the degrees of the characteristic polynomials are

$$
\begin{aligned}
&1, 2, 2, 3, 3, 5, 5, 8, 9, 14, 16, 26, 31, 49, 64, 99, 133, 209, 291, 455, 657, 1022, 1510, 2359,\\
&3545, 5536, 8442, 13201, 20319, 31836, 49353, 77436, 120711, 189674, 296854, 467160,\\
&733363, 1155647, 1818594, 2869378, 4524081, 7146483, \ldots
\end{aligned}
\tag{6.67}
$$

where we find there is a "mod 6" effect.

6.B Partition functions at $z = -1$

Successive powers of transfer matrices always satisfy a linear recursion relation, since any matrix satisfies its own characteristic polynomial. Therefore, any linear function of the matrix or its components which is independent of the power of the matrix will also satisfy the same linear recursion relation. The usual functions involved in creating partition functions from transfer matrices, the trace of the matrix, dot products with boundary vectors, and modified traces to account for Möbius and Klein bottle boundary conditions, all cause the respective partition functions to satisfy the same linear recursion relation as their transfer matrix, its characteristic polynomial. In particular, the Klein bottle partition function $Z^{KC}_{L_v,L_h}(z)$ satisfies the same linear recursion relation in L_v as the torus $Z^{CC}_{L_v,L_h}(z)$, since it is constructed from the same transfer matrix $T_C(z; L_h)$, and the cylinder partition function $Z^{CF}_{L_v,L_h}(z)$ satisfies the same recursion relation in L_v as the Möbius partition function $Z^{MF}_{L_v,L_h}(z)$ since they are both constructed from the same transfer matrix $T_F(z; L_h)$.

Therefore, the generating functions for the partition functions for a given L_h and for general z are rational functions in z and $x = L_v$ whose denominators are the characteristic polynomials of the L_h transfer matrix and whose numerators are polynomials given by the product of the characteristic polynomial and the initial terms of the series (the numerator has degree 1 less in x than the degree of the characteristic polynomial).

When the transfer matrix can be block diagonalized and the boundary vector dot products cause the partition function to be a function of only a restricted set of matrices in the direct sum, the partition function will satisfy a recursion relation of smaller order than the order of the full transfer matrix. As an example, $T_C(z; L_h)$ can be block diagonalized into different momentum sectors, and $Z^{FC}_{L_v,L_h}(z)$ is only a function of the reflection symmetric zero momentum sector 0^+, so that the cylinder $Z^{FC}_{L_v,L_h}(z)$ will satisfy a recursion relation in L_v of the order of the 0^+ sector and not the order of the full $T_C(z; L_h)$ matrix. Likewise, $Z^{FF}_{L_v,L_h}(z)$ satisfies a recursion relation in L_v of the order of the positive parity sector of $T_F(z; L_h)$.

Beyond restrictions to particular matrix sectors, however, in general the polynomials in the numerator and denominator of the generating functions do not partially cancel, regardless of the initial conditions of the recursion relation, so that partition functions in z generally satisfy a recursion relation of the same order as its transfer matrix. This holds generically for hard hexagons and hard squares even if at particular values of z some cancellations can occur in the generating function.

For hard squares at $z = -1$ the denominators of the generating functions simplify to the expressions given in appendix A, whose orders grow according to the order of the transfer matrices. The numerators, however, are such that massive cancellations occur, so that the partition functions as a function of $x = L_v$ at $z = -1$ satisfy linear recursion relations of much smaller degree than than the partition function does for general z. The form of the numerator is dependent on the initial conditions of the recursion relation, that is, the partition function value at $z = -1$ for the first several values of L_v. This, in turn, is dependent on boundary conditions: both the torus and the Klein bottle partition functions satisfy the same linear recursion relation of their transfer matrix $T_C(-1; L_h)$, but the numerators of their generating functions are different, so that the Klein bottle exhibits much more massive cancellations than the torus for a given L_h. Likewise, the cylinder $Z^{CF}_{L_v,L_h}(-1)$ and the Möbius band have different recursion relation orders due to different amounts of cancellations at $z = -1$.

The cylinder has the property that for odd L_h, $Z^{FC}_{L_v,L_h}(-1) = -2$ whenever $\gcd(L_h - 1, L_v) = 0 \mod 3$, and $Z^{FC}_{L_v,L_h}(-1) = 1$ otherwise [132]. Therefore, the linear recursion relation of $Z^{FC}_{L_v,L_h}(-1)$ for odd L_h is always of order 1 or 2, even though for generic z the partition function $Z^{FC}_{L_v,L_h}(z)$ satisfies a linear recursion relation of the order of the 0^+ sector of the $T_C(z; L_h)$ transfer matrices, which grows as $N_G^{L_h}$. The initial conditions for the cylinder for odd L_h, therefore, are able to effect incredible cancellations to its generating function whose denominators are given in Appendix A.

