Packing dimers on $(2p+1)\times(2q+1)$ lattices

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We use computational method to investigate the number of ways to pack dimers on $m\times n$ lattices, where both m and n are odd. In this case, there is always a single vacancy in the lattices. We show that the dimer configuration numbers on $(2k+1)\times(2k+1)$ odd square lattices have some remarkable number-theoretical properties in parallel to those of close-packed dimers on $2k\times 2k$ even square lattices, for which an exact solution exists. Furthermore, we demonstrate that there is an unambiguous logarithmic term in the finite size correction of free energy of odd-by-odd lattice strips with any width $n\geqslant 1$. This logarithmic term determines the distinct behavior of the free energy of odd square lattices. These findings reveal a deep and previously unexplored connection between statistical physics models and number theory and indicate the possibility that the monomer-dimer problem might be solvable.

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I. INTRODUCTION

The dimer model has been investigated for many years to represent adsorption of diatomic molecules on a surface. In the model, the surface is represented as a regular plane lattice and the diatomic molecules as rigid dimers, which fit into the lattice so that each dimer occupies two adjacent lattice sites and no lattice site is covered by more than one dimer. The model is closely related to another well-studied lattice model, the Ising model. A central problem of the model is to enumerate the dimer configurations on the lattice. An exact solution exists only for the special case when the lattices of size $m\times n$ is completely covered by dimers if at least one of m and n is even (the close-packed dimer problem) [1,2]. The general monomer-dimer problem where there are vacancies in the lattice, like the general Ising model in an external field, however, remains unsolved and is usually considered computationally intractable [3]. One exception is a recent analytic solution to the special case where there is a single vacancy at certain specific sites on the boundary of the lattice [4].

In this report, we use a computational method to investigate the number of ways to pack dimers on lattices of size $m\times n$, where both m and n are odd. We call this kind of lattices *odd* lattices in the following. In this case, there is always a single vacancy in the lattices. If at least one of m and n is even, the lattices are called *even* lattices. The computation method is outlined in Sec. II. In Sec. III, we show that the leading coefficients of the partition functions (a_N) on odd $(2k+1)\times(2k+1)$ square lattices have some surprising number-theoretical properties, in parallel to those found in even $2k\times 2k$ square lattices [5]. We also show that the average free energy of odd square lattices of finite sizes differs dramatically from that of even square lattices. Unlike that of even square lattices, the average free energy of odd square lattices approaches the thermodynamic limit nonmonotonically, descending first for small lattices to reach a minimum before ascending as the size of the lattice increases. In contrast, the free energy of even square lattices approaches the thermodynamic limit monotonically. The behavior of the free energy of finite size odd square lattices also differs from that of lattices where there is a single vacancy restricted at certain specific sites on the boundary of the lattices [4]. In this latter case, the free energy behaves in much the same way as that of close-packed even square lattices without vacancy.

To investigate further the origin of the different behaviors of free energy in odd and even square lattices, in Sec. IV we calculate the free energy on strip lattices of size $m\times n$, where both m and n are odd. The data show unambiguously that there is a logarithmic term in the free energy of odd lattices, which is absent in the free energy when m or n is even. We demonstrate that it is this logarithmic term in the finite size correction of the free energy in odd lattices that leads to the nonmonotonicity and minimum in the free energy of the odd square lattices. In Sec. V, we discuss our findings in a broader prospective and explore their potential relation with the theory of computational complexity.

II. COMPUTATIONAL METHOD

Here we use computational method to enumerate the dimers on plane lattices. The computational method we use is similar to the one introduced previously where symmetry of the dimer configurations is used to obtain a recurrence of the partition functions and to reduce the complexity of the problem [6]. The computational method is outlined below. For a lattice of size $m\times n$, the property we are interested in is the configurational grand canonical partition function

$$Z_{m,n}(x,y,z)=\sum_{N_x,N_y,N_z} g_{m,n}(N_x,N_y,N_z)x^{N_x}y^{N_y}z^{N_z},$$

where x, y, and z are the activities of the x dimers, y dimers, and monomers, respectively, and $g_{m,n}(N_x,N_y,N_z)$ is the number of ways to place N_x dimers in the x (horizontal) direction, N_y dimers in the y (vertical) direction, and N_z monomers on the sites that are not occupied by dimers. Without losing generality, we can let $z=1$, so that the partition function can be written as

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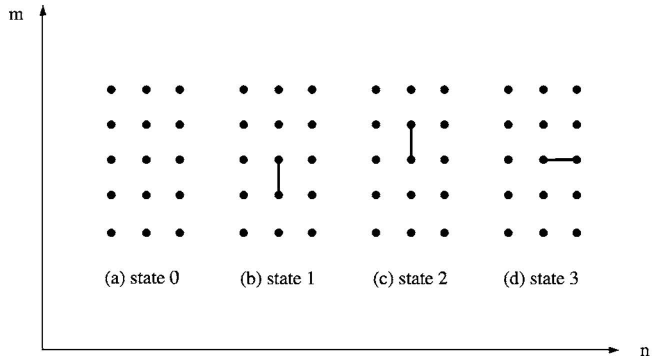

FIG. 1. The configurational states of one lattice site. Suppose the strip with width n is expanding in the vertical direction. The four states that each site can have are depicted here for the *central site* in the figure. (a) State 0: the site is empty; (b) state 1: the site is occupied by the first half of a vertical dimer; (c) state 2: the site is occupied by the second half of a vertical dimer; (d) state 3: the site is occupied by a horizontal dimer. Since the lattice strip is growing vertically, for horizontal dimers, we do not need to distinguish first half or second half.

$$Z_{m,n}(x,y) = \sum_{N_x,N_y} g_{m,n}(N_x,N_y)x^{N_x}y^{N_y}. \tag{1}$$

Since there is no interaction between dimers except for the constraint that no site can be occupied by more than one dimer, the partition function of a strip lattice with width of n is totally determine by the configurations of dimers on two adjacent rows of the lattice, each row itself being a one-dimensional linear lattice of size n [6]. A square matrix M_n is set up based on these two rows (see below). The vector Ω_m, which consists of partition function of Eq. (1) as well as other *contracted* partition functions [6] on a $m\times n$ strip, is calculated by the following recurrence

$$\Omega_m = M_n\Omega_{m-1}. \tag{2}$$

To construct the matrix M_n, we notice that each lattice site can have four dimer configurational states, as shown in Fig. 1 for the center site: (a) state 0, the monomer state, where the site is empty; (b) state 1, the site is occupied by the first half of a vertical dimer; (c) state 2, the site is occupied by the second half of a vertical dimer; (d) state 3, the site is occupied by a horizontal dimer. Since the lattice strip is growing vertically (n is fixed and m is changing), for horizontal dimers, we do not need to distinguish first half or second half. For each lattice site (i,j), we denote $s(i,j)$ as its state.

