Symmetry, Sliding Windows and Transfer Matrices.

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In this paper we study 1D k-neighbor Ising model. Variational approach using modified nearest-neighbor interaction strength is developed, but the optimization of the coupling constant appears at least as hard as the exact solution in the general case. For the exact solution two formulations of transfer matrix are studied: the block-spin approach yielding matrix T and the 'sliding window' approach yielding matrix T_s . Equivalence between the two is established with $T_s^k = T$ holding universally. Matrix T_s is sparse and possesses apparent symmetries, giving hope for analytical computation of eigenvalues. Special cases are worked out explicitly. Finally, in the appendix we compute the exact partition function for the 2D Ising model on an anisotropic triangular lattice, using graphical techniques as shown in [1].

PACS numbers:

I. INTRODUCTION

Despite its seeming simplicity, Ising models hold many theoretical challenges, especially when it comes to exact analytical calculations. The significance of the obtaining such results lies in their Universality (c.f. e.g. [1]), meaning that the insights obtained from Ising model will be applicable to a variety of real physical systems, too complicated to study in their full generality.

The 1D nearest-neighbor Ising model has been solved exactly with arbitrary magnetic field. Following the work of Onsager ([2]), and consequent simplifications of the treatment, the exact solution for 2D lattices has been achieved, with zero magnetic field.

In this paper, we investigate analytic approaches to k-neighbor Ising model (kNIM). In Section II A we develop a variational formulation for kNIM. Following the apparent difficulty of analytical optimization of the parameters of the variational anzats, we investigate the connections between two alternative formulations of transfer matrices. In Section II B we show that the two approaches are indeed equivalent and explore some of the consequences of the new formulation. In Appendix we discuss the general case and conclude with the exact partition function for the 2D anisotropic triangular lattice.

II. K-NEIGHBOR 1D ISING MODEL

The Hamiltonian, with indices taken modulo N is:

$$-\beta H = \sum_{i=1}^{k} K_j \sum_{i=1}^{N} S_i S_{i+j} = \sum_{i=1}^{N} \sum_{j=1}^{k} K_j S_i S_{i+j}.$$

A. Variational Estimates

Here we give an estimate of the free energy of the radius-k model through the variational principle, with the exactly solvable single parameter nearest-neighbor model as the trial distribution.

The well-known variational principle states

$$\beta F \le \beta \tilde{F} \equiv \min_{I} \left\{ \beta F_0 + \langle \beta H - \beta H_0 \rangle_0 \right\},\tag{1}$$

where $\langle \rangle_0$ refer to averages taken with respect to the trial distribution.

Our trial distribution is the nearest neighbor Ising model with the Hamiltonian:

$$\beta H_0 = J \sum_{i=1}^{N} S_i S_{i+1},$$

where again all the indices are understood modulo N. For such a model, denoting $t = \tanh J$

$$\beta F_0 = -\ln Z_0 = -\left(N\ln\left[2\cosh J\right] + \ln\left[1 + t^N\right]\right) = -N\ln 2 + \frac{N}{2}\ln(1 - t^2) - \ln\left[1 + t^N\right].$$

Moreover,

$$\langle S_i S_{i+j} \rangle_0 = \frac{t^j + t^{N-j}}{1 + t^N}. \tag{2}$$

Using (2),

$$\langle \beta H_0 \rangle_0 = J \sum_{i=1}^N \langle S_i S_{i+1} \rangle_0 = N J \frac{t + t^{N-1}}{1 + t^N},$$

$$\langle \beta H \rangle_0 = \sum_{i=1}^N \sum_{j=1}^k K_j \langle S_i S_{i+j} \rangle_0 = N \sum_{j=1}^k K_j \frac{t^j + t^{N-j}}{1 + t^N}$$

Consequently,

$$\beta \tilde{F} = -N \ln 2 + \min_{t} \left\{ \frac{N}{2} \ln(1 - t^{2}) - \ln\left[1 + t^{N}\right] + \frac{N}{1 + t^{N}} \left(\sum_{j=1}^{k} K_{j}(t^{j} + t^{N-j}) - J(t + t^{N-1}) \right) \right\}.$$