In [130] it was proven that for the torus partition function, $Z^{CC}_{L_v,L_h}(-1) = 1$ whenever L_v, L_h are co-prime. Since for each L_h the torus at $z = -1$ satisfies a linear recursion relation, its initial conditions happen to be exactly suited to allow for this number theoretic property. This property does not extend to other boundary conditions even when they satisfy the same overall linear recursion relation. The Klein bottle satisfies the same $T_C(-1; L_h)$

linear recursion relation that the torus also satisfies, but its initial conditions do not cause it to share in the torus' co-primality property.

A repeating sequence with period n will have a generating function of the form $p(x)/(1-x^n)$. Therefore, since all of the eigenvalues of the transfer matrices $T_C(-1;L_h)$ and $T_F(-1;L_h)$ are roots of unity, as long as the denominators have only square-free factors, the sequences of partition function values at $z=-1$ will be repeating, with a period given by the lcm of the exponents n_j in the factors $(1-x^{n_j})$. Most sequences below are repeating, with a period often much larger than the order of the transfer matrix. For the limited cases considered below, all generating functions along a periodic direction (including a twist for Möbius bands and Klein bottles) are repeating. Along the free direction, the sequences are not always repeating; the cylinder for $L_h = 0 \bmod 4$ is non-repeating and the free-free partition function is non-repeating for four of the L_h considered. In [4] a general form for the generating functions of $Z^{FC}_{L_v,L_h}(-1)$ for even L_h is conjectured, along with the conjecture that for even L_h the only repeating sequences for $Z^{FC}_{L_v,L_h}(-1)$ are when $L_h = 2 \bmod 4$. We make the following conjecture:

Conjecture 1 *Along a periodic direction (including twists) all generating functions are repeating.*

We further find below that along the periodic direction, all repeating sequences are sums of repeating sub-sequences of period p_j which have value zero except at locations $p_j - 1 \bmod p_j$ where their value is an integer multiple of p_j. Often the value is exactly p_j. Therefore, the generating functions along a periodic direction are logarithmic derivatives of a product of factors of the form $(1-x^{p_j})^{m_j}$, where m_j is an integer. We conjecture that this always holds:

Conjecture 2 *Along a periodic direction (including twists), all generating functions are logarithmic derivatives of products of the form $\prod_j (1-x^{p_j})^{m_j}$, where p_j and m_j are integers.*

As it turns out, for the limited cases considered below, we find surprisingly that the generating functions for the torus and the cylinder along the periodic direction are exactly the negative of the logarithmic derivative of the characteristic polynomial of their transfer matrices at $z=-1$, so that we have the further conjecture:

Conjecture 3 *The generating functions of the torus and cylinder (along the periodic direction) are equal to the negative of the logarithmic derivative of their characteristic polynomials, that is, $G^{CC}_{L_h} = -\frac{d}{dx}\ln\left(P^{CC}_{L_h}\right)$ and $G^{CF}_{L_h} = -\frac{d}{dx}\ln\left(P^{CF}_{L_h}\right)$, respectively.*

This is similar to a conjecture in [1]. We note that this does not hold for general z, nor for Möbius bands or Klein bottles at $z=-1$. Due to this conjecture, we can use the results from appendix 6.A to further the tables of periods for the sequences $Z^{CC}_{L_v,L_h}(-1)$ and $Z^{CF}_{L_v,L_h}(-1)$, where we notice a mod 3 pattern.

For $Z^{CC}_{L_v,L_h}(-1)$, for $L_h = 0 \bmod 3$ we conjecture that the periods are given by the $\mathrm{lcm}(L_h, 2L_h, \ldots, nL_h)$, where n is often given by $n = L_h/3 - 1$.

For $Z^{CF}_{L_v,L_h}(-1)$, for $L_h = 1 \bmod 3$ we conjecture that the periods are given by the $\text{lcm}(6, 12, \ldots, 6n)$, where n is often $2(L_h - 4)/3 + 1$.

We also note that the periods of the cylinder (along the periodic L_v direction), the Möbius band, and the free-free plane are all equal, and the periods of the Klein bottle and cylinder (along the free L_v direction) are equal.

Below we list both the generating functions and tables of values for all boundary conditions, since number theoretic properties such as the torus's co-primality property can be missed by simply considering the generating functions. The periods of repeating sequences are tabulated, along with the minimal order of the recursion relations. All generating functions listed were determined by computing all partition function values up to the order of the transfer matrix and canceling the numerator and denominators of the generating function to arrive at the minimal order linear recursion relation; however, we extend the table of values to higher L_h.