The total number of dimer configurations $t(n)$ in a one-dimensional lattice with length n is $t(n)=4^n$. Some of these configurations are not valid: when dimers occupy horizontally, they have to occupy an even number of consecutive sites. The total number of valid configurations $v(n)$ is given by the generating function $1/(1-3x-x^2)$. This generating function can be derived from the obvious recurrence $v(n)=3v(n-1)+v(n-2)$.

The size and elements of matrix M_n are determined by the unique relative configurations of the dimers on two adjacent rows of the lattice. The basic method of Ref. [6] is to express *contracted* partition functions of one row with contracted partition functions of the next row. A particular contracted partition function is the partition function of the lattice when states of lattice sites in one row are fixed in a given configuration. For dimers on row $j+1$, there are only two *effective* configurational states of dimers on row j if the states of dimers in row j are fixed in a given configuration. When dimers on row j are in states $s(i,j)=0$, 1, or 3, they will contribute the same expansion coefficients when the contracted partition functions of row $j+1$ are expressed with the contracted partition functions of row j. In other words, for the purpose of building up the matrix M_n to calculate the partition functions recursively in the vertical direction, the occupancy of a horizontal dimer on site (i,j) has the same effect as having an empty site on site (i,j). So does the occupancy of the first half of a dimer on site (i,j). By grouping these states together, and taking symmetry into account, the total number of *unique* configurational states is given by formula $u(n)=2^{n-1}+2^{\lfloor (n+1)/2\rfloor -1}$.

The detailed algorithm to construct matrix M_n is given below. (1) For a strip lattice with a given width of n, the $t(n)=4^n$ configurations are enumerated. (2) Only $v(n)$ valid configurations are kept. Those that are not valid are filtered out. (3) Based on symmetry and the grouping of dimer states mentioned above, each valid configuration is assigned into a group. (4) For each of the $u(n)$ groups say group p, pick a configuration $c_p(\alpha)$ in the group and loop through all the valid configurations determined in step (2) to check their compatibility with $c_p(\alpha)$.

The possible *compatible* combinations of states in lattice sites (i,j) and $(i,j+1)$ are $\{[s(i,j)\in\{0,1,3\}$ and $s(i,j+1)\in\{0,2,3\}]$ or $[s(i,j)=2$ and $s(i,j+1)=1]\}$. All other combinations of states are not feasible. They either lead to contradiction to the definition of the states, or violate the constraint that each lattice site cannot be multiply occupied. For example, the combination $\{s(i,j)=0$ and $s(i,j+1)=1\}$ belongs to the first category, while $\{s(i,j)=2$ and $s(i,j+1)=2\}$ belongs to the second category.

Suppose the configuration being checked for compatibility with $c_p(\alpha)$ is from group q, and is labeled as $c_q(\beta)$. The check of compatibility is carried out for all the lattice sites along the horizontal direction for the configuration, that is, for $i=1,\ldots,n$. Only when all sites of $c_q(\beta)$ are compatible with sites of $c_p(\alpha)$ does the configuration $c_q(\beta)$ make contributions to the matrix element $M_n(p,q)$. As an example, the matrix for $n=3$ is given below.

$$M_3 = \begin{bmatrix} 1+2x & 2y+2xy & y & 2y^2 & y^2 & y^3 \\ 1+x & y & y & y^2 & 0 & 0 \\ 1 & 2y & 0 & 0 & y^2 & 0 \\ 1 & y & 0 & 0 & 0 & 0 \\ 1 & 0 & y & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The following example gives the various sizes of $t(n)$, $v(n)$, and $u(n)$. For $n=19$, the numbers of total, total valid, and total unique configurations are $t(19)=274\,877\,906\,944$,

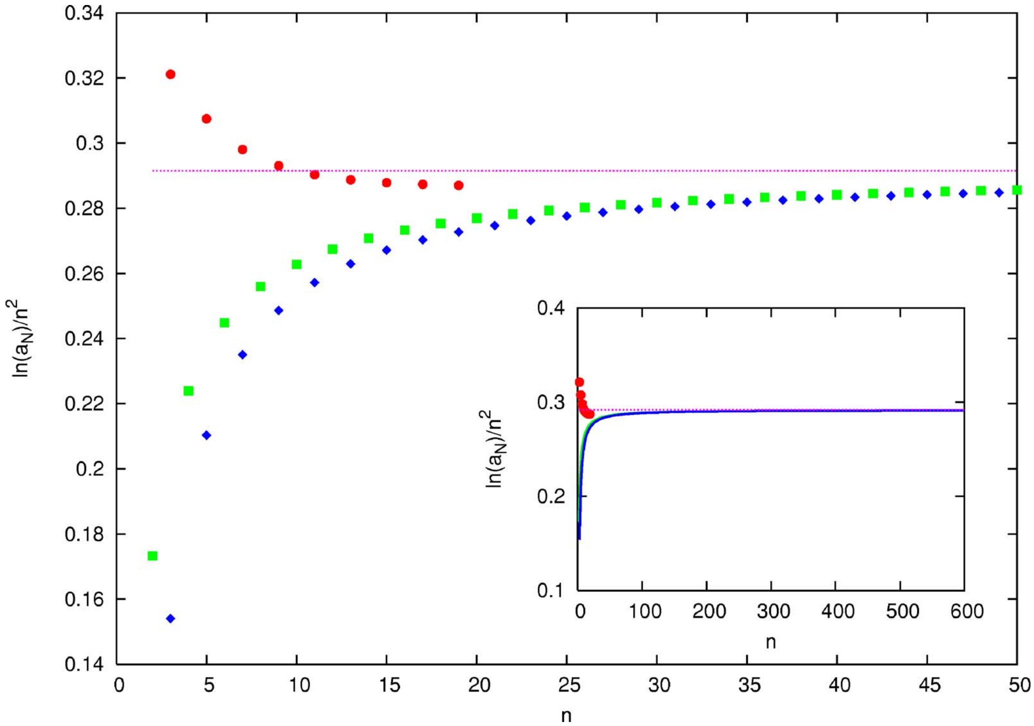

FIG. 2. (Color online) Free energy per lattice site ($\ln a_N/n^2$) of odd and even square lattices in unit of $-k_BT$ as a function of n, the size of the lattice. The values for odd square lattices are in solid circle, those for even square lattices in solid square. The value in the thermodynamic limit, $\lim_{n\to\infty} n^{-2}\ln a_N(n)=0.291\,560\,904$, is also shown as the dotted horizontal line. The values for even square lattices beyond $n=20$ are calculated from the exact results [1,2]. In the inset, more data are shown for the even square lattices to make it clearer how $\ln a_N/n^2$ approaches the thermodynamic limit. Also shown in solid diamonds are the values from lattices where there is a single vacancy restricted at certain specific sites on the boundary of the lattices [4].

