Monomer-dimer model in two-dimensional rectangular lattices with fixed dimer density

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© dated: March 23, 2024

I. INTRODUCTION

The monomer-dimer problem has received a lot of attention not only from statistical physics but also from theoretical computer science. As one of the classical lattice statistical mechanical models, the monomer-dimer model was first used to describe the absorption of a binary molecule of unequal sizes on a crystal surface. In the model, the regular lattice sites are either covered by monomers or dimers. The diatomic molecules are modeled as rigid dimers which occupy two adjacent sites in a regular lattice and no lattice site is covered by more than one dimer. The lattice sites that are not covered by the dimers are regarded as occupied by monomers. A central problem of the model is to enumerate the dimer configurations on the lattice. In 1941, an elegant analytical solution was found for a special case of the problem, namely when the planar lattice is completely covered by dimers (the close-packed dimer problem, or dimer covering problem). For the general monomer-dimer problem where there are vacancies in monomer sites in the lattice, there is no exact solution. For three-dimensional lattices, there is no exact solution for the special case of close-packed dimer problem. One recent advance is an analytic solution to the special case of the problem in two-dimensional lattices where there is a single vacancy at certain specific sites on the boundary of the lattice. The monomer-dimer problem also serves as a prototypical problem in the field of computational complexity. It has been shown that two-dimensional monomer-dimer problem belongs to the \#P-complete class and hence is computationally intractable.

Even though there is a lack of progress in the analytical solution to the monomer-dimer problem, many rigorous results exist, such as series expansions, lower and upper bounds on free energy, and exact solutions for certain cases. Some approximate methods have also been proposed. For example, the monomer-dimer constant $h_d$ (the exponential growth rate) of the number of all configurations with different number of dimers has also been calculated. By using sequential importance sampling and Monte Carlo methods, the dimer covering constant for a three-dimensional periodic lattice has been estimated. The importance of monomer-dimer models comes from the fact that there is one to one mapping between the Ising model and the monomer-dimer model: the Ising model in the absence of an external field is mapped to the pure dimer model, and the Ising model in the presence of an external field is mapped to the generalized monomer-dimer model.

The major purposes of this paper are (1) to show it is possible to calculate accurately the free energy of the monomer-dimer problem in two-dimensional rectangular lattices at a fixed dimer density by using the proposed computational methods (Sections II, IV, VII, and VIII),
and (2) to use the computational methods to probe the physical properties of the monomer-dimer model, especially at the high dimer density \( \lim x \). The high dimer density \( \lim x \) is considered to be more difficult and more interesting than the low dimer density \( \lim x \). The major result is the asymptotic expression Eq. (24). The third purpose of the paper is to introduce the asymptotic theory of Penant and Wison [25], which not only gives a theoretical explanation of the origin of the logarithmic correction term found by computational methods reported in this paper (Section III), but also has the potential to be applicable to other statistical models.

The following notation and definitions will be used throughout the paper. The configurational grand canonical partition function of the monomer-dimer system in a \( \times \) two-dimensional lattice is

\[
Z_{m,n}(x) = a_n(x;\eta) \eta^{m + 1} + a_u(\eta;\eta)x^{m + 1} + \ldots \ldots a_m(\eta;\eta)x^m,
\]

where \( a_n(\eta;\eta) \) is the number of distinct ways to arrange \( n \) dimers on the \( m \times n \) lattice, \( N = m + n \), and \( x \) can be taken as the activity of a dimer. The average number of sites covered by dimers (i.e., the average number of dimers) of this grand canonical ensemble is given by

\[
\frac{\ln Z_{m,n}(x)}{m} = \frac{2}{m} \ln \frac{x}{1 - x} = \frac{2}{m} \sum_{n=0}^{N} \frac{a_n(\eta;\eta)x^n}{n}.
\]

The limit of this average for large lattices is denoted as \( \Gamma(\eta) \): \( \Gamma = \lim_{m,n \to \infty} \ln Z_{m,n}(x) \). In general we use \( a(\eta) \) for the average number of sites covered by dimers in a \( \times \) \( \times \) \( d \)-dimensional \( n \) site lattice when the dimer activity is \( x \).

