

The Statistics of Dimers on a Three-Dimensional Lattice. II. An Improved Lower Bound

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The model proposed in the previous paper is used to improve the Hammersley lower bound for three-dimensional dimer problem.

KEY WORDS: Dimers; correlation functions; lower bound.

1. INTRODUCTION

In the previous paper,⁽¹⁾ hereafter referred to as I, we dealt with the number of ways of dissecting an N -brick (with sides of length l_1, l_2, l_3) into dimers. We have considered dissections that do not generate any closed path on the set of points with only even (A_0 sublattice) or only odd (B_0 sublattice) coordinates. It was found that the number of such dissections is

$$\varphi'_N = \exp \left\{ \sum_{a_1=0}^{l_1/2-1} \sum_{a_2=0}^{l_2/2-1} \sum_{a_3=0}^{l_3/2-1} \ln \left[4 \sum_{j=1}^3 \sin^2 \left(\frac{2\pi a_j}{l_j} \right) \right] \right\}$$

The dissections considered can be found among all the possible dissections of an N -brick; therefore, the following inequality is true for the number of arbitrary dissections:

$$\varphi_N \geq \varphi'_N$$

For the limiting value

$$\lambda = \lim_{N \rightarrow \infty} (1/N) \ln \varphi_N$$

we have the bound

$$\lambda \geq \lambda' = \frac{1}{4\pi} \int_0^\pi \int_0^\pi \int_0^\pi d\alpha_1 d\alpha_2 d\alpha_3 \ln \left[4 \sum_{j=1}^3 \sin^2 \alpha_j \right] \quad (1)$$

which coincides with the lower bound obtained by Hammersley.⁽²⁾

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In this paper we improve the lower bound in (1). To this end in Section 2 we consider a class of dissections of an N -brick, which generate at least one closed path. Their contribution to φ_N can be evaluated by using correlation functions of the exact solvable model considered in I (model I). In Section 3 a general expression for the correlation functions is derived. Numerical results for these functions and the improved lower bound for λ are presented in Section 4.

2. A CLASS OF FORBIDDEN CONFIGURATIONS

It will be convenient to use below the following equivalent formulation of the dimer problem. An N -brick is the union of N unit cubes. Define, as in I, a lattice L with sites in the centers of the cubes and with edges connecting the nearest sites. Every dissection of the N -brick into dimers corresponds to a dissection of the lattice L into nonintersecting pairs of adjacent sites. Here a dimer is an edge together with the pair of sites incident to it.

Let C be an arbitrary dissection obeying the rules of the model I. A closed nonintersecting line composed of the lattice edges, one half of which are dimers, will be called a contour. If x_1, x_2, \dots, x_n are the lattice sites belonging to the contour and $(x_1x_2), (x_3x_4), \dots, (x_{n-1}x_n)$ are the dimers, then by the "shift" of these dimers along the contour we will understand their substitution by dimers $(x_2x_3), (x_4x_5), \dots, (x_nx_1)$. The shift of dimers along any contour leads to a dissection C' different from C . It may turn out that C' generates closed paths on the sublattices of L .

In fact, consider two configurations of seven dimers Ω_1 and Ω_2 (Fig. 1). The dimers a, b, c and dotted edges form a contour. The dissections containing Ω_1 and generating no closed path transform into dissections with the closed path on the sites 1, 2, 3, 4 under the shift of dimers a, b, c along the contour.

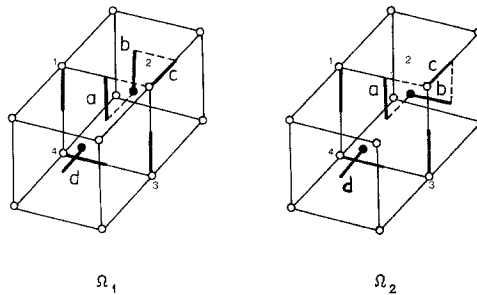


Fig. 1.