$v(19)=6\,616\,217\,487$, and $u(19)=262\,656$. Since the size of matrix M_n is determined by $u(n)$, for $n=19$, M_{19} is of size $262\,656\times 262\,656$, with each element as a polynomial of x and y. All computations are carried out in a 32-bit LINUX workstation with 2 GB memory. Exact integers, instead of floating number approximations, are used in the calculations.

III. NUMBER-THEORETICAL PROPERTIES AND FREE ENERGY OF PACKING DIMERS ON ODD SQUARE LATTICES

Once the matrix M_n is set up, the partition functions can be obtained recursively from Eq. (2). Although the full partition function of Eq. (1) can be obtained from the method, here we are especially interested in a_N [12], the coefficient of the leading term in the partition function Eq. (1) when $x=y$, where $N=\lfloor mn/2\rfloor$

$$Z_{m,n}(x) = a_N x^N + a_{N-1}x^{N-1} + \cdots + a_0.$$

When $n=2k$, the square lattice $n\times n$ can be fully covered by $N=n^2/2$ dimers, and we can take advantage of the available exact results for this cases [1,2]. We refer these kinds of lattices as even square lattices in the following. When $n=2k+1$, the square lattice can at most accommodate $N=(n^2-1)/2$ dimers. In this case, there is always a single vacancy in the lattice. We refer to the lattices as odd square lattices. The free energy per lattice site $\ln a_N/(mn)$ (divided by $-k_BT$) for the odd and even square lattices as a function of n, the size of the lattice, is shown in Fig. 2. The exact result for the even lattices [1,2] shows that in the thermodynamic limit,

$$\lim_{n\to\infty} n^{-2}\ln a_N(n) = G/\pi = 0.291\,560\,904,$$

where G is the Catalan number. For the fully packed lattices, the difference between the even and odd lattices is the existence of a single vacancy site in the odd lattices. The effects of this single vacancy site are evident for small lattices, but as the size of the lattice increases, the effects become smaller. The parity of even and odd square lattices will manifest its greatest effects in terms of $\ln a_N/n^2$ when n is small. This is shown in Fig. 2. As can be seen from the figure, in the beginning for small lattices, the free energy of even and odd square lattices approaches the thermodynamic limit from different directions, with that of even square lattices smaller than the asymptotic value, and that of odd square lattices greater than the asymptotic value. However, it is interesting to note that the free energy of odd square lattices soon reaches and passes over the thermodynamic limit value at about $n=11$. Since $\ln a_N/n^2$ is a well-defined thermodynamic property, it should approach the same value in the thermodynamic limit as n approaches infinity for both even and odd square lattices. Accordingly, it is expected that the free energy of the odd square lattices will reach a minimum, after

TABLE I. The values of a_N, the coefficients of the leading term in the partition functions of dimers on $n\times n$ square lattices, and their factorizations.

n	a_N	Factors of $a_N=2^k c_k$	$c_k \bmod 2^4$
2	2	2	1
3	18	2×3^2	−7
4	36	$2^2\times 3^2$	−7
5	2180	$2^2\times 5\times 109$	1
6	6728	$2^3\times 29^2$	−7
7	2200776	$2^3\times 3\times 107\times 857$	−7
8	12988816	$2^4\times 17^2\times 53^2$	−7
9	20355006224	$2^4\times 7\times 31\times 5862617$	1
10	258584046368	$2^5\times 241^2\times 373^2$	−7
11	1801272981919008	$2^5\times 3\times 13\times 19\times 139\times 546508031$	−7
12	53060477521960000	$2^6\times 5^4\times 31^2\times 53^2\times 701^2$	1
13	1560858753560238398528	$2^6\times 313\times 439\times 177490360930511$	1
14	112202208776036178000000	$2^7\times 3^{10}\times 5^6\times 19^2\times 29^4\times 61^2$	1
15	13428038397958481723104394368	$2^7\times 948517\times 110600600710425473093$	−7
16	2444888770250892795802079170816	$2^8\times 101^2\times 9929^2\times 5849^2\times 16661^2$	1
17	1157111379933346772804754279450353920	$2^8\times 5\times 903993265572927166253714280820589$	1
18	548943583215388338077567813208427340288	$2^9\times 37^4\times 457^2\times 1597^2\times 33629^2\times 30817^2$	1
19	1004777133003025735713513459537724394989392384	$2^9\times 3\times 206870980007\times 2578470886559 \times 1226356459698559963$	−7

which it would approach the thermodynamic limit monotonically above the values of the even square lattices. The same conclusion can also be obtained from the existence theory of the dimer system, which asserts that the limit of $\ln a_N/n^2$ exists as n approaches infinity [7]. The behavior of the free energy of odd square lattices is to contrast with that of the even square lattices, which approaches the thermodynamic limit monotonically from the very beginning. The current calculation shows that the minimum of the odd square lattices will be reached when $n\geqslant 19$. We will discuss the origin of the minimum in the free energy of odd square lattices after we discuss the logarithmic correction term found in the finite size correction in Sec. IV.

Also shown in Fig. 2 is the free energy of lattices where there is a single vacancy restricted at certain specific sites on the boundary of the lattices [4]. The free energy for these lattices approaches the thermodynamic limit monotonically, in the same way and the same direction as that of even square lattices, and behaves quite differently from that of odd square lattices. The data show that removing the restriction of the location of the vacancy on the lattice boundary leads to significant changes in the nature of the problem.