The total number of configurations of dimers is given by \( Z_{m,n}(1) \) at \( x = 1 \), and the monomer-dimer constant for a two-dimensional is defined as

\[
h_2 = \lim_{m,n \to \infty} \ln Z_{m,n}(1). \quad (3)
\]

In general, we denote \( h_d \) as the monomer-dimer constant for a \( d \)-dimensional \( n \) site lattice, and \( h_2 \) as the grand potential per lattice site at any dimer activity \( x \). For a two-dimensional is defined as

\[
h_2(x) = \lim_{m,n \to \infty} \ln Z_{m,n}(x) / m. \quad (4)
\]

In this paper we focus on the number of dimer configurations at a given dimer density \( x \). In this sense we are working on the canonical ensemble. The connection between the canonical ensemble and the grand canonical ensemble is discussed in Appendix A. We define the dimer density for the canonical ensemble as the ratio

\[
x = \frac{2s}{m}. \quad (5)
\]

When the lattice is fully covered by dimers, \( x = 1 \). For a \( m \times n \) lattice, the number of dimers at a given dimer density is \( s = \frac{m+n}{2} \). In the following we use \( a_{m,n}(x) \) as the number of distinct dimers and monomer configurations at the given dimer density \( x \). By using this definition, Eq. (6) can be rewritten as

\[
Z_{m,n}(x) = a_{m,n}(x)x^m, \quad (6)
\]

The free energy per lattice site at a given dimer density is defined as

\[
f_{m,n}(x) = \ln a_{m,n}(x) / mn \quad \text{and the free energy at a given dimer density for a semi-infinite lattice strip of length } n \text{ is}
\]

\[
f_{1,n}(x) = \frac{\ln a_{1,n}(x)}{1}, \quad \text{and the free energy for } \ln(1) \text{ is}
\]

\[
f_2(1) = \frac{G}{1} = 0.291560904
\]

where \( G \) is the Catalan's constant. For other values of \( x \), no analytical result is known, although several bounds are developed in [11-12]. We will show below that by using the exact calculation method developed previously [27,28,29], we can calculate \( f_2(x) \) at an arbitrary dimer density with high accuracy.

The article is organized as follows. In Section III, the computational method is outlined. In Section IV, we show a logarithmic correction term in the semi-infinite correction of \( f_{m,n}(x) \) for any fixed dimer density \( 0 < x < 1 \). The coefficient of this logarithmic correction term is exactly \( 1 = 2 \), for both cylinder lattices and lattices with free boundaries. We give a theoretical explanation for this logarithmic correction term and its coefficient using the newly developed asymptotic theory of Penant and Wison [25]. In this section we use the universality of this logarithmic correction term with coefficient 1 = 2. This term is not unique to the monomer-dimer model: a large class of lattice models has this term when the density of the models is fixed. Moreover, in applications of this asymptotic method to the monomer-dimer model in particular, and statistical models in general, can be found in Section V. In Section VI, we calculate \( f_{1,n}(x) \) on a cylinder strip of length \( n \) for \( n = 1; \ldots 17 \) with cylinder boundary condition. The sequence of \( f_{1,n}(x) \) on cylinder lattices converges very
fast so that we can obtain $f_2()$ quite accurately. To the best of our knowledge, the results presented here are the most accurate for monomer end-mer problem in two-dimensional rectangular lattices at an arbitrary dim er density. In Section VI, similar calculations of $f_{m,n}(\cdot)$ are carried out on lattice strips $1 \times n$ with free boundaries for $n = 1; \ldots ; 16$. Compared with the sequence with cylinder boundary condition, the sequence $f_{1,n}(\cdot)$ with free boundaries converges slower. In Section VII, the position and values of the maximum of $f_2(\cdot)$ are located: $f_2(\cdot) = 0.562798972834$ at $n = 0.56381231$. These results give an estimation of the monomer end-mer constant with 11 correct digits. The previous best result is with 9 correct digits \cite{2}. The results are also compared with those obtained by series expansions and eik-theoretical methods. The maximum value of $f_2(\cdot)$ is equal to the two-dimensional monomer end-mer constant $h_2$. This is one special case of the more general relations between the calculated values in the canonical ensemble and those in the grand canonical ensemble, and these relations are further discussed in Appendix B.