6.B.1 The torus $Z^{CC}_{Lv,L_h}(-1)$

$\mathbf{L_h \backslash L_v}$	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	1	-1	1	3	1	-1	1	3	1	-1	1	3	1	-1	1	3	1	-1	1	3
3	1	1	4	1	1	4	1	1	4	1	1	4	1	1	4	1	1	4	1	1
4	1	3	1	7	1	3	1	7	1	3	1	7	1	3	1	7	1	3	1	7
5	1	1	1	1	-9	1	1	1	1	11	1	1	1	1	-9	1	1	1	1	11
6	1	-1	4	3	1	14	1	3	4	-1	1	18	1	-1	4	3	1	14	1	3
7	1	1	1	1	1	1	1	1	1	1	1	1	1	-27	1	1	1	1	1	1
8	1	3	1	7	1	3	1	7	1	43	1	7	1	3	1	7	1	3	1	47
9	1	1	4	1	1	4	1	1	40	1	1	4	1	1	4	1	1	76	1	1
10	1	-1	1	3	11	-1	1	43	1	9	1	3	1	69	11	43	1	-1	1	13
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
12	1	3	4	7	1	18	1	7	4	3	1	166	1	3	4	7	1	126	1	7
13	1	1	1	1	1	1	1	1	1	1	1	1	-51	1	1	1	1	1	1	1
14	1	-1	1	3	1	-1	-27	3	1	69	1	3	1	55	1	451	1	-1	1	73
15	1	1	4	1	-9	4	1	1	4	11	1	4	1	1	174	1	1	4	1	11

Table 6.B.7: $Z^{CC}_{L_v,L_h}(-1)$

The generating functions $G^{CC}_{L_h}$ as a function of $x = L_v$ are given below.

$$
\begin{aligned}
G^{CC}_1 &= \frac{1}{(1-x)}, \qquad G^{CC}_2 = G^{CC}_1 + \frac{4x^3}{(1-x^4)} - \frac{2x}{(1-x^2)}, \qquad G^{CC}_3 = G^{CC}_1 + \frac{3x^2}{(1-x^3)}, \\
G^{CC}_4 &= G^{CC}_2 + \frac{4x}{(1-x^2)}, \qquad G^{CC}_5 = G^{CC}_1 + \frac{20x^9}{(1-x^{10})} - \frac{10x^4}{(1-x^5)}, \\
G^{CC}_6 &= G^{CC}_3 - G^{CC}_1 + G^{CC}_2 + \frac{12x^5}{(1-x^6)}, \qquad G^{CC}_7 = G^{CC}_1 + \frac{56x^{27}}{(1-x^{28})} - \frac{28x^{13}}{(1-x^{14})}, \\
G^{CC}_8 &= G^{CC}_4 + \frac{40x^9}{(1-x^{10})}, \qquad G^{CC}_9 = G^{CC}_3 + \frac{36x^{17}}{(1-x^{18})} + \frac{36x^8}{(1-x^9)}, \\
G^{CC}_{10} &= G^{CC}_2 + \frac{70x^{13}}{(1-x^{14})} + \frac{10x^4}{(1-x^5)} + \frac{40x^7}{(1-x^8)}, \\
G^{CC}_{11} &= G^{CC}_1 + \frac{110x^{54}}{(1-x^{55})} + \frac{176x^{43}}{(1-x^{44})} - \frac{88x^{21}}{(1-x^{22})}. \qquad (6.68)
\end{aligned}
$$

Z^{CC} L_h	1	2	3	4	5	6	7	8	9	10	11
T_C order	2	3	4	7	11	18	29	47	76	123	199
min rec order	1	3	3	4	6	8	15	12	18	24	77
period	1	4	3	4	10	12	28	20	18	280	220

Table 6.B.8: The minimal order of the recursion relation and the period of the repeating sequence of $Z^{CC}_{L_v,L_h}(-1)$ as a function of L_v.

6.B.2 The Klein bottle $Z^{KC}_{L_v,L_h}(-1)$ with twist in L_v direction

$\mathbf{L_h \backslash L_v}$	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	-1	-3	-1	1	-1	-3	-1	1	-1	-3	-1	1	-1	-3	-1	1	-1	-3	-1	1
3	-1	-1	2	-1	-1	2	-1	-1	2	-1	-1	2	-1	-1	2	-1	-1	2	-1	-1
4	-1	5	-1	1	-1	5	-1	1	-1	5	-1	1	-1	5	-1	1	-1	5	-1	1
5	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3	-1	3
6	1	-5	4	-1	1	-2	1	-1	4	-5	1	2	1	-5	4	-1	1	-2	1	-1
7	1	-3	1	5	1	-3	1	5	1	-3	1	5	1	-3	1	5	1	-3	1	5
8	1	7	1	3	1	7	1	3	1	7	1	3	1	7	1	3	1	7	1	3
9	1	5	4	5	1	8	1	5	4	5	1	8	1	5	4	5	1	8	1	5
10	-1	-7	-1	-3	-1	-7	13	5	-1	-7	-1	-3	-1	-7	-1	5	-1	-7	-1	-3
11	-1	-5	-1	3	9	-5	-1	3	-1	5	-1	3	-1	-5	9	3	-1	-5	-1	13
12	-1	9	2	5	-1	12	-1	5	2	9	-1	8	-1	9	2	5	-1	12	-1	5
13	-1	7	-1	7	-1	7	13	7	-1	7	-1	7	-1	21	-1	7	-1	7	-1	7
14	1	-9	1	3	1	-9	1	-29	1	1	23	3	1	-9	1	3	1	-9	1	13