The values of a_N up to $n=19$ are listed in the second column of Table I. One of the advantages of using exact integer calculations instead of approximation calculations is that the number-theoretical nature of the coefficients of the partition functions can be studied in more details. For the even lattices $2k\times 2k$, it is first conjectured and later proved [5] by using the explicit formulas [1,2] that $a_N=2^k c_k=2^k b_k^2$, where c_k and b_k are integers, and b_k has the following property:

$$b_k=\begin{cases} k+1 & \pmod{2^4} \quad \text{if } k \text{ is even} \\ (-1)^{(k-1)/2} & \pmod{2^4} \quad \text{if } k \text{ is odd} \end{cases}.$$

From these results it is easy to show that for even square lattices

$$c_k=b_k^2=\begin{cases} 1 & \pmod{2^4} \quad \text{if } k=8p+q,\ q=0,1,6,7 \\ -7 & \pmod{2^4} \quad \text{if } k=8p+q,\ q=2,3,4,5 \end{cases}.$$

So for the $2k\times 2k$ lattices, the sequence of $a_N/2^k (\bmod 2^4)$ is, starting with $k=1$: 1, −7, −7, −7, −7, 1, 1, 1, 1, −7,….

From Table I, we can see that parallel but distinct properties also hold for the odd square lattices. We have the following conjectures for odd lattice with size $(2k+1)\times(2k+1)$:

Conjecture 1. For odd lattice $(2k+1)\times(2k+1)$, a_N can be factored as

$$a_N=2^k c_k,$$

where c_k is an odd integer. Furthermore, when $k>1$, c_k is squarefree: its prime decomposition contains no repeated factors.

Conjecture 2. For odd lattice $(2k+1)\times(2k+1)$, we have

$$c_k=\begin{cases} 1 & \pmod{2^4} \quad \text{if } k \text{ is even} \\ -7 & \pmod{2^4} \quad \text{if } k \text{ is odd} \end{cases}.$$

The sequence of $a_N/2^k (\bmod 2^4)$ is, starting from $k=1$: −7, 1, −7, 1, −7, 1….

Since very large numbers and big matrices are involved in

TABLE II. Fitting $\ln a_N/(mn)$ to Eq. (3) for odd values of m. Only data with $m \geqslant m_0 = 101$ are used in the fitting.

n	a_0	a_1	a_2	a_3	a_4	h
3	0.219493	−0.11012	−0.172442	0.127814	−0.0964287	1
5	0.252922	−0.0562601	−0.162238	0.0964196	−0.0648308	1
7	0.265557	−0.0491038	−0.152149	0.0711154	−0.0466402	1
9	0.272073	−0.0514573	−0.145208	0.0503154	−0.0373426	1
11	0.276016	−0.0561077	−0.140372	0.0319921	−0.034609	1
13	0.278649	−0.0611249	−0.136868	0.0151006	−0.037443	1
15	0.280527	−0.0659264	−0.134236	−0.00090841	−0.045399	1
17	0.281932	−0.0703454	−0.132197	−0.0163402	−0.0583437	1
19	0.283023	−0.0743568	−0.130576	−0.0313702	−0.076415	1

the calculations, it is important to check the correctness of the results. The correctness of the data can be confirmed in several ways. First, the method mentioned in Sec. II applies to strip lattices with width n no matter whether n is even or odd. For even n, the exact results [1,2] can be used to check the correctness of the results. Second, for a lattice strip of size $m\times n$ with a given width of n when n is odd, the recurrence of Eq. (2) will calculate *both* even and odd values of m using the *same* matrix M_n. For those even values of m, the exact formula [1,2] can be used to check the correctness of the results. For example, when $n=19$, the values of a_N calculated from Eq. (2) for $m=18$ and $m=20$ are

$$83\,575\,338\,913\,384\,268\,749\,982\,379\,454\,805\,917\,136\,051,$$

and

$$3\,911\,222\,696\,776\,012\,972\,239\,561\,518\,359\,338\,259\,546\,415\,835,$$

respectively, which are exactly what the exact formula gives. The value a_N of $m\times n=19\times 19$ lattice is calculated from that of 18×19 lattice, and the value a_N of 20×19 lattice is calculated from that of the 19×19 lattice.

Third, the numbers can be cross-checked based on the fact that a_N for a lattice of size $m\times n$ should be the same as that for a lattice of size $n\times m$, even though different matrices M_n and M_m are involved. For example, the value of a_N for the 19×17 lattice, which is calculated from matrix M_{17} of a size $65\,792\times 65\,792$, gives the same value as that calculated from the 17×19 lattice, which is calculated from matrix M_{19}. The value is

$$18\,985\,861\,771\,720\,893\,262\,968\,550\,933\,152\,139\,575\,482.$$

Much larger values have been checked for these tests, some of which are shown in Sec. IV.

TABLE III. Fitting $\ln a_N/(mn)$ to Eq. (3) for even values of m. Only data with $m \geqslant m_0 = 100$ are used in the fitting. Numbers in square brackets denote powers of 10.

n	a_0	a_1	a_2	a_3	a_4	h
3	0.219493	−0.0791336	−1.51574[−8]	1.46224[−6]	−5.93864[−5]	−8.41131[−11]
5	0.252922	−0.102613	−1.09579[−8]	4.6246[−7]	1.1226[−6]	−1.65381[−10]
7	0.265557	−0.114309	4.47355[−8]	−4.20078[−6]	0.000166702	5.96032[−10]
9	0.272073	−0.121309	4.4861[−8]	−4.25669[−6]	0.000170225	7.58016[−10]
11	0.276016	−0.125966	1.7632[−9]	−6.40388[−7]	4.02706[−5]	−9.03742[−11]
13	0.278649	−0.129288	−5.39512[−9]	−9.39239[−8]	2.35758[−5]	−3.1035[−10]
15	0.280527	−0.131777	7.97321[−8]	−7.59505[−6]	0.000305046	2.24049[−9]
17	0.281932	−0.13371	1.08088[−7]	−8.71801[−6]	0.000312377	4.42329[−9]
19	0.283023	−0.135256	3.1797[−7]	−2.0882[−5]	0.000640364	1.91347[−8]