In Section VII, the relations developed in Appendix A are used to compare the results of the computational method presented in this paper with those of other exact \cite{3}. Form monomer end-mer ovals, the more interesting properties are at the more dilute high dimer density limit. In Section VIII, asymptotic behavior of the free energy $f_{m,n}(\cdot)$ is examined for high dimer density near close packing. For lattices with finite width, a dependence of the free energy $f_{m,n}(\cdot)$ on the parity of the lattice with $n$ is found \cite{4}, consistent with the previous results when the number of monomers is $n/2\cdot$ The combination of the results in this section and those of Section II leads to the asymptotic expression Eq. \(2b\) for near close packing dimer density. The asymptotic expression of $f_2(\cdot)$, the free energy on an an in $d$-dimensional lattice, is also investigated near close packing. The results support the functional forms obtained previously through series expansions \cite{5}, but quantitatively the value of the exponent is lower than previously conjectured. In Appendix A, we put together in one place various exact formulas for the one-dimensional lattices ($n = 1$). These formulas can be used to check the formulas developed for the more general situations where $n > 1$. As an illustration, an explicit application of the Fermi-Dirac and Wilson asymptotic method is also given for $n = 1$.

\section{Computational Methods}

The basic computational strategy is to use exact calculations to obtain a series of partition functions $Z_{m,n}(x)$ of lattice strips $m \times n$. Then for a given dimer density $\rho$, $f_{m,n}(\cdot)$ can be calculated using arbitrary precision arithmetic. By fitting $f_{m,n}(\cdot)$ to a given function (Sections \(\text{VIA}\) and \(\text{VII}\)), $f_{m,n}(\cdot)$ can be estimated with high accuracy. From $f_{m,n}(\cdot), f_2(\cdot)$ can then be estimated using the special convergent properties of the sequence $f_{m,n}(\cdot)$ on the cylinder lattice strips (Section \(\text{V}\)).

\subsection{A. Calculation of the partition functions}

The computational methods used here have been described in details previously \cite{6,7,8}. The full partition functions (Eq. \(1\)) are calculated recursively for lattice strips on cylinder lattices and lattices with free boundaries. As before, all calculations of the terms $a_n(m,n)$ in the partition functions use exact integers, and when logarithms are taken to calculate free energy $f_{m,n}(\cdot)$, the calculations are done with precisions much higher than the machine floating-point precision. The bigm library used is GNU mp library (GMP) for arbitrary precision arithmetic (version 4.2) \cite{9}. The details of the calculations on lattices with free boundaries can be found in Ref. \cite{10}, so in the following only information on cylinder lattices is given.

For a $m \times n$ lattice strip, a square matrix $M_{n,m}$ is set up based on two rows of the lattice strip with proper boundary conditions. The vector $\text{v}_{m,n}$, which consists of partition function of Eq. \(2b\) as well as other contracted partition functions \cite{11,12}, is calculated by the following recurrence

$$m = M_{n,m};$$

\text{v}_{m,n} = \text{v}_{m,n} \cdot \text{y}_{m,n}$$

where $\text{v}_{m,n}$ is Euler's totient function, which gives the number of integers relatively prime to integer $m$. The size of matrix $M_{n,m}$ is $u_n(n)$, and $u_n(n)$ is the number of odd and even numbers in the sequence $v_{n}$. The first 17 terms of the sequence $v_{n}$ are: 2, 3, 4, 6, 8, 13, 18, 30, 46, 78, 126, 224, 380, 687, 1224, 2250, and 4112. It is noted that the sequence $u_n(n)$ is exactly the same as that shown in column 2, Table 1 of Ref. \cite{11}. Calculations based on the dominant eigenvalues of the $M$ matrices of the cylinder lattice strips for $n = 4, 6, 8, 10$ are carried out by Runnels \cite{12}. The sizes of $M_{n,m}$ for cylinder lattice strips are smaller when compared with the corresponding matrices of lattices with free boundaries \cite{12}, which allows for calculations on wider lattice strips.