We need to minimize

$$\Psi = \frac{N}{2}\ln(1-t^2) - \ln\left[1+t^N\right] + \frac{N}{1+t^N} \left(\sum_{j=1}^k K_j(t^j+t^{N-j}) - J(t+t^{N-1})\right).$$

$$\frac{d\Psi}{dt} = \frac{Nt}{1-t^2} - \frac{Nt^{N-1}}{1+t^N} - \frac{N^2t^{N-1}}{(1+t^N)^2} \left(\sum_{j=1}^k K_j(t^j + t^{N-j}) - J(t+t^{N-1}) \right)
+ \frac{N}{1+t^N} \left(\sum_{j=1}^k K_j(jt^{j-1} + (N-j)t^{N-j-1}) - J(1+(N-1)t^{N-2}) - \frac{t+t^{N-2}}{1-t^2} \right).$$

Unfortunately, it is impossible to solve for $\frac{d\Psi}{dt}=0$ analytically, since it involves solving for general roots of polynomial of degree N. One conceivable approximation would be small-coupling, large N (such that one could neglect terms of the order of Nt^N etc.), but this is not much simpler than solving the exact model.

B. Exact Partition Function for 1D NNN Ising Model

Here we compute the exact partition function for the Next-Nearest-Neighbor Cyclic 1D Ising model. We do it in two different ways, both by the method of transfer matrices, differing in the way the transfer matrix is defined. The second way is somewhat less orthodox and the purpose of the exercise in this Section is to convince ourselves that these approaches are indeed equivalent. The benefit of the less orthodox approach is that the transfer matrix is sparse and has symmetries that could potentially enable exact computations for arbitrary k.

The Hamiltonian for the NNN case (again all indices are modulo N) is

$$-\beta H = \sum_{i=1}^{N} S_i (K_1 S_{i+1} + K_2 S_{i+2}).$$

The topology of the model is shown in Figure 1.

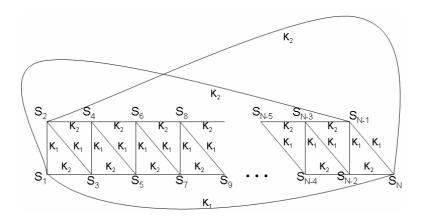


FIG. 1: 1D NNN Ising model

1. The Conventional Transfer Matrix

Let us employ the conventional transfer matrix approach, having 1 or $e^{\alpha k_1 + \beta k_2}$ as its entries.

$$\begin{split} Z &= \sum_{\{S_i\}} \prod_{i=1}^N e^{S_i \sum_{j=1}^k K_j S_{i+j}} = tr[\quad \left\langle S_1 S_2 | e^{K_1(S_1 S_2 + S_2 S_3) + K_2(S_1 S_3 + S_2 S_4)} | S_3 S_4 \right\rangle \\ & \cdot \quad \left\langle S_3 S_4 | e^{K_1(S_3 S_4 + S_4 S_5) + K_2(S_3 S_5 + S_4 S_6)} | S_5 S_6 \right\rangle \\ & \vdots \\ & \cdot \quad \left\langle S_{N-1} S_N | e^{K_1(S_{N-1} S_N + S_N S_1) + K_2(S_{N-1} S_1 + S_N S_2)} | S_1 S_2 \right\rangle] \\ & = tr \ [\ T^{N/2} \], \end{split}$$

where T is a 4x4 transfer matrix with elements $\langle S_1 S_2 | T | S_3 S_4 \rangle = e^{K_1(S_1 S_2 + S_2 S_3) + K_2(S_1 S_3 + S_2 S_4)}$, explicitly

$$T = \begin{pmatrix} e^{2(k_1 + k_2)} & e^{2k_1} & 1 & e^{-2k_2} \\ e^{-2k_1} & e^{-2k_1 + 2k_2} & e^{-2k_2} & 1 \\ 1 & e^{-2k_2} & e^{-2k_1 + 2k_2} & e^{-2k_1} \\ e^{-2k_2} & 1 & e^{2k_1} & e^{2(k_1 + k_2)} \end{pmatrix}$$