Let $P(n_1)$ be the probability that in a given dissection one can find n_1 configurations of the type Ω_1 . The shifts of dimers along each of contours contained in these configurations produce dissections absent from the φ'_N dissections obeying the conditions of model I. Hence, using also convexity of the exponential we have

$$\varphi_N \geq \varphi'_N \sum_{n_1} 2^{n_1} P(n_1) \geq \varphi'_N 2^{\bar{n}_1} \tag{2}$$

where $\bar{n}_1 = \sum_{n_1} n_1 P(n_1) = \langle \Omega_1 \rangle N/8$, $N/8$ is the number of sublattice sites. Here we introduced the correlation function $\langle \Omega_1 \rangle$ defined as the ratio of the number of dissections that contain Ω_1 in a given sublattice site to the total number of dissections obeying the conditions of model I.

To improve the bound in (2), consider additionally configurations of the type Ω_2 (Fig. 1) and note that the dimer d in Ω_1, Ω_2 can occupy five different positions. For a fixed position of the dimer d there exist 8 ways to arrange the dimer b and dimers on the sites 1, 2, 3, 4 to obtain a configuration of the type Ω_i . To each indicated configuration there corresponds a configuration reflected with respect to the square 1234, which can be also oriented in three directions. The number of configurations under consideration should be doubled because of symmetry with respect to the replacement of sublattice A_0 by sublattice B_0 . We get 96 configurations of each type Ω_i^δ where δ labels the five positions of the dimer d and $i = 1, 2$.

Note that contours in different configurations can possess common dimers and no shift can thus be made along every contour independently. To determine the number of possible shifts, we ascribe to each contour from the set of Ω_i -type configurations a point of a graph G . If two contours have common dimers, the two corresponding points of G are connected by an arc.

It can easily be verified by construction that every dimer belongs at most to two contours. So, the number of arcs emerging from each point of G does not exceed 3. Let i be an arbitrary point of G . We may imagine i to be colored black if one shifts dimers along the contour, corresponding to i , and white otherwise. Then, the number of possible shifts in the set of contours equals the number of ways in which points of G ($\text{deg } i \leq 3$ for all $i \in G$) can be colored with two colors such that adjacent points have never the black color.

The needed number can be bounded above by the series

$$1 + \mathfrak{N} + \frac{\mathfrak{N}(\mathfrak{N} - 4)}{2!} + \frac{\mathfrak{N}(\mathfrak{N} - 4)(\mathfrak{N} - 8)}{3!} + \dots = 5^{\mathfrak{N}/4}$$

where \mathfrak{N} is the number of points of the graph G .

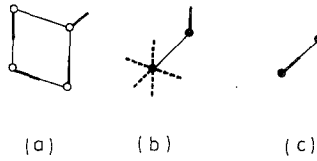


Fig. 2.

Taking into account the obvious identity $\langle \Omega_1^\delta \rangle = \langle \Omega_2^\delta \rangle$ we have

$$\mathcal{F} = 24N \sum_{\delta=1}^5 \langle \Omega_1^\delta \rangle$$

which leads to the estimate

$$\lambda \geq \lambda' + 6 \sum_{\delta=1}^5 \langle \Omega_1^\delta \rangle \ln 5 \quad (3)$$

As was pointed out in I, dimers on the sublattices A_0 and B_0 are arranged independently, so $\langle \Omega_1^\delta \rangle$ can be decoupled into two correlation functions. The configuration of dimers on the sublattice A_0 is shown in Fig. 2a and the corresponding correlation function is denoted by ω_1 . The dotted lines in Fig. 2b show five positions of the dimer d on the sublattice B_0 with the fixed position of the dimer b . The sum of two-point correlation functions over all dotted dimer positions is $\langle \omega_2 \rangle$. The correlation functions $\langle \omega_2 \rangle$ and $\langle \omega_3 \rangle$ (see Fig. 2c) are related by the simple identity

$$\langle \omega_2 \rangle + \langle \omega_3 \rangle = 1/6 \quad (4)$$

following from symmetry of the model.

We then obtain from (3) and (4)

$$\lambda \geq \lambda' + \langle \omega_1 \rangle (1 - 6\langle \omega_3 \rangle) \ln 5 \quad (5)$$

and thus we should calculate two correlation functions of the model I $\langle \omega_1 \rangle$ and $\langle \omega_2 \rangle$.