For cylinder lattice strips, full partition functions are calculated for $n = 1; \ldots ; 17$, with length up to $m = 1000$ for
In this paper the main quantity to be calculated is \( f_2(s) \). The starting point of the calculations is the full partition function Eq. 4 for different values of \( n \) and \( m \). Finite values of \( n \) and \( m \) only lead to discrete values of dimer density, as defined in Eq. 5. For example, when \( n = 7 \) and \( m = 11 \), the number of dimers takes the values of \( 0; 1; \ldots ; 38 \), and dimer density of this lattice can only be one of the following values: \( 0; 2; \ldots ; 76 = 77 \). In general, for fixed \( n \) and \( m \), only a rational number:

\[
\frac{p}{q} = \frac{m n}{2q}
\]

where \( p \) and \( q \) are positive integers. When expressed as a rational number, the number of dimers is given by

\[
s = \frac{m n}{2} = \frac{m n p}{2q}.
\]

This expression is only meaningful if \( m n p \) can be divided by \( 2q \). When we write the grand canonical partition function in the form of Eq. 6 for fixed \( m \) and \( n \), we implicitly imply that Eq. 8 is satisfied.

In the following we use the rational dimer density \( \frac{p}{q} \), whenever possible so that the value of \( a_{m,n}(s) \) can be read directly from the partition function of fixed lattice size. Depending on the values of \( p \) and \( q \), some dimer densities, such as \( 1 = 2 \), can be realized in any lattice, while others can only be realized in small numbers of lattices with special combinations of values of \( m \) and \( n \). In many situations it becomes possible to use rational values of \( m \) and \( n \). For example, in Section V I, the location of the maximum of \( f_2(s) \) is searched within a very small region of \( s \), and in Section V I I, in order to compare the results from different methods, the output values of other computational methods \( \frac{p}{q} \). In such situations, if the rational form of \( m \) and \( n \) was used, \( p \) and \( q \) would become so big that not enough data points which satisfy Eq. 8 could be found for the fitting of the \( m \) and \( n \) lattice strip. To calculate \( f_{m,n}(s) \) for an arbitrary real number \( 0 < s < 1 \), interpolation of the exact data points is needed. Since full partition functions have been calculated for fairly large lattice sizes, proper interpolation procedure can yield highly accurate values of \( f_{m,n}(s) \) for an arbitrary real number \( s \). For interpolation, we use the standard Bullough-Kostera rational function interpolation method \( \frac{p}{q} \). For any real number \( s \), Eq. 8 is used to calculate the corresponding number of dimers \( s \), which may not be an integer. On each side of this value of \( s \), 30 exact values of \( a_{m,n}(s) \) are used (if possible) in the interpolation. If on one side there are not enough exact data points of \( a_{m,n}(s) \), extra data points on the other side of \( s \) are used to make the total number of exact data points as 60.

For the high dimer density case (Section V I I I), the total number of data points used is changed to 30. We also take care that no extrapolation is used: if \( s \) is greater than the maximum dimer density for a given \( m \) and \( n \), the data point from this lattice is not used. Let's look at the above example of \( s = 7 \) lattice again. For this lattice, the highest dimer density is 76 = 77. If calculation is done for a dimer density \( s = 0.99 \), since \( 0.99 < 76 = 77 = 0.987 \), the data point from this lattice will not be used in the following steps to avoid inaccuracy introduced by unreliable extrapolations.