Table 6.B.9: $Z^{KC}_{L_v,L_h}(-1)$

The generating functions $G_{L_h}^{KC}$ as a function of $x = L_v$ are given below.

$$G_1^{KC} = \frac{1}{(1-x)}, \qquad G_2^{KC} = -G_1^{KC} + \frac{4x^3}{(1-x^4)} - \frac{2x}{(1-x^2)}, \qquad G_3^{KC} = -G_1^{KC} + \frac{3x^2}{(1-x^3)},$$
$$G_4^{KC} = -G_2^{KC} - 2G_1^{KC} + \frac{4x}{(1-x^2)}, \qquad G_5^{KC} = G_4^{KC} + G_2^{KC} + G_1^{KC},$$
$$G_6^{KC} = -G_4^{KC} + G_3^{KC} + G_1^{KC}, \qquad G_7^{KC} = 2G_2^{KC} + 3G_1^{KC}, \qquad G_8^{KC} = G_4^{KC} + 2G_1^{KC},$$
$$G_9^{KC} = G_5^{KC} + G_3^{KC} + 3G_1^{KC}, \qquad G_{10}^{KC} = -G_8^{KC} - \frac{14x^{13}}{(1-x^{14})} + \frac{8x^7}{(1-x^8)} + \frac{14x^6}{(1-x^7)},$$
$$G_{11}^{KC} = G_7^{KC} - 2G_1^{KC} + \frac{10x^4}{(1-x^5)}. \tag{6.69}$$

Z^{KC} L_h	1	2	3	4	5	6	7	8	9	10	11
T_C order	2	3	4	7	11	18	29	47	76	123	199
min rec order	1	3	2	4	2	5	3	4	4	20	7
period	1	4	3	4	2	12	4	4	6	56	20

Table 6.B.10: The minimal order of the recursion relation and the period of the repeating sequence of $Z_{L_v,L_h}^{KC}(-1)$ as a function of L_v.

6.B.3 The cylinder $Z_{Lv,L_h}^{FC}(-1) = Z_{Lh,L_v}^{CF}(-1)$

The generating functions $G_{L_h}^{FC}$ as a function of $x = L_v$ are given below. For odd L_h there are only two cases:

$$G_{3n\pm1}^{FC} = \frac{1}{(1-x)} \qquad G_{3n}^{FC} = G_{3n\pm1}^{FC} - \frac{3}{(1-x^3)}$$

$L_h \backslash L_v$	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1
3	-2	1	1	-2	1	1	-2	1	1	-2	1	1	-2	1	1	-2	1	1	-2	1
4	-1	3	-3	5	-5	7	-7	9	-9	11	-11	13	-13	15	-15	17	-17	19	-19	21
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	2	-1	1	4	-1	-1	4	1	-1	2	1	1	2	-1	1	4	-1	-1	4	1
7	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
8	-1	3	5	5	3	7	1	1	-1	3	-3	5	3	7	1	9	-1	3	-3	5
9	-2	1	1	-2	1	1	-2	1	1	-2	1	1	-2	1	1	-2	1	1	-2	1
10	-1	-1	1	1	9	-1	1	1	-11	-1	1	11	9	-1	1	-9	-11	-1	11	11
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
12	2	3	-3	8	-5	7	8	9	-9	14	-11	13	2	15	-15	8	-17	19	-4	21
13	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
14	-1	-1	1	1	-1	13	1	1	13	-1	15	1	-1	-15	1	15	-15	-1	-13	15
15	-2	1	1	-2	1	1	-2	1	1	-2	1	1	-2	1	1	-2	1	1	-2	1
16	-1	3	5	5	3	7	1	33	-1	3	13	5	3	7	-31	9	-1	35	-3	5

Table 6.B.11: $Z^{FC}_{L_v,L_h}(-1) = Z^{CF}_{L_h,L_v}(-1)$

For even L_h:

$$
\begin{aligned}
G^{FC}_2 = G^{FC}_1 - \frac{2(1+x)}{(1-x^4)}, \qquad G^{FC}_4 &= \frac{x}{(1-x^2)} - \frac{(1-x)^2}{(1-x^2)^2}, \qquad G^{FC}_6 = -G^{FC}_3 + G^{FC}_2 + G^{FC}_1, \\
G^{FC}_8 &= \frac{1}{5}G^{FC}_4 - \frac{4}{5}\frac{(1+x)(1-x^5)^2}{(1-x^{10})(1-x)^2} + \frac{8}{5}\frac{x(1+x)(x^3+3)(1-x^5)}{(1-x^{10})(1-x)}, \\
G^{FC}_{10} &= G^{FC}_2 + \frac{10x(1+x)(1+x^2)}{(1-x^8)} - \frac{10x(x^2+x+1)}{(1-x^7)}, \\
G^{FC}_{12} &= \frac{7}{9}G^{FC}_4 - \frac{4(1-x^6)(1-x^9)}{(1-x^{18})} + \frac{2}{3}\frac{(1+x)(1-x^2)(1-x^3)^2}{(1-x^6)^2} + \frac{(2x^5+2x^4+55x^3+55)}{9(1-x^6)}, \\
G^{FC}_{14} &= G^{FC}_2 + \frac{28x^3 p^{FC}_{14}}{(1-x^{16})} - \frac{14x^3(x^7+x^6+x^2+x+1)}{(1-x^{11})} - \frac{14x^3(1+x)}{(1-x^5)}, \\
G^{FC}_{16} &= \frac{243G^{FC}_4 + 2108G^{FC}_1}{455} + \frac{16(1+x)(1-x^{13})p^{FC}_{16;1}}{13(1-x^{26})} + \frac{32(1+x)(1-x^7)p^{FC}_{16;2}}{7(1-x^{14})} + \frac{8(1-x^2)p^{FC}_{16;3}}{5(1-x^{10})},
\end{aligned}
\tag{6.70}
$$