3. CORRELATION FUNCTIONS

In I we have found a generating function for dimer configurations of the model I containing points of one of the sublattices A_0 or B_0 :

$$\begin{aligned} \phi(Z_1, Z_2, Z_3) &= \prod_{a_1=0}^{l_1/2-1} \prod_{a_2=0}^{l_2/2-1} \prod_{a_3=0}^{l_3/2-1} \sum_{j=1}^3 \left(2Z_j - 2Z_j \cos \frac{4\pi a_j}{l_j} \right) \\ &= 2^{N/8} (Z_1 + Z_2 + Z_3)^{N/8} \prod_{a_1=0}^{l_1/2-1} \prod_{a_2=0}^{l_2/2-1} \prod_{a_3=0}^{l_3/2-1} (1 - \lambda_{a_1 a_2 a_3}) \quad (6) \end{aligned}$$

where

$$\lambda_{a_1 a_2 a_3} = (Z_1 + Z_2 + Z_3)^{-1} \sum_{j=1}^3 Z_j \cos \frac{4\pi a_j}{l_j}$$

are eigenvalues of a “random walk” matrix Λ .

Let $\beta_t(\mu_1, \mu_2, \mu_3)$ be the sum over all t -step paths ending in a lattice point with coordinates (μ_1, μ_2, μ_3) . If one ascribes a weight $w_j = Z_j 2^{-1} (Z_1 + Z_2 + Z_3)^{-1}$ to each step in a direction j ($j = 1, 2, 3$), then Λ is the matrix of coefficients of the recurrence relation following from Eq. (10) of I:

$$\begin{aligned} \beta_t(\mu_1, \mu_2, \mu_3) = & w_1 \beta_{t-1}(\mu_1 - 1, \mu_2, \mu_3) + w_1 \beta_{t-1}(\mu_1 + 1, \mu_2, \mu_3) \\ & + w_2 \beta_{t-1}(\mu_1, \mu_2 - 1, \mu_3) + w_2 \beta_{t-1}(\mu_1, \mu_2 + 1, \mu_3) \\ & + w_3 \beta_{t-1}(\mu_1, \mu_2, \mu_3 - 1) + w_3 \beta_{t-1}(\mu_1, \mu_2, \mu_3 + 1) \end{aligned} \quad (7)$$

Thus, we have

$$\phi(Z_1, Z_2, Z_3) = 2^{N/8} (Z_1 + Z_2 + Z_3)^{N/8} \det(I - \Lambda) \quad (8)$$

where I is the $(N/8) \times (N/8)$ unit matrix. Denote by i ($i = 1, \dots, 6$) all possible directions of the path exit from a given point m belonging to the sublattice A_0 (B_0). Let k dimers in points m_1, m_2, \dots, m_k be oriented in fixed directions i_1, i_2, \dots, i_k . The generating function of dimer configurations $\phi'(Z_1, Z_2, Z_3)$ containing the given collection of k dimers is defined by the matrix $\Lambda' = \Lambda + \delta$. A defect matrix δ should be such that a matrix element of Λ' equals 1 for the transition from the point m_ν ($\nu = 1, 2, \dots, k$) in the direction i_ν and equals zero for other directions.

Defining $w(i_\nu)$ by

$$w(i_\nu) = \begin{cases} w_1 & \text{if } i_\nu = 1, 2 \\ w_2 & \text{if } i_\nu = 3, 4 \\ w_3 & \text{if } i_\nu = 5, 6 \end{cases}$$

we can write $\phi'(Z_1, Z_2, Z_3)$ as

$$\phi'(Z_1, Z_2, Z_3) = 2^{N/8} (Z_1 + Z_2 + Z_3)^{N/8} \prod_{\nu=1}^k w(i_\nu) \det(I - \Lambda - \delta) \quad (9)$$

The correlation function defined by

$$K = \frac{\phi'(Z_1, Z_2, Z_3)}{\phi(Z_1, Z_2, Z_3)} = \prod_{\nu=1}^k w(i_\nu) \frac{\det(I - \Lambda - \delta)}{\det(I - \Lambda)} \quad (10)$$

can be written as

$$K = \prod_{\nu=1}^k w(i_\nu) \det(I - A^{-1}\delta) \tag{11}$$

where A^{-1} is the inverse of $A = I - \Lambda$.