C. Fitting procedure

The fitting experiments are carried out by using the \( \texttt{texp} \) function of software gnuplot (version 4.0) \( \frac{p}{q} \) on a 64-bit Linux system. The algorithm implemented is the nonlinear least-squares (NLLS) Levenberg-Marquardt method \( \frac{p}{q} \). All fitting experiments use the default value as the initial value for each parameter, and each fitting experiment is done independently. As done previously \( \frac{p}{q} \), only those \( a_{m,n}(s) \) with \( m = 100 \) are used in the fitting. Since \( a_{m,n}(s) \) is calculated for relatively large lattice strips (in the \( m \) direction, see Section V I), the estimates of \( f_{m,n}(s) \) are usually quite accurate, up to 12 or 13 decimal places. The accuracy for this fitting step is limited by the machine oating-point precision, since gnuplot uses machine oating-point representations, instead of arbitrary precision arithmetic etc. We would have used the GMP library to implement a fitting program with arbitrary precision arithmetic etc. This would increase the accuracy in the estimation of \( f_2(s) \) when is small. For the major objective of this paper, i.e., to investigate the behavior of \( f_2(s) \) when \( s \) \( \approx \) 1 (Section V I I I), however, the current accuracy is adequate. At high dimer density \( s \) towards \( s \) \( \approx \) 1, the convergence of \( f_{m,n}(s) \) towards \( f_2(s) \) is much slower than at low dimer density \( s \approx 0 \). With lattice width \( n = 17 \) used for the current calculations, \( f_{m,n}(s) \) is far from converging to the machine oating-point precision when \( s \approx 1 \).

III. LOGARITHMIC CORRECTIONS OF THE FREE ENERGY AT FIXED DIMER DENSITY

For lattice strips \( m \) with a fixed width \( n \) and a given dimer density, the coefficients \( a_{m,n}(s) \) of the partition functions are extracted to the following:

\[
f_{m,n}(s) = \ln a_{m,n}(s) = \frac{m n}{m} C_0 + \frac{C_1}{m} + \frac{C_2}{m^2} + \frac{C_3}{m^3} + \frac{C_4}{m^4} + \frac{1}{n} \ln (m + 1)
\]

where \( C_0 = f_{1,1}(s) \).
For both cylinder lattices and lattices with free boundaries, the fitting experiments clearly show that \( s = 1 \leq 2 \), accurate up to at least six decimal places, for any dimer density \( 0 < \rho < 1 \). This result holds for both odd \( n \) and even \( n \). This is in contrast with the results reported earlier for the situation with a fixed number of monomers (or vacancies), where the logarithmic correction coefficient depends on the number of monomers present and the parity of the width of the lattice strip \( (2g, 2s) \). We notice that a coefficient \( 1=2 \) also appears in the logarithmic correction term of the free energy studied in Ref. \( [27] \); this is a special case of the monomer-dimer problem where there is a single vacancy at certain specific sites on the boundary of the lattice.

For the general monomer-dimer model, to our best knowledge, this logarithmic correction term with coefficient \( 1=2 \) has not been reported before in the literature. The recently developed multivariate asymptotic theory by Penante and Wilson \( [28] \), however, gives an explanation of this term and its coefficient. This theory applies to combinatorial problems when the multivariate generating function of the model is known. For univariate generating functions, asymptotic methods are well known and have been used for a long time. The situation is quite different for multivariate generating functions. Until recently, techniques to get asymptotic expressions from multivariate generating functions were almost entirely missing \( (29) \) (for review, see Ref. \( [26] \)). The new technique developed by Penante and Wilson method applies to a large class of multivariate generating functions in a systematic way. In general, the theory applies to generating functions with multiple variables, and for the bivariate case that we are interested in here, the generating function of two variables takes the form

\[
F(x; y) = \frac{G(x; y)}{H(x; y)} = \sum_{m=0}^{\infty} a_m x^m y^m \tag{10}
\]

where \( G(x; y) \) and \( H(x; y) \) are analytic, and \( H(0; 0) \neq 0 \). In this case, Penante and Wilson method gives the asymptotic expression as

\[
a_m = \left( \frac{G(x_0; y_0)}{H(x_0; y_0)} \right) \frac{x_0^m y_0^m}{m! Q(x_0; y_0)} \tag{11}
\]

where \( (x_0; y_0) \) is the positive solution to the two equations

\[
H(x; y) = 0; \quad m x \frac{\partial H}{\partial x} = s y \frac{\partial H}{\partial y} \tag{12}
\]

and \( Q(x; y) \) is defined as

\[
(\ln H_x)(\ln H_y)^2 (\ln H_y)(\ln H_x)^2 [(\ln H_y)^2 (\ln H_{xx})^2 + (\ln H_x)^2 (\ln H_{yy})^2 + 2(\ln H_x)(\ln H_y)(\ln H_{xy})];
\]

where \( H_x, H_y, \) etc. are partial derivatives \( \partial H/\partial x, \partial H/\partial y, \) and so on. One of the advantages of the method over previous ones is that the convergence of Eq. \( (11) \) is uniform when \( s = m + n = 2 \) are bounded.