$$
\begin{aligned}
p_{14}^{FC} &= x^{12}+x^{11}+x^7+x^6+x^5+x^2+x+1, \\
p_{16;1}^{FC} &= -2x^{11}+6x^9-3x^8+4x^7-9x^6+5x^5-5x^4+9x^3-4x^2+3x-6, \\
p_{16;2}^{FC} &= -x^5+3x^3-x^2+x-3, \\
p_{16;3}^{FC} &= 7x^7+7x^6-3x^5+x^4-5x^3+12x^2+6x+10.
\end{aligned} \tag{6.71}
$$

Z^{FC} L_h	2	4	6	8	10	12	14	16
T_{C0^+} order	2	3	5	8	14	26	49	99
min rec order	2	3	5	7	13	15	25	29
period	4	–	12	–	56	–	880	–

Table 6.B.12: The minimal order of the recursion relation and the period of the repeating sequence of $Z^{FC}_{L_v,L_h}(-1)$ as a function of L_v.

The generating functions $G_{L_h}^{CF}$ as a function of $x = L_v$ are given below.

$$
\begin{aligned}
G_1^{CF} &= \frac{6x^5}{(1-x^6)} - \frac{3x^2}{(1-x^3)} - \frac{2x}{(1-x^2)} + \frac{1}{(1-x)}, \qquad G_2^{CF} = \frac{4x^3}{(1-x^4)} - \frac{2x}{(1-x^2)} + \frac{1}{(1-x)}, \\
G_3^{CF} &= \frac{8x^7}{(1-x^8)} - \frac{4x^3}{(1-x^4)} + \frac{1}{(1-x)}, \qquad G_4^{CF} = G_1^{CF} + G_2^{CF} + \frac{4x}{(1-x^2)} - \frac{1}{(1-x)}, \\
G_5^{CF} &= G_3^{CF} + \frac{10x^9}{(1-x^{10})} - \frac{2x}{(1-x^2)}, \qquad G_6^{CF} = 2G_2^{CF} + \frac{14x^{13}}{(1-x^{14})} + \frac{2x}{(1-x^2)} - \frac{1}{(1-x)}, \\
G_7^{CF} &= G_3^{CF} - G_2^{CF} + G_1^{CF} + \frac{18x^{17}}{(1-x^{18})} + \frac{12x^{11}}{(1-x^{12})}, \\
G_8^{CF} &= -G_3^{CF} + \frac{22x^{21}}{(1-x^{22})} + \frac{32x^{15}}{(1-x^{16})} + \frac{4x^3}{(1-x^4)} + \frac{2}{(1-x)}, \\
G_9^{CF} &= G_6^{CF} - G_5^{CF} + G_2^{CF} + \frac{26x^{25}}{(1-x^{26})} + \frac{60x^{19}}{(1-x^{20})} + \frac{16x^7}{(1-x^8)} - \frac{24x^3}{(1-x^4)}, \\
G_{10}^{CF} &= G_4^{CF} - G_3^{CF} + G_2^{CF} + \frac{30x^{29}}{(1-x^{30})} + \frac{72x^{23}}{(1-x^{24})} + \frac{36x^{17}}{(1-x^{18})}.
\end{aligned}
\tag{6.72}
$$

Z^{CF} L_h	1	2	3	4	5	6	7	8	9	10
T_F order	2	3	5	8	13	21	34	55	89	144
min rec order	2	3	5	6	13	16	26	36	60	60
period	6	4	8	12	40	28	72	176	3640	360

Table 6.B.13: The minimal order of the recursion relation and the period of the repeating sequence of $Z_{L_v,L_h}^{CF}(-1)$ as a function of L_v.