The Λ has been diagonalized by the Fourier transform (11) of I. Elements of the matrix A^{-1} can be found by the inverse transform

$$a^{-1}(\mu_1, \mu_2, \mu_3; \mu'_1, \mu'_2, \mu'_3) = \sum_{a_1=0}^{l_1/2-1} \sum_{a_2=0}^{l_2/2-1} \sum_{a_3=0}^{l_3/2-1} \exp\left[-2\pi i \sum_{j=1}^3 \frac{2a_j(\mu_j - \mu'_j)}{l_j}\right] (1 - \lambda_{a_1 a_2 a_3})^{-1} \tag{12}$$

which in the limit $N \rightarrow \infty$ gives

$$a^{-1}(\mu_1, \mu_2, \mu_3; \mu'_1, \mu'_2, \mu'_3) = \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\alpha_1 d\alpha_2 d\alpha_3 \times \left\{ \exp\left[-i \sum_{j=1}^3 (\mu_j - \mu'_j) \alpha_j\right] / \left(1 - 2 \sum_{j=1}^3 w_j \cos \alpha_j\right) \right\} \tag{13}$$

The calculation of the determinant in formula (11) is straightforward, because almost all the elements of the matrix are zero. Then formula (11) acquires the form

$$K = \prod_{\nu=1}^k w(i_\nu) \det(I - Q)$$

where Q is the matrix obtained from δA^{-1} by crossing out rows and columns containing only zeros.

Define the six-component vector $\Delta(m', n)$ for two arbitrary sublattice points m and n with coordinates (μ_1, μ_2, μ_3) and (ν_1, ν_2, ν_3) :

$$\{\delta(\mu_1 - 1, \mu_2, \mu_3; \nu_1, \nu_2, \nu_3), \delta(\mu_1 + 1, \mu_2, \mu_3; \nu_1, \nu_2, \nu_3), \delta(\mu_1, \mu_2 - 1, \mu_3; \nu_1, \nu_2, \nu_3), \delta(\mu_1, \mu_2 + 1, \mu_3; \nu_1, \nu_2, \nu_3), \delta(\mu_1, \mu_2, \mu_3 - 1; \nu_1, \nu_2, \nu_3), \delta(\mu_1, \mu_2, \mu_3 + 1; \nu_1, \nu_2, \nu_3)\} \tag{14}$$

and vector $A^{-1}(n, m')$:

$$\{a^{-1}(\nu_1, \nu_2, \nu_3; \mu_1 - 1, \mu_2, \mu_3), a^{-1}(\nu_1, \nu_2, \nu_3; \mu_1 + 1, \mu_2, \mu_3), a^{-1}(\nu_1, \nu_2, \nu_3; \mu_1, \mu_2 - 1, \mu_3), a^{-1}(\nu_1, \nu_2, \nu_3; \mu_1, \mu_2 + 1, \mu_3), a^{-1}(\nu_1, \nu_2, \nu_3; \mu_1, \mu_2, \mu_3 - 1), a^{-1}(\nu_1, \nu_2, \nu_3; \mu_1, \mu_2, \mu_3 + 1)\} \tag{15}$$

For a four-point correlation function $K(m_1, m_2, m_3, m_4)$ the matrix Q becomes

$$Q = \begin{bmatrix} A^{-1}(m_1, m'_1)\Delta(m'_1, m_1) & A^{-1}(m_1, m'_2)\Delta(m'_2, m_2) & & & & & & & \\ A^{-1}(m_2, m'_1)\Delta(m'_1, m_1) & & \dots & & & & & & \\ A^{-1}(m_3, m'_1)\Delta(m'_1, m_1) & & & \dots & & & & & \\ A^{-1}(m_4, m'_1)\Delta(m'_1, m_1) & & & & \dots & & & & \\ & & & & & \dots & A^{-1}(m_1, m'_4)\Delta(m'_4, m'_4) & & \\ & & & & & & \dots & \dots & \\ & & & & & & & \dots & \\ & & & & & & & & \dots & A^{-1}(m_4, m'_4)\Delta(m'_4, m_4) \end{bmatrix} \quad (16)$$

Crossing out the two last rows and columns from (16) we get the matrix Q for a two-point correlation function.