2. The 'Sliding Window' Transfer Matrix

Alternatively,

$$Z = \sum_{\{S_i\}} \prod_{i=1}^{N} e^{S_i \sum_{j=1}^{k} K_j S_{i+j}} = tr[\quad \langle S_1 S_2 | e^{S_1(K_1 S_2 + K_2 S_3)} | S_2 S_3 \rangle$$

$$\cdot \quad \langle S_2 S_3 | e^{S_2(K_1 S_3 + K_2 S_4)} | S_3 S_4 \rangle$$

$$\vdots$$

$$\cdot \quad \langle S_i S_{i+1} | e^{S_i(K_1 S_{i+1} + K_2 S_{i+2})} | S_{i+1} S_{i+2} \rangle$$

$$\vdots$$

$$\cdot \quad \langle S_N S_1 | e^{S_N(K_1 S_1 + K_2 S_2)} | S_1 S_2 \rangle]$$

$$= tr \ [T_s^N],$$

where T_s is a 4x4 transfer matrix with elements $\langle S_1 S_2 | T | S_2 S_3 \rangle = e^{S_1(K_1 S_2 + K_2 S_3)}$, naively written as

$$T_s = \begin{pmatrix} e^{k_1 + k_2} & e^{k_1 - k_2} & 0 & 0\\ 0 & 0 & e^{-k_1 + k_2} & e^{-(k_1 + k_2)}\\ e^{-(k_1 + k_2)} & e^{-k_1 + k_2} & 0 & 0\\ 0 & 0 & e^{k_1 - k_2} & e^{k_1 + k_2} \end{pmatrix}.$$

It is really tempting to rearrange (relabeling) the rows of T_s , toobtain a block-diagonal matrix

$$T_s^{(b)} = \begin{pmatrix} e^{k_1 + k_2} & e^{k_1 - k_2} & 0 & 0\\ e^{-(k_1 + k_2)} & e^{-k_1 + k_2} & 0 & 0\\ 0 & 0 & e^{-k_1 + k_2} & e^{-(k_1 + k_2)}\\ 0 & 0 & e^{k_1 - k_2} & e^{k_1 + k_2} \end{pmatrix}.$$

However, unfortunately, in the general case, T_s and $T_s^{(b)}$ will not have the same eigenvalues, since they are not connected by similarity transformation.

3. Comparison of the Two Approaches

Examining the two formulations, it becomes obvious that they are completely equivalent provided $T = T_s^2$ holds, and it indeed holds:

$$T_s^2 = \begin{pmatrix} e^{k_1 + k_2} & e^{k_1 - k_2} & 0 & 0 \\ 0 & 0 & e^{-k_1 + k_2} & e^{-(k_1 + k_2)} \\ e^{-(k_1 + k_2)} & e^{-k_1 + k_2} & 0 & 0 \\ 0 & 0 & e^{k_1 - k_2} & e^{k_1 + k_2} \end{pmatrix}^2 = \begin{pmatrix} e^{2(k_1 + k_2)} & e^{2k_1} & 1 & e^{-2k_2} \\ e^{-2k_1} & e^{-2k_1 + 2k_2} & e^{-2k_2} & 1 \\ 1 & e^{-2k_2} & e^{-2k_1 + 2k_2} & e^{-2k_1} \\ e^{-2k_2} & 1 & e^{2k_1} & e^{2(k_1 + k_2)} \end{pmatrix} = T.$$

Since we have shown equivalence at the level of transfer matrices, it is cleat that all derived quantities will agree too. Moreover, the derivations are by no means unique to the NNN model and hold for a general k-neighbors also. We thus have established the equivalence of the two approaches for transfer matrix computations.

To compute the exact NNN partition function, lets use T_s . The eigenvalues of the matrix T_s are:

$$\lambda_{1\pm} = e^{K_2} \left(\cosh K_1 \pm \sqrt{(\sinh K_1)^2 + e^{-4K_2}} \right),$$

$$\lambda_{2\pm} = e^{K_2} \left(\sinh K_1 \pm \sqrt{(\cosh K_1)^2 - e^{-4K_2}} \right).$$

Consequently,

$$Z = e^{NK_2} \left[\left(\cosh K_1 + \sqrt{(\sinh K_1)^2 + e^{-4K_2}} \right)^N + \left(\cosh K_1 - \sqrt{(\sinh K_1)^2 + e^{-4K_2}} \right)^N + \left(\sinh K_1 + \sqrt{(\cosh K_1)^2 - e^{-4K_2}} \right)^N + \left(\sinh K_1 - \sqrt{(\cosh K_1)^2 - e^{-4K_2}} \right)^N \right].$$

III. DISCUSSION AND FUTURE DIRECTIONS

In this paper we considered analytical approaches to Ising models with long-range interactions. The symmetry structure of the newly developed 'sliding window' transfer matrix is promising and merits further research. It is shown for instance, that NNNN partition function is computable exactly using these symmetries. It would be interesting to continue the investigation of the symmetry properties and ways to use them to obtain non-trivial exact results.