$L_h \backslash L_v$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	1	-1	-2	-1	1	2	1	-1	-2	-1	1	2	1	-1	-2	-1	1	2	1	-1
2	-1	-3	-1	1	-1	-3	-1	1	-1	-3	-1	1	-1	-3	-1	1	-1	-3	-1	1
3	-1	-1	-1	-5	-1	-1	-1	3	-1	-1	-1	-5	-1	-1	-1	3	-1	-1	-1	-5
4	-1	3	-4	-1	-1	6	-1	-1	-4	3	-1	2	-1	3	-4	-1	-1	6	-1	-1
5	-1	1	-1	-3	9	1	-1	5	-1	1	-1	-3	-1	1	9	5	-1	1	-1	-3
6	1	-5	1	3	1	-5	15	3	1	-5	1	3	1	-5	1	3	1	-5	1	3
7	1	-3	-2	-3	1	12	1	5	-20	-3	1	0	1	-3	-2	5	1	12	1	-3
8	1	5	1	-3	1	5	1	-27	1	5	-21	-3	1	5	1	5	1	5	1	-3
9	1	3	1	-5	1	3	-13	3	1	-47	1	-5	27	3	1	3	1	3	1	5
10	-1	-7	-4	-3	-1	-4	-1	5	-40	-7	-1	72	-1	-7	26	5	-1	-4	-1	-3
11	-1	-5	-1	-1	-1	-5	-1	-9	-1	-5	87	-1	-1	93	-1	7	-35	-5	-1	-1
12	-1	7	-1	-5	-1	7	-1	3	-1	57	-1	-5	155	7	-1	-125	-1	7	-39	5

Table 6.B.14: $Z^{MF}_{L_v,L_h}(-1)$

6.B.4 The Möbius band $Z^{MF}_{L_v,L_h}(-1)$ with twist in the L_v direction

The generating functions $G^{MF}_{L_h}$ as a function of $x = L_v$ are given below.

$$
\begin{aligned}
G^{MF}_1 &= \frac{6x^5}{(1-x^6)} - \frac{3x^2}{(1-x^3)} - \frac{2x}{(1-x^2)} + \frac{1}{(1-x)}, \qquad G^{MF}_2 = \frac{4x^3}{(1-x^4)} - \frac{2x}{(1-x^2)} - \frac{1}{(1-x)},\\
G^{MF}_3 &= \frac{8x^7}{(1-x^8)} - \frac{4x^3}{(1-x^4)} - \frac{1}{(1-x)}, \qquad G^{MF}_4 = -G^{MF}_2 + G^{MF}_1 + \frac{4x}{(1-x^2)} - \frac{3}{(1-x)},\\
G^{MF}_5 &= G^{MF}_3 - \frac{10x^9}{(1-x^{10})} + \frac{10x^4}{(1-x^5)} + \frac{2x}{(1-x^2)},\\
G^{MF}_6 &= 2G^{MF}_2 - \frac{14x^{13}}{(1-x^{14})} + \frac{14x^6}{(1-x^7)} - \frac{2x}{(1-x^2)} + \frac{3}{(1-x)},\\
G^{MF}_7 &= G^{MF}_3 + G^{MF}_2 + G^{MF}_1 + \frac{18x^{17}}{(1-x^{18})} - \frac{12x^{11}}{(1-x^{12})} - \frac{18x^8}{(1-x^9)} + \frac{12x^5}{(1-x^6)} + \frac{2}{(1-x)},\\
G^{MF}_8 &= -3G^{MF}_3 - 5G^{MF}_2 + \frac{22x^{21}}{(1-x^{22})} + \frac{32x^{15}}{(1-x^{16})} - \frac{22x^{10}}{(1-x^{11})} - \frac{6x}{(1-x^2)} - \frac{7}{(1-x)},\\
G^{MF}_9 &= -G^{MF}_6 + G^{MF}_3 + G^{MF}_2 - \frac{26x^{25}}{(1-x^{26})} + \frac{60x^{19}}{(1-x^{20})} + \frac{26x^{12}}{(1-x^{13})} - \frac{50x^9}{(1-x^{10})} - \frac{2x}{(1-x^2)} + \frac{4}{(1-x)},\\
G^{MF}_{10} &= 2G^{MF}_7 - G^{MF}_3 - G^{MF}_1 - \frac{30x^{29}}{(1-x^{30})} - \frac{72x^{23}}{(1-x^{24})} + \frac{30x^{14}}{(1-x^{15})} + \frac{96x^{11}}{(1-x^{12})} - \frac{24x^5}{(1-x^6)} - \frac{3}{(1-x)}.
\end{aligned}
\tag{6.73}
$$

Z^{MF} L_h	1	2	3	4	5	6	7	8	9	10
T_F order	2	3	5	8	13	21	34	55	89	144
min rec order	2	3	5	5	13	16	23	35	60	59
period	6	4	8	12	40	28	72	176	3640	360

Table 6.B.15: The minimal order of the recursion relation and the period of the repeating sequence of $Z^{MF}_{L_v,L_h}(-1)$ as a function of L_v.