4. NUMERICAL RESULTS

Let m_1, m_2, m_3, m_4 be positions of the points 1, 2, 3, 4 shown in Fig. 2a. To calculate $\langle w_1 \rangle$ we put

$$m_1 = (0, 0, 0), \quad m_2 = (0, 0, 1), \quad m_3 = (0, -1, 1), \quad m_4 = (0, -1, 0)$$

From the definition (14) it follows that

$$\begin{aligned} \Delta(m'_1, m_1) &= \{-w_1, -w_1, -w_2, -w_2, -w_3, (1-w_3)\} \\ \Delta(m'_2, m_2) &= \{-w_1, -w_1, (1-w_2), -w_2, -w_3, -w_3\} \\ \Delta(m'_3, m_3) &= \{-w_1, -w_1, -w_2, -w_2, (1-w_3), -w_3\} \\ \Delta(m'_4, m_4) &= \{(1-w_1), -w_1, -w_2, -w_2, -w_3, -w_3\} \end{aligned} \quad (17)$$

The scalar product of $A(m_1, m')$ and $\Delta(m'_1, M_1)$ gives, according to (12), (15), (16), and (17),

$$\begin{aligned} Q_{11} &= \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\alpha_1 d\alpha_2 d\alpha_3 \\ &\quad \times \left(e^{i\alpha_3}/2 - \sum_{j=1}^3 w_j \cos \alpha_j \right) / \left(1/2 - \sum_{j=1}^3 w_j \cos \alpha_j \right) \end{aligned} \quad (18)$$

At $z_1 = z_2 = z_3 = 1$ we have $w_1 = w_2 = w_3 = 1/6$ and $Q_{11} = 0$. The matrix

element Q_{12} is given by

$$Q_{12} = \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\alpha_1 d\alpha_2 d\alpha_3 \times \left(e^{i(\alpha_3 - \alpha_2)} / 2 - \sum_{j=1}^3 w_j \cos \alpha_j \right) / \left(1/2 - \sum_{j=1}^3 w_j \cos \alpha_j \right) \quad (19)$$

At $z_1 = z_2 = z_3 = 1$ (19) becomes

$$Q_{12} = \frac{3}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi d\alpha_1 d\alpha_2 d\alpha_3 \frac{(1 + \cos \alpha_2) \cos \alpha_3}{3 + \cos \alpha_1 + \cos \alpha_2 + \cos \alpha_3} \equiv 6k_1 \quad (20)$$

Similarly, we have

$$Q_{14} = -Q_{13} = Q_{23} = -Q_{31} = Q_{34} = -Q_{42} = Q_{41} = 6k_1 \\ Q_{22} = Q_{33} = Q_{44} = 0, \quad Q_{21} = Q_{32} = Q_{43} = 1$$

The element Q_{24} is

$$Q_{24} = -\frac{3}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi d\alpha_1 d\alpha_2 d\alpha_3 \frac{(1 + \cos \alpha_1) \cos \alpha_2 \cos \alpha_3}{3 + \cos \alpha_1 + \cos \alpha_2 + \cos \alpha_3} \equiv -6k_2 \quad (21)$$

By using (11), the correlation function $\langle \omega_1 \rangle$ takes the form

$$\langle \omega_1 \rangle = \det \begin{vmatrix} 1/6 & -k_1 & k_1 & -k_1 \\ -1/6 & 1/6 & -k_1 & k_2 \\ k_1 & -1/6 & 1/6 & -k_1 \\ -k_1 & k_1 & -1/6 & 1/6 \end{vmatrix} \quad (22)$$

The calculations of integrals (20) and (21) give $k_1 = -0.0308729 \dots$ and $k_2 = 0.0116130 \dots$. Substituting these values into (22) we obtain

$$\langle \omega_1 \rangle = 0.0012718 \dots$$

The configuration ω_3 is a fragment of the configuration ω_1 and we easily find

$$\langle \omega_3 \rangle = \det \begin{pmatrix} 1/6 & -k_1 \\ -1/6 & 1/6 \end{pmatrix} = 0.0329232 \dots$$

Using (4) we obtain $\langle \Omega_1 \rangle = 3.40189 \dots \times 10^{-5}$. Then from (3) it follows that

$$\lambda \geq \lambda' + 0.001642$$

The numerical value of the Hammersley bound is $\lambda' = 0.418347$. The improved lower bound is

$$\lambda \geq 0.419989 \dots$$

Here we have evaluated the contribution to λ from the simplest dissections generating closed paths on the sublattices. The method suggested allows one to take into account the contribution of dissections with a more complex closed path though it becomes more difficult to establish the independence of contours.

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