IV. APPENDIX

A. Why the Exact Partition Function for the 1D Ising Model With K neighbors is Still Not Computed

Now that we have convinced ourselves through simple example that the two alternative transfer matrix formulations are indeed equivalent, the treatment for the k-neighbor Ising model follows as a simple generalization of the k=2 case.

$$Z = \sum_{\{S_i\}} \prod_{i=1}^{N} e^{S_i \sum_{j=1}^{k} K_j S_{i+j}} = tr[\quad \langle S_1 S_2 \cdots S_k | e^{S_1 \sum_{j=1}^{k} K_j S_{1+j}} | S_2 S_3 \cdots S_{k+1} \rangle$$

$$\cdot \quad \langle S_2 S_3 \cdots S_{k+1} | e^{S_2 \sum_{j=1}^{k} K_j S_{2+j}} | S_3 S_4 \cdots S_{k+2} \rangle$$

$$\vdots$$

$$\cdot \quad \langle S_i S_{i+1} \cdots S_{k+i-1} | e^{S_i \sum_{j=1}^{k} K_j S_{i+j}} | S_{i+1} S_{i+2} \cdots S_{k+i} \rangle$$

$$\vdots$$

$$\cdot \quad \langle S_N S_1 \cdots S_{k-1} | e^{S_N \sum_{j=1}^{k} K_j S_{N+j}} | S_1 S_2 \cdots S_k \rangle]$$

$$= tr \left[T_{S(k)}^N \right],$$

where $T_{s(k)}$ is a $2^k x 2^k$ 'sliding window' transfer matrix with entries

$$\langle S_1 S_2 \cdots S_k | T_{s(k)} | S_1' S_2' \cdots S_k' \rangle = \begin{cases} e^{S_1 \sum_{j=1}^k K_j S_j'} & \text{If } (S_2, S_3, ..., S_k) = (S_1', S_2', ..., S_{k-1}'), \\ 0 & \text{Otherwise (since mutually inconsistent)}. \end{cases}$$

It is important to note that each row and column of $T_{s(k)}$ has exactly 2 entries $\langle S_1 S_2 \cdots S_k | T_{s(k)} | S_2 S_3 \cdots S_{k+1} \rangle = e^{S_1 \sum_{j=1}^k K_j S_{1+j}}$, and the rest are zeros. The matrix $T_{s(k)}$ is sparse, with the number of non-zero entries linear in matrix size. For instance, for NNNN model, we have the following matrix (denote $\kappa_i = e^{K_i}$):

1		$ +++\rangle$	$ ++-\rangle$	$ + -+ \rangle$	$ +\rangle$	$ -++\rangle$	$ -+-\rangle$	$ +\rangle$	$ \rangle$
	$\langle + + + $	$\kappa_1 \kappa_2 \kappa_3$	$\kappa_1 \kappa_2 / \kappa_3$	0	0	0	0	0	0
ı	$\langle + + - $	0	0	$\kappa_1 \kappa_3 / \kappa_2$	$\kappa_1/(\kappa_2\kappa_3)$	0	0	0	0
ı	$\langle + - + $	0	0	0	0	$\kappa_2 \kappa_3 / \kappa_1$	$\kappa_2/(\kappa_1\kappa_3)$	0	0
ı	$\langle + $	0	0	0	0	0	0	$\kappa_3/(\kappa_1\kappa_2)$	$1/(\kappa_1\kappa_2\kappa_3)$
ı	$\langle -++ $	$1/(\kappa_1\kappa_2\kappa_3)$	$\kappa_3/(\kappa_1\kappa_2)$	0	0	0	0	0	0
ı	$\langle -+- $	0	0	$\kappa_2/\kappa_1\kappa_3$	$(\kappa_2\kappa_3)/\kappa_1$	0	0	0	0
l	$\langle+ $	0	0	0	0	$\kappa_1/(\kappa_2\kappa_3)$	$\kappa_1 \kappa_3 / \kappa_2$	0	0
/	$\langle $	0	0	0	0	0	0	$\kappa_1 \kappa_2 / \kappa_3$	$\kappa_1 \kappa_2 \kappa_3$

The matrix has a pronounced symmetry, which gives hope for an analytical solution for the eigenvalues. Actually, the solution for NNNN is possible, since it involves quartic polynomials. Due to a severe lack of time we have not been able to conclude our calculations for NNNN.