6.B.5 The free-free plane $Z^{FF}_{L_v,L_h}(-1)$

$\mathbf{L_h \backslash L_v}$	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
1	0	-1	-1	0	1	1	0	-1	-1	0	1	1	0	-1	-1	0	1	1	0	-1
2	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1
3	-1	1	-1	-1	1	-1	1	1	-1	1	-1	-1	1	-1	1	1	-1	1	-1	-1
4	0	1	-1	2	-1	3	-2	3	-3	4	-3	5	-4	5	-5	6	-5	7	-6	7
5	1	-1	1	-1	1	1	-1	3	-1	1	1	-3	3	-1	1	3	-3	3	-1	-1
6	1	-1	-1	3	1	-3	1	5	-1	-5	3	5	-3	-3	5	3	-5	-1	5	1
7	0	1	1	-2	-1	1	2	3	-1	-2	-1	-1	4	3	-1	-2	-3	3	4	1
8	-1	1	1	3	3	5	3	3	3	3	-1	1	-3	-1	-3	1	-3	1	1	5
9	-1	-1	-1	-3	-1	-1	-1	3	3	1	5	1	5	5	1	1	-3	-5	-5	-5
10	0	-1	1	4	1	-5	-2	3	1	2	-1	3	-4	-7	7	10	-1	-7	-4	5
11	1	1	-1	-3	1	3	-1	-1	5	-1	1	1	-1	-3	-1	7	-1	-3	-3	3
12	1	1	-1	5	-3	5	-1	1	1	3	1	5	-1	17	-1	5	1	-1	-1	3
13	0	-1	1	-4	3	-3	4	-3	5	-4	-1	-1	2	1	-1	0	5	-3	10	-9

Table 6.B.16: $Z^{FF}_{L_v,L_h}(-1)$

The generating functions $G_{L_h}^{FF}$ as a function of $x = L_v$ are given below.

$$
\begin{aligned}
G_1^{FF} &= \frac{2x^4(1+x)}{(1-x^6)} + \frac{1}{(1-x^3)} - \frac{1}{(1-x)}, \qquad G_2^{FF} = \frac{2x^2(1+x)}{(1-x^4)} - \frac{1}{(1-x)},\\
G_3^{FF} &= \frac{2x^3(x-1)(1+x^2)}{(1-x^8)} + \frac{2x}{(1-x^2)} - \frac{1}{(1-x)},\\
G_4^{FF} &= \frac{1}{3}G_1^{FF} - \frac{(1-x)^2}{3(1-x^2)^2} + \frac{x}{3(1-x^2)} + \frac{1}{3(1-x)},\\
G_5^{FF} &= G_3^{FF} + \frac{10x^3(1-x) + 4(1-x)^2(2x^2+x+2)}{5(1-x^5)} + \frac{2}{5(1-x)},\\
G_6^{FF} &= 2G_2^{FF} + \frac{2(1-x)(5x^5+10x^4+x^3-x^2+11x+9)}{7(1-x^7)} + \frac{3}{7(1-x)},\\
G_7^{FF} &= G_3^{FF} + \frac{p_7^{FF}(x^6+x^3+1)(1-x^2)}{3(1-x^{18})} + \frac{(1-x)(1-x^2)^2(x^2+x+1)^2}{3(1-x^6)^2} + \frac{1}{3(1-x)},\\
G_8^{FF} &= \frac{-3G_4^{FF} + G_1^{FF}}{11} + \frac{2(1+x)(1-x^{11})p_{8;1}^{FF}}{11(1-x^{22})} + \frac{2(1-x^8)p_{8;2}^{FF}}{(1-x^{16})} - \frac{15}{11(1-x)},\\
G_9^{FF} &= G_3^{FF} + \frac{p_{9;1}^{FF}}{(1-x^{20})} + \frac{p_{9;2}^{FF}}{(1-x^{14})} + \frac{2(1-x)p_{9;3}^{FF}}{13(1-x^{13})} + \frac{2}{13(1-x)},\\
G_{10}^{FF} &= \frac{1}{9}G_4^{FF} + \frac{4p_{10;1}^{FF}}{3(1-x^{18})} + \frac{2p_{10;2}^{FF}}{5(1-x^{15})} - \frac{p_{10;3}^{FF}}{2(1-x^{12})} - \frac{p_{10;4}^{FF}}{90(1-x^6)^2} + \frac{p_{10;5}^{FF}}{90(1-x^6)} + \frac{4}{15(1-x)},\\
G_{11}^{FF} &= G_3^{FF} + \frac{p_{11;1}^{FF}}{(1-x^{34})} + \frac{p_{11;2}^{FF}}{(1-x^{16})} - \frac{2(1-x^2)p_{11;3}^{FF}}{7(1-x^{14})} + \frac{(1-x)p_{11;4}^{FF}}{11(1-x^{11})} + \frac{27}{77(1-x)},
\end{aligned}
\tag{6.74}
$$