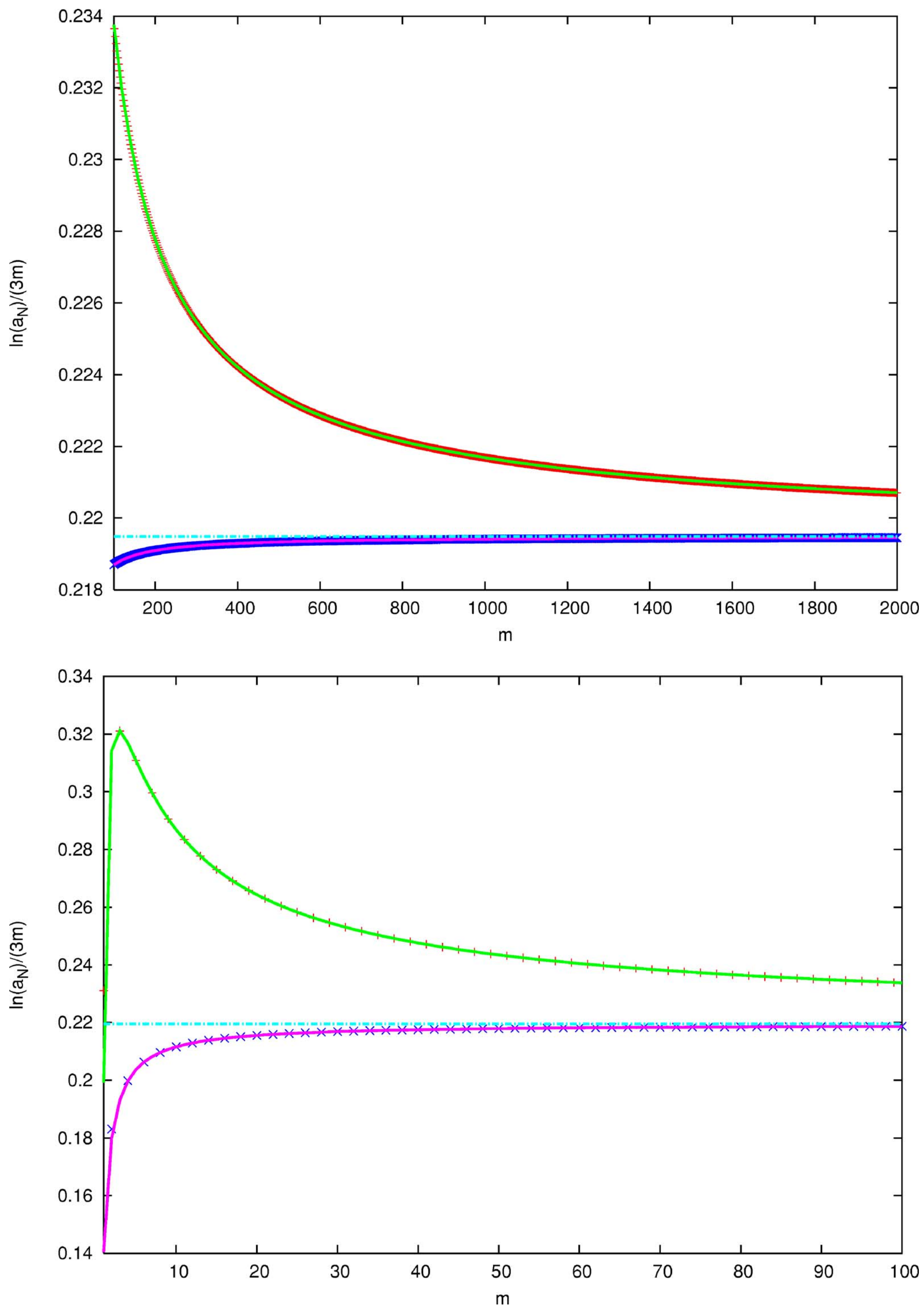

FIG. 3. (Color online) The original data of $\ln(a_N)/(mn)$ for $n=3$ and the fitted curves. In each panel, the data points and curve in the upper part are for odd m, and those in the lower part are for even m. The dashed horizontal line is $a_0^e(3)=0.219\,493$ from exact expression Eq. (5). The data $m \geqslant m_0=100$ are used in the fitting, and they are shown in the top panel. In the bottom panel, the same curves are shown together with the original data for $1 \leqslant m < m_0=100$, which are not used in the fitting.

IV. FINITE SIZE CORRECTION

The data shown in Fig. 2 clearly indicate that the finite size correction of free energy of odd square lattices differs significantly from that of even square lattices. Finite size correction is investigated in Refs. [8,9] for the close-packed dimer model on $m \times n$ lattices with at least one of m or n being even, and in Ref. [4] for lattices where there is a single vacancy restricted at certain specific sites on the boundary of