For the monomer-dimer model discussed here, with \( n \) as the single width of the lattice strip, \( m \) as the length, and \( s \) as the number of dimers, we can construct the bivariate generating function \( F(x; y) \) as

\[
F(x; y) = \sum_{m=0}^{\infty} a_m (\ln n; n)x^m y^m = Z_{n; n}(x; y); \quad m = 0, n = 0 \tag{13}
\]

For the monomer-dimer model, as well as a large class of lattice models in statistical physics, the bivariate generating function \( F(x; y) \) is always in the form of Eq. \( (11) \), with \( G(x; y) \) and \( H(x; y) \) as polynomials in \( x \) and \( y \). In fact, we can get \( H(x; y) \) directly from matrix \( M \) in Eq. \( (7) \). It is closely related to the characteristic function of \( M \); \( H(x; y) = \det M_{n \times n} = y^s, \) where \( s \) is the size of the matrix \( M_{n \times n} \). As an illustration, the bivariate generating function \( F(x; y) \) for the one-dimensional lattice \( (n = 1) \) is shown in Eq. \( (10) \) of Appendix B.

When the dimer density is fixed, which is the case discussed here, \( s = n = 2 \). If we substitute this relation into Eq. \( (12) \), then we see that the solution \( (x_0; y_0) \) of Eq. \( (12) \) only depends on \( n \) and does not depend on \( m \) or \( s \). Substituting this solution \( (x_0; y_0) \) into Eq. \( (11) \) we obtain

\[
\ln n \ln (x_0; y_0) + 1 \ln m z_{n; m} + 1 \ln G(x_0; y_0) \frac{G(x_0; y_0)}{H(x_0; y_0)} \tag{14}
\]

From this asymptotic expansion we obtain the logarithmic correction term with coefficient \( 1=2 \) exactly, for
any value of n. In fact, this asymptotic theory predicts that there exists such a logarithmic correction term with coefficient of 1/2 for a large class of lattice models when the two variables involved are proportional, that is, when the m odds are at fixed density. For those lattice models which can be described by bivariate generating functions, this logarithmic correction term with coefficient of 1/2 is universal when those models are at fixed density. For the monomer-dimer model, this proportional relation is for s and m with s = m/2. An explicit calculation for n = 1 is shown in Appendix A.

For a fixed density and a fixed lattice width n, the first term of Eq. (14) is a constant and does not depend on m. We identify it as $f_{1,m,n}$

$$f_{1,m,n} = \frac{1}{n} \ln \left( \alpha \right)$$

In all the following fitting experiments, we set $\alpha = 1/2$ for Eq. (17).

IV. CYLINDER LATTICES

For the monomer-dimer problem at a given density in cylinder lattice strips, the sequence $f_{1,m,n}$ converges very fast to $f_1(n)$, as can be seen from a few sample data in Table I. In the table, values of $f_{1,m,n}$ for $m = 1, 2, 3, 4, 5$ and $n = 1$ are listed. Two obvious features can be observed: (1) The function $f_{1,m,n}$ is an increasing function of odd n, but a decreasing function of even n. Furthermore, for nine integer values of m and k,

$$f_{1,m,k} > f_1(n) > f_{1,m,k+1}$$

The value $f_{1,m,n}$ oscillates around the limit value $f_1(n)$ from even n to odd n. (2) The smaller the value of $m$, the faster the rate of convergence of $f_{1,m,n}$ towards $f_1(n)$. Rational values of n are used for the calculations in Table I and no interpolation of $a_{m,n}$ is used. The number of data points used in the fitting are listed in the parentheses.