Unfortunately, tempting as it is, in spite of the fact that $T_{s(k)}$ can be cast into a block-diagonal term by the cyclic shift of one of it's coordinates, this will change the eigenvalues.

1	,	$ + + + \rangle$	$ ++-\rangle$	$ + -+ \rangle$	$ +\rangle$	$ -++\rangle$	$ -+-\rangle$	$ + \rangle$	$ \rangle$	
1	$\langle + + + $	$\kappa_1 \kappa_2 \kappa_3$	$\kappa_1 \kappa_2 / \kappa_3$	0	0	0	0	0	0	
1	$\langle -++ $	$1/(\kappa_1\kappa_2\kappa_3)$	$\kappa_3/(\kappa_1\kappa_2)$	0	0	0	0	0	0	ı
1	$\overline{\langle + + - }$	0	0	$\kappa_1 \kappa_3 / \kappa_2$	$\kappa_1/(\kappa_2\kappa_3)$	0	0	0	0	
1	$\langle -+- $	0	0	$\kappa_2/\kappa_1\kappa_3$	$(\kappa_2\kappa_3)/\kappa_1$	0	0	0	0	١.
1	$\overline{\langle +-+ }$	0	0	0	0	$\kappa_2 \kappa_3 / \kappa_1$	$\kappa_2/(\kappa_1\kappa_3)$	0	0	
1	$\langle+ $	0	0	0	0	$\kappa_1/(\kappa_2\kappa_3)$	$\kappa_1 \kappa_3 / \kappa_2$	0	0	
1	$\overline{\langle + }$	0	0	0	0	0	0	$\kappa_3/(\kappa_1\kappa_2)$	$1/(\kappa_1\kappa_2\kappa_3)$	
/	(0	0	0	0	0	0	$\kappa_1 \kappa_2 / \kappa_3$	$\kappa_1 \kappa_2 \kappa_3$ /	

The determinant, $\prod_i \lambda_i$ is correct and can be computed easily. Since we were not sure of the utility of the calculation, we did not pursue this explicitly.

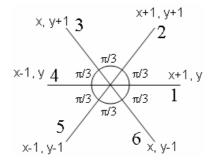


FIG. 2: Direction labels for 2D triangular lattice

B. Exact Partition Function for the Ising Model on 2D Triangular Lattice

Here we develop the exact partition function for the Ising model on 2D triangular lattice, using graphic techniques. It is easy to see that the same approach that worked for the square lattice works also here. Denoting $t_i = tanh(K_i)$, and repeating the steps in [1], we get

$$\frac{\ln Z}{N} = \ln(2\prod_{i=1}^{3} \cosh(K_i)) - \frac{1}{2N} \sum_{\overline{q}} tr \ln(1 - T^*(\overline{q})) = \ln(2\prod_{i=1}^{3} \cosh(K_i)) - \frac{1}{2} \int \frac{d^2 \overline{q}}{(2\pi)^2} \ln \det(1 - T^*(\overline{q})),$$

where in the last equality we used the fact that $tr \ln(1 - T^*(\overline{q})) = \ln \det(1 - T^*(\overline{q}))$. The directions for building the T^* matrix are shown in Figure 2. Using these, we have the following directions map

/	$\rightarrow * \rightarrow$	$\rightarrow *$ \nearrow	$\rightarrow * $ $^{\setminus}$	$\rightarrow * \leftarrow$	→ * <u>/</u>	$\rightarrow * \nearrow$	\
l	$\nearrow * \rightarrow$	/*/	/ * \	/* * ←	/*/	/* \	1
	/ * \	\\ * \\ \	*\	\ * ←	* \	\ * \	l
l	<u>←*</u> <u></u>	← * /	← * \	← * ←	← * ✓	← * ✓	'
l	✓ * \	/*/	✓ * \	∠ * ←	/ * /	/* \	
/	<u>*\</u>	*/	/*/	_ * ←	*/	_*_	/