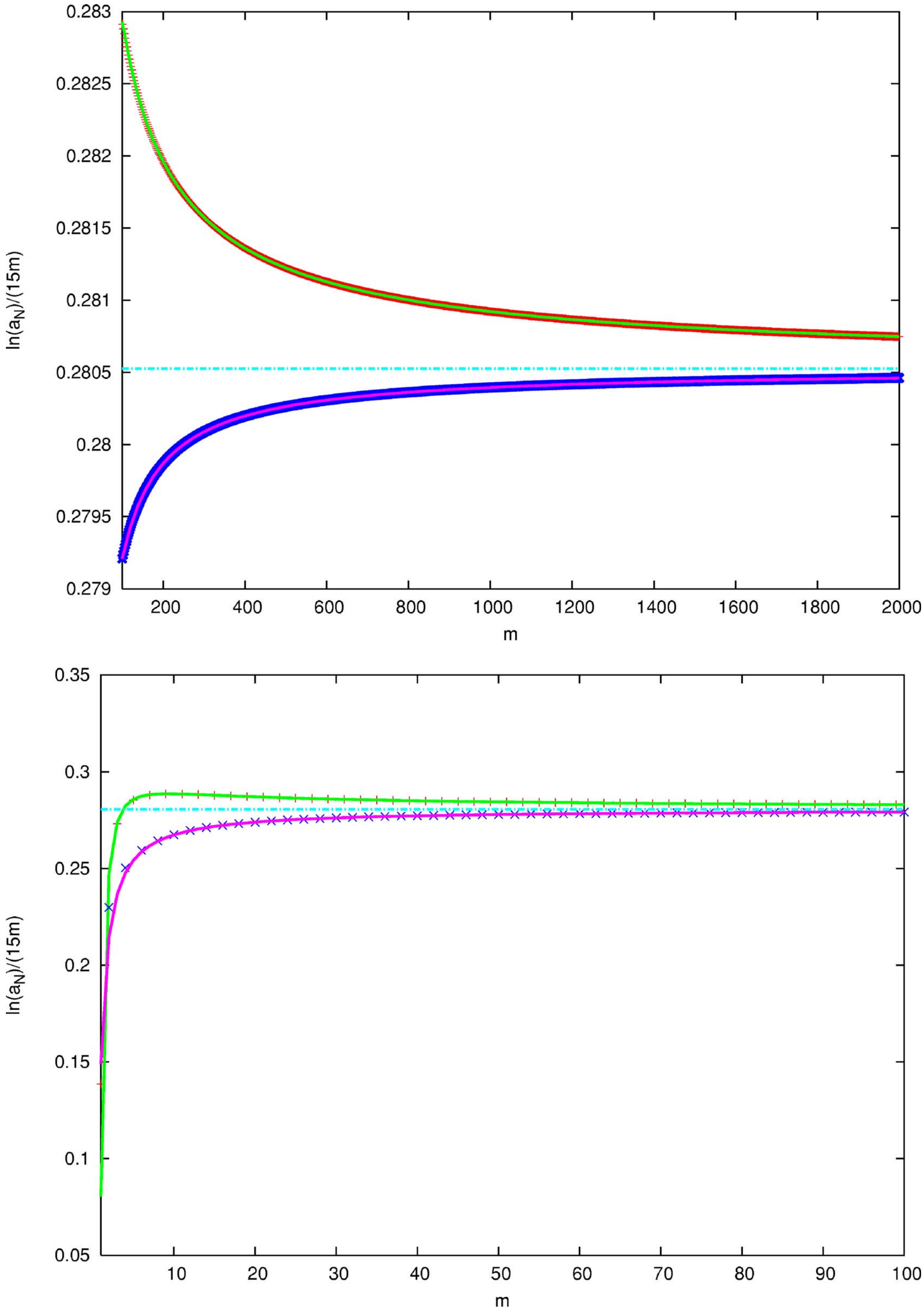

FIG. 4. (Color online) The original data of $\ln(a_N)/(mn)$ for $n=15$ and the fitted curves. The dashed horizontal line is $a_0^e(15)=0.280\,527$ from exact expression Eq. (5). See the legend of Fig. 3.

the lattices. In these models, exact solutions are known and finite size corrections can be obtained from expansions of the exact expressions.

To investigate the finite size correction of free energy of dimers in odd lattices where there is always a vacancy, we calculate the partition functions for long strip lattices $m\times n$

TABLE IV. Fitting $\ln a_N/(mn)$ to Eq. (3) for odd values of m, with a_0 fixed as a_0^e given by Eq. (5). Only data with $m \geqslant m_0 = 101$ are used in the fitting.

n	a_0^e	a_1	a_2	a_3	a_4	h
3	0.219493	−0.11012	−0.172442	0.12782	−0.096693	1
5	0.252922	−0.0562601	−0.162238	0.0964239	−0.0649986	1
7	0.265557	−0.0491038	−0.152149	0.0711184	−0.04676	1
9	0.272073	−0.0514573	−0.145208	0.0503178	−0.0374353	1
11	0.276016	−0.0561077	−0.140372	0.0319939	−0.0346786	1
13	0.278649	−0.0611249	−0.136868	0.0151016	−0.0374833	1
15	0.280527	−0.0659264	−0.134236	−0.00090856	−0.0453931	1
17	0.281932	−0.0703454	−0.132197	−0.0163431	−0.0582417	1
19	0.283023	−0.0743568	−0.130576	−0.0313809	−0.0760878	1

using Eq. (2) for $n=1,\ldots,19$, and fit a_N with the following function:

$$\frac{\ln a_N}{mn} = a_0 + \frac{a_1}{m} + \frac{a_2}{m^2} + \frac{a_3}{m^3} + \frac{a_4}{m^4} + \frac{h}{n}\frac{\ln(m+1)}{m}. \tag{3}$$

The reason to choose $\ln(m+1)$ instead of $\ln(m)$ in Eq. (3) is that for $n=1$, we have the following exact results:

$$a_N = \begin{cases} (m+1)/2 & m \text{ is odd} \\ 1 & m \text{ is even} \end{cases}. \tag{4}$$

The fitting results are equally unambiguous if $\ln(m)$ were used (data not shown).

In the following discussions, we use n as the fixed width of the strip lattice and m as the expanding length. For each $n=3,\ldots,19$, we calculate a_N from $m=1$ to $m=2000$, except for $n=17$, where $m \leqslant 1000$, and for $n=19$, where $m \leqslant 500$. Values of odd and even lattices of the same strip width n are fitted separately. The results of the fitting are shown in Table II for odd values of m and Table III for even values of m. In these fittings, only $m \geqslant m_0 = 100$ are used in the fitting. The effect of m_0 on the fitting is discussed later. The curves of fitting for two values of n, $n=3$, and $n=15$, are shown in Fig. 3 and Fig. 4, respectively.

Several features can be observed directly from these results of fitting the data to Eq. (3). First, for odd values of m, the coefficient h of $(mn)^{-1}\ln(m+1)$ is equal to 1, for *all* values of n (Table II). This logarithmic term is clearly absent when m is even (Table III). It is noted that there is also a logarithmic term in the finite size correction of lattices where the single vacancy is restricted at specific sites on the boundary of the lattices [4]. However, the logarithmic correction there is quite different from the logarithmic correction discovered here. Not only the sign and magnitude are different ($-1/2$ in Ref. [4]), more importantly, the logarithmic correction in Ref. [4] only becomes significant when *both* m and n become large. On the contrary, the logarithmic correction term for odd lattices appears in *all* lattices, even when $n=1$ as shown in Eq. (4).

Second, the linear term a_0 agrees exactly between odd m values and even m values, and they both agree with the exact expression for *infinitely* long strips of finite width n [1]

$$a_0^e(n) = \frac{1}{n}\ln\left\{\prod_{l=1}^{n/2}\left[\cos\frac{l\pi}{n+1} + \left(1+\cos^2\frac{l\pi}{n+1}\right)^{1/2}\right]\right\}. \tag{5}$$

This agreement is expected, as m goes into infinity, the property of odd and even lattices should approach the same value. If we fix the values of a_0 to those given by Eq. (5) and fit the data for the other parameters, there is little changes in the fitting results. The fitting results with fixed a_0 are shown in

TABLE V. Fitting $\ln a_N/(mn)$ to Eq. (3) for even values of m, with a_0 fixed as a_0^e given by Eq. (5). Only data with $m \geqslant m_0 = 100$ are used in the fitting. Numbers in square brackets denote powers of 10.