$$
\begin{aligned}
p_7^{FF} &= x^9 + x^8 + 2x^6 - 7x^5 + 4x^4 - 4x^3 + 7x^2 - 2x + 1, \\
p_{8;1}^{FF} &= 8x^9 + 9x^7 - 2x^6 + x^5 + 5x^4 - 5x^3 - x^2 + 2x - 9, \\
p_{8;2}^{FF} &= -x^7 - x^6 - 2x^5 - x^4 + x + 2, \\
p_{9;1}^{FF} &= 2(2x^5 + x^4 - x - 2)(1 + x^2)(1 - x^{10}), \\
p_{9;2}^{FF} &= 2(-x^5 - x^3 + x^2 - x + 1)(1 + x)(1 - x^7), \\
p_{9;3}^{FF} &= 14x^{11} + 28x^{10} + 16x^9 + 17x^8 - 8x^7 - 7x^6 + 7x^5 + 21x^4 + 35x^3 + 36x^2 + 11x + 12, \\
p_{10;1}^{FF} &= x(1 - x)(x^6 + x^3 + 1)(1 - x^6), \\
p_{10;2}^{FF} &= (1 + x)(1 - x^3)(2x^{10} - 4x^8 + 4x^7 + 4x^6 - 7x^5 + x^4 + 7x^3 - 4x^2 - 2x + 4), \\
p_{10;3}^{FF} &= (1 - x^6)(5x^5 + 5x^4 - 4x^3 - 7x^2 + 7x + 4), \\
p_{10;4}^{FF} &= (1 - x)(1 - x^2)^2(37x^4 + 86x^3 + 111x^2 + 86x + 37), \\
p_{10;5}^{FF} &= (97x^3 + 97x^2 + 48x + 49)(1 - x^2), \\
p_{11;1}^{FF} &= 2x^2(1 + x)(1 - x^{17})(x^{13} - 2x^9 + x^8 + x^6 + x^5 - x^4 - x^3 - x + 2), \\
p_{11;2}^{FF} &= (1 - x^8)(x^7 + x^6 + x^5 - 3x^4 - x^3 + x^2 + 3x - 1), \\
p_{11;3}^{FF} &= 8x^{11} + 8x^{10} + 2x^9 + 9x^8 - 4x^7 - 4x^6 - 3x^5 + 11x^4 + 12x^3 + 12x^2 - x + 6, \\
p_{11;4}^{FF} &= -4x^9 - 8x^8 - 56x^7 - 16x^6 + 24x^5 + 20x^4 - 28x^3 - 32x^2 + 8x + 48.
\end{aligned} \tag{6.75}
$$

Z^{FF} L_h	1	2	3	4	5	6	7	8	9	10	11
T_{F+} order	2	2	4	5	9	12	21	30	51	76	127
min rec order	2	2	4	5	9	9	17	21	31	35	51
period	6	4	8	–	40	28	–	–	3640	–	20944

Table 6.B.17: The minimal order of the recursion relation and the period of the repeating sequence of $Z_{L_v,L_h}^{FF}(-1)$ as a function of L_v.

6.C Hard square equimodular curves as $|z| \to \infty$

Consider hard squares for a system of width $L_h = 2L$ sites. The boundary conditions can be free or periodic, but not restricted by parity or momentum. We wish to show that the transfer matrices $T_C(z; L_h)$ and $T_F(z; L_h)$ both have $2L$ branches of equimodular curves going out to $|z| \to \infty$.

Let A (resp. B) denote the maximally packed state with L particles occupying the even (resp. odd) numbered sites. Similarly, for $k \ll L$, let A_k denote the classes of states having $L - k$ particles of which $O(L)$ have positions overlapping with those of A and $O(1)$ overlap with those of B. More loosely, the states A_k have the same order as A, up to small local perturbations. The states B_k are similarly defined from B.

To discuss the $|z| \to \infty$ limit we replace z by z^{-1} and consider a perturbation theory for $|z| \ll 1$. After division by an overall factor, the Boltzmann weight of state A is 1, and each of the states in the class A_k have weight z^k.

To order zero (i.e., considering only states A and B) the transfer matrix is the permutation matrix of size 2, with eigenvalues $\lambda_1 = 1$ and $\lambda_2 = -1$.

To order $k \ll L$ it is easy to see that the only non-zero matrix elements connect an A-type state to a B-type state and vice versa. Physically this means that if we start from a state which has predominantly particles on the even sublattice, it will remain so forever: we stay in the same ordered phase. Mathematically it is not hard to see that this implies that the eigenvalues λ_1 and λ_2 will continue to just differ by an overall sign, order by order in perturbation theory. Other eigenvalues are $O(z)$, hence play no role since then cannot be equimodular with λ_1 and λ_2.

The perturbative result $\lambda_1 + \lambda_2 = 0$ breaks down at an order k which is sufficiently high to create a domain wall across the strip/cylinder/torus between the two different ordered states. This happens precisely for $k = L$. It follows that $\lambda_1 + \lambda_2 = O(z^L)$, implying that

$$\lambda_2/\lambda_1 = -1 + O(z^L)\,. \tag{6.76}$$

To obtain equimodularity, the left-hand side must be on the unit circle. For $|z| \ll 1$ this will happen when z^L is perpendicular to -1, so that $\arg(z^L) = \pm\pi/2$. It follows that there are $2L$ equimodular curves going out of $z = 0$ with the angles

$$\arg(z) = \frac{(1+2k)\pi}{2L} \text{ with } k = 0, 1, \ldots, 2L-1. \tag{6.77}$$

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