Consequently,

$$T^*(q) = \begin{pmatrix} t_1 e^{-iq_x} & t_1 e^{-i(q_x + \pi/3)} & t_1 e^{-i(q_x + 2\pi/3)} & 0 & t_1 e^{-i(q_x - 2\pi/3)} & t_1 e^{-i(q_x - \pi/3)} \\ t_2 e^{-i(q_x + q_y - \pi/3)} & t_2 e^{-i(q_x + q_y)} & t_2 e^{-i(q_x + q_y + \pi/3)} & t_2 e^{-i(q_x + q_y + 2\pi/3)} & 0 & t_2 e^{-i(q_x + q_y - 2\pi/3)} \\ t_3 e^{-i(q_y - 2\pi/3)} & t_3 e^{-i(q_y - \pi/3)} & t_3 e^{-iq_y} & t_3 e^{-i(q_y + \pi/3)} & t_3 e^{-i(q_y + 2\pi/3)} & 0 \\ 0 & t_1 e^{i(q_x + 2\pi/3)} & t_1 e^{i(q_x + \pi/3)} & t_1 e^{iq_x} & t_1 e^{i(q_x - \pi/3)} & t_1 e^{i(q_x - 2\pi/3)} \\ t_2 e^{i(q_x + q_y - 2\pi/3)} & 0 & t_2 e^{i(q_x + q_y + 2\pi/3)} & t_2 e^{i(q_x + q_y + \pi/3)} & t_2 e^{i(q_x + q_y)} & t_2 e^{i(q_x + q_y - \pi/3)} \\ t_3 e^{i(q_y - \pi/3)} & t_3 e^{i(q_y - 2\pi/3)} & 0 & t_3 e^{i(q_y + 2\pi/3)} & t_3 e^{i(q_y + \pi/3)} & t_3 e^{i(q_y + \pi/3)} \end{pmatrix}$$

Denoting $X \equiv e^{iq_x}$, $Y \equiv e^{iq_y}$, $\Omega \equiv e^{i\pi/3}$,

$$T^*(q) = \begin{pmatrix} \frac{t_1 X^{-1}}{t_2 (XY)^{-1}\Omega} & t_1 X^{-1}\Omega^{-1} & t_1 X^{-1}\Omega^{-2} & 0 & t_1 X^{-1}\Omega^2 & t_1 X^{-1}\Omega \\ \frac{t_2 (XY)^{-1}\Omega}{t_3 Y^{-1}\Omega} & t_2 (XY)^{-1} & t_2 (XY)^{-1}\Omega^{-1} & t_2 (XY)^{-1}\Omega^{-2} & 0 & t_2 (XY)^{-1}\Omega^2 \\ \hline t_3 Y^{-1}\Omega^2 & t_3 Y^{-1}\Omega & t_3 Y^{-1} & t_3 Y^{-1}\Omega^{-1} & t_3 Y^{-1}\Omega^{-2} & 0 \\ \hline 0 & t_1 X\Omega^2 & t_1 X\Omega & t_1 X & t_1 X\Omega^{-1} & t_1 X\Omega^{-2} \\ \hline t_2 XY\Omega^{-2} & 0 & t_2 XY\Omega^2 & t_2 XY\Omega & t_2 XY & t_2 XY\Omega^{-1} \\ \hline t_3 Y\Omega^{-1} & t_3 Y\Omega^{-2} & 0 & t_3 Y\Omega^2 & t_3 Y\Omega & t_3 Y \end{pmatrix}$$

Using Mathematica, we arrive at the following expression

$$\det(1 - T^*(q)) = \frac{\prod_{i=1}^{3} \cosh(2K_i) - \prod_{i=1}^{3} \sinh(2K_i) - \sinh(2K_1) \cos(q_x) - \sinh(2K_2) \cos(q_y) - \sinh(2K_3) \cos(q_x + q_y)}{\cosh^2(K_1) \cosh^2(K_2) \cosh^2(K_3)}.$$

Summarizing,

$$\ln \frac{Z}{2} = \frac{N}{2} \int_0^{2\pi} \frac{dq_x^2 dq_y^2}{(2\pi)^2} \ln \left[\prod_{i=1}^3 \cosh(2K_i) - \prod_{i=1}^3 \sinh(2K_i) - \sinh(2K_1) \cos(q_x) - \sinh(2K_2) \cos(q_y) - \sinh(2K_3) \cos(q_x + q_y) \right].$$

- [1] M. Kardar, "Statistical Physics of Fields," Cambridge University Press, 2007.
- $[2]\ L$ Onsager, Phys. Rev. 65, 117 (1944).