n	a_0^e	a_1	a_2	a_3	a_4	h
3	0.219493	−0.0791336	7.47107[−9]	−9.44524[−7]	4.45608[−5]	2.27359[−11]
5	0.252922	−0.102613	1.94042[−8]	−2.4284[−6]	0.000113707	9.98152[−11]
7	0.265557	−0.114309	1.52227[−8]	−1.92429[−6]	9.08621[−5]	1.08499[−10]
9	0.272073	−0.121309	1.33789[−8]	−1.63273[−6]	7.50474[−5]	1.28054[−10]
11	0.276016	−0.125966	1.13578[−8]	−1.42994[−6]	6.72433[−5]	1.27535[−10]
13	0.278649	−0.129288	1.87165[−8]	−2.35995[−6]	0.000111213	2.48496[−10]
15	0.280527	−0.131777	1.53596[−8]	−1.93301[−6]	9.09871[−5]	2.3596[−10]
17	0.281932	−0.13371	2.90394[−8]	−3.27894[−6]	0.000144225	6.13228[−10]
19	0.283023	−0.135256	5.2761[−8]	−4.99251[−6]	0.000194123	1.61671[−9]

TABLE VI. The fitting of Eq. (3) for $n=15$ with different values of m_0, the minimal value of m used in the fitting.

m_0	a_1	a_2	a_3	a_4	h
1	−0.0646792	−0.141833	−0.0446463	0.0632163	0.996424
31	−0.0659261	−0.134254	0.000154746	−0.0674233	1
51	−0.0659264	−0.134236	−0.000905825	−0.0454885	1
101	−0.0659264	−0.134236	−0.000908559	−0.0453931	1
201	−0.0659264	−0.134236	−0.000908559	−0.0453931	1
301	−0.0659264	−0.134236	−0.000908559	−0.0453931	1

Tables IV and V. For odd m, there is virtually no change in a_1, a_2, and h, and for even m, there is no change in a_1.

From Figs. 3 and 4, we can see that there are good matches between the fitted curves and the original data, for both odd and even values of m. In both figures, the top panels display the fitted curves and the data used in the fitting ($m \geqslant m_0=100$). The bottom panels display the fitted curves and the data *not* used in the fitting ($1 \leqslant m < m_0=100$). Even for those data points that are not used in the fitting, the match between fitted curves and the original data is good. From these figures it can also be seen that the free energy converges slower when m is odd than when m is even.

The effects of m_0 on the fitting results are shown in Table VI for $m\times 15$ lattices. From the table, we can see that the fitting results converge quickly as a function of m_0, the minimal value of m used in the fitting.

From these fitting experiments, it is clear that there is an additional logarithmic term for the free energy of odd lattices. In this case, the asymptotic expression of $\ln a_N$ is given by

$$\ln a_N \approx mnf_b + (m+n)f_s + \ln(m+1) + \ln(n+1), \qquad (6)$$

where f_b and f_s are the "bulk" and "surface" terms, respectively [8]

$$f_b = G/\pi = 0.291\,560\,904$$

and

$$f_s = G/\pi - \frac{1}{2}\ln(1+\sqrt{2}) = -0.149\,125\,89.$$

With this asymptotic expression, we revisit the free energy $\ln a_N/n^2$ of odd square lattices with size $n\times n$ shown in Fig. 2 and investigate the origin of the nonmonotonicity and minimum found in $\ln a_N/n^2$ for odd square lattices. For even square lattices, the exact results of close-packed lattices give the asymptotic expression of even square lattices as [9]

$$\begin{aligned}\frac{\ln a_N}{n^2} &\approx f_b + \frac{2f_b - \ln(1+\sqrt{2})}{n} + \frac{\ln 2 + f_b - \ln(1+\sqrt{2})}{n^2}\\ &= 0.291\,560\,904 - 0.298\,251\,779n^{-1}\\ &\quad + 0.103\,334\,497\,7n^{-2},\end{aligned}$$

which increases monotonically with n when $n \geqslant 1$. In contrast, the logarithm term in odd lattices introduces a minimum into the function.

For odd square lattices, if we fit the data of $\ln a_N/n^2$ to the following equation,

$$\frac{\ln a_N}{n^2} = f_b + \frac{2f_s}{n} + \frac{b_2}{n^2} + \frac{b_3}{n^3} + \frac{2\ln(n+1)}{n^2}, \qquad (7)$$

we obtain $b_2=-2.064\,12$ and $b_3=2.390\,28$. The fitting uses data in the range of $9 \leqslant n \leqslant 19$. The fitted curve together with the original data is shown in Fig. 5. If we fit the data with the coefficient of $\ln(n+1)/n^2$ as a free parameter, we would get 1.746 47 as the coefficient. The derivation from the expected value of 2 is attributed to the fact that the values of n used in the fitting are not large enough. For the same reason, the values of b_2 and b_3 mentioned above are of limited accuracy.

If we fit the same Eq. (7) to $\ln a_N/n^2$ of even square lattices with the coefficient of $\ln(n+1)/n^2$ as a free parameter (using data in the range of $100 \leqslant n \leqslant 1000$), we obtain $\ln a_N/n^2 \approx 0.291\,560\,904 - 0.298\,251\,779n^{-1} + 0.103\,144n^{-2} + 0.006\,684\,42n^{-3} + 0.000\,03\ln(n+1)/n^2$. This result again shows the absence of the logarithmic term for the even lattices, as shown before in Tables III and V. The coefficient of n^{-2} agrees well with the exact result. The different behaviors of free energy in odd and even square lattices are dominantly determined by the presence of the logarithmic term in odd square lattices.

V. DISCUSSION

We report here the exact values of a_N, the coefficients of the leading term in the partition functions of dimers on odd lattices through extensive computations using an extended method originally developed in Ref. [6]. At first, we investigate a_N on $(2k+1)\times(2k+1)$ odd square lattices, and from these exact values, we investigate the different behaviors of the average free energy of the odd square lattices compared with that of the even square lattices. Although no exact solution exists for the odd lattices, the values of a_N show some remarkable features (Table I). Based on their number-theoretical properties, we put forth a couple of *conjectures* about a_N.

The average free energy of the odd square lattices approaches the thermodynamic limit in a way that is quite different from that of the even square lattices, as well as that of the lattices where a single vacancy is restricted at certain specific sites on the lattice boundary (Fig. 2).

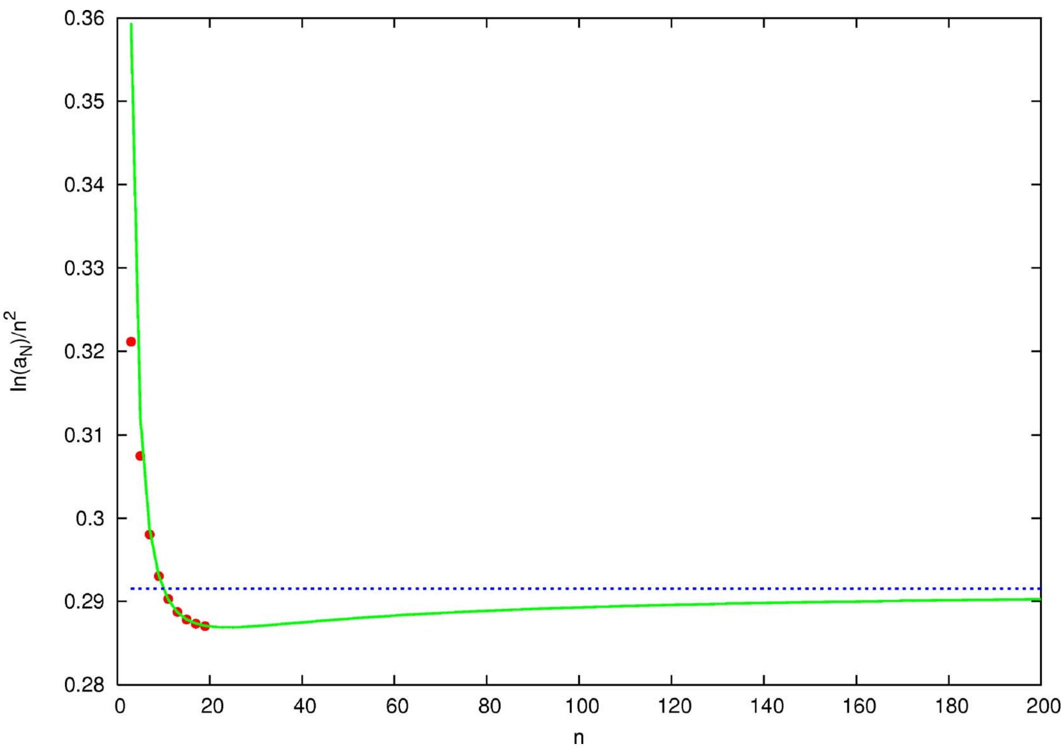

FIG. 5. (Color online) Fitting of $\ln a_N/n^2$ on odd square lattices to Eq. (7). Data in the range of $9 \leqslant n \leqslant 19$ are used in fitting. The dashed horizontal line is the value in the thermodynamic limit: 0.291 560 904.

Comparison with this latter case shows that the removal of the restriction on the location of the vacancy changes the nature of the problem: while in both cases, there is a single vacancy in the whole lattice, the restriction of the vacancy on the lattice boundary significantly reduces the dimer configuration numbers. In fact, when the vacancy is restricted on the lattice boundary, a_N on a lattice of size $(2k+1)\times(2k+1)$ is asymptotically a $\sqrt{2k+1}$ multiplicative factor smaller than a_N in an even lattice of size $(2k+2)\times 2k$ [4]. On the contrary, the a_N on the odd lattices discussed in this report is *bigger* than that of even lattices. For example, the value a_N of an odd square 19×19 lattice reported in Table I is 68 times bigger than the value of a_N for an even 18×20 lattice, which is

$$a_N = 14\ 766\ 712\ 169\ 803\ 333\ 833\ 186\ 604\ 776\ 310\ 955\ 189\ 771\ 941.$$

In Sec. IV, we investigate a_N on odd strip lattices of size $m\times n$, where n is the fixed width of the lattice. We find *unambiguously* that there is a logarithmic term in the finite size correction of the free energy $\ln a_N/mn$. This term is clearly absent in the free energy of even lattices. We also demonstrate that it is this logarithmic correction term that creates the distinct pattern of free energy in odd lattices. From these results, we show that in the asymptotic expression of the free energy per site for odd lattices, in addition to the usual bulk and surface terms of close-packed lattices [8,9], we have an additional term $\ln(m+1)(n+1)$ as shown in Eq. (6). It is also noted that this logarithmic finite size correction term is present for strip lattices of any width $n\geqslant 1$. This is in contrast to the logarithmic term in lattices where the vacancy is restricted to the lattice boundary, where the term only becomes significant when *both* m and n are large [4].

Since the exact solution to the close-packed dimer model was discovered in 1961, little progress has been made for the general two-dimensional monomer-dimer problem. The problem is usually considered to be computationally intractable [3]. More precisely, in the language of computational complexity, it has been shown to be in the "#*P-complete*" class. The #*P*-complete class plays the same role for counting problems (such as counting dimer configurations in two-dimensional lattices, as discussed in this paper) as the more familiar *NP-complete* class plays for the decision problems. #*P*-complete problems belong to the class of problems called the #*P* class, which has the same status as the *NP* class for the decision problems. Among the problems in the #*P* class, the #*P*-complete problems are the "hardest": every problem in #P class can be *reduced* to them in polynomial time. Hence if *any* problem in the #P-complete class is found to be solvable, every problem in the #P class is solvable. Currently it is not clear whether there exists any such solution to the #P-complete class problems, and "P versus NP" problem is the perhaps the major outstanding problem in theoretical computer science.

Although currently, we still do not have an exact solution to the problem of packing dimers on odd lattices, the number-theoretical properties demonstrated for the square lattices and the unambiguous logarithmic term in the finite size correction point to the possibility that the model may actually be solvable. It is hoped that the conjectures and the exact coefficients of the partition functions reported here would give some hints to the elusive exact solutions, and act as references for other approaches to the problem, such as Monte Carlo simulations. It would be interesting to see if other unsolved models in statistical mechanics show the similar patterns in their enumerations. It is our hope that the results shown here will open up new avenues and stimulate new mathematical and computational approaches to the unsolved statistical models.

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[12] The coefficient of the leading term in the partition function gives directly the total work required to saturate the lattice with the N dimers $\Delta G_N = -k_B T \ln a_N$, where k_B is the Boltzmann constant and T is the temperature [10,11]. The average work to ligate one dimer is given by $-(\ln a_N)/N$ in unit of $k_B T$. This concept is not very often mentioned in statistical physics literature, but it plays an important role in studying cooperative binding phenomena in biology and chemistry [10,11]. The value of x_m in $\ln x_m = -(\ln a_N)/N$ is usually called "Wyman median ligand activity" [10] or "mean ligand activity" [11].