As a check of the accuracy of the results, the data at n = 1 can be compared with the exact solution. For a cylinder lattice strip 1 x n, the exact expression for $f_{1,m,1}$ reads as

$$f_{1,m,1} = \frac{1}{n} \ln \left( \frac{2}{1} \right) + \frac{\sin (\pi \frac{2}{1})}{n} + 1 + \sin^2 (\pi \frac{2}{1})$$

The results from Eq. (17) are listed as the last column in Table I. As mentioned in the previous section, all input data are exact integers and the logarithm of these integers is taken with high precision before the fitting. The only places where accuracy can be lost are in the fitting procedure as well as the approximation introduced by the fitting function Eq. (10). Comparisons of the data in the last two columns of Table I show that, as far as the fitting procedure is concerned, the calculation accuracy is up to 12 or 13 decimal places.

Another check for the accuracy of the fitting procedure is through the exact expression Eq. (18) of one-dimensional strip (n = 1) at various density. The data are listed in the first row of Table II. By using Eq. (15) of the Fermi-Dirac and Wilson asymptotic method, we can also compute the fitting results with exact asymptotic values for small values of n (data not shown). All these checks confirm that the accuracy of the fitting procedure is up to 12 or 13 decimal places. See Section V for further discussions on this issue.

The fast convergence of $f_{1,m,n}$ and the property of Eq. (10) make it possible to obtain $f_1(n)$ quite accurately, especially when n is not too close to 1. Some of the values of $f_2(n)$ at rational $p = \frac{p}{q}$ for small $p$ and $q$ are listed in Table II. As in Table I, no interpolation of $a_{m,n}$ is used. The number of data points in square brackets indicate the next digit for n = 16 (upper bound) and n = 17 (lower bound). The data show that when n = 0.55, the $f_2(n)$ is accurate up to at least 10 decimal places. It should be pointed out that the data listed are just raw data, showing digits that have already converged for n = 16 and n = 17. If the pattern of convergence of these raw data is explored and extrapolation technique is used, as is done in Section V, it is possible to get even more correct digits. As shown in Section V, the true value of $f_2(n)$ is not the average of $f_{1,m,n}(n)$ and $f_{1,m,n}(n+1)$. Instead, it should be closer to $f_{1,m,n}(n)$.

V. LATTICES WITH FREE BOUNDARIES

We also carry out similar calculations for lattice strips on m x n two-dimensional lattices with free boundaries, for n = 2, ..., 16. A few sample data are shown in Table II. In the table, values of $f_{1,m,n}$ for $m = 1, 2, 3, 4, 5$ and $n = 1$ are listed. The data in Table II show that the sequence of $f_{1,m,n}$ in lattices with free boundaries converges slower than that in cylinder lattices. Furthermore, in contrast to the situation in cylinder lattices, $f_{1,m,n}(n)$ is an increasing function of n for $0 < k < 1$; $f_{1,m,n}(n)$ approaches $f_1(n)$ (the same value as that for cylinder lattices) monotonically from below. When $n = 1$, the functions $f_{1,m,n}(1)$ and $f_{1,m,n}(1)$ are increasing functions, with $f_{1,m,n}(1) > f_{1,m,n}(1)$ and $f_{1,m,n}(1) > f_{1,m,n}(1)$. Due to the slow convergence rate and the lack of property of Eq. (16), it is difficult to obtain $f_1(n)$ reliably from the data on the lattice strips with free boundaries.

As we did in the previous Section, we also take advantage of the known exact solution for $n = 1$ as a check for the numerical accuracy of the fitting procedure. The exact result for lattice strips with free boundaries is given...
TABLE I: The cosine coefficient $c_0$ ($f_{0,m}$) for dihedral angles and on cylinder lattice strips $1/n$. The numbers in parentheses are the number of data points used in the fitting. The first row for $n=1$ is from the exact expression Eq. 6. The last column is from the exact expression Eq. 11 when $\alpha = 1$. Rational $1/n$ is used here and no interpolation of $a_{n,m}$ is used.

| $1/n$ | $2/n$ | $3/n$ |
|-------|-------|-------|
| 0.4068321918785 | 0.0000000000000 | 0.0000000000000 |
| 0.4068321918785 | 0.0000000000000 | 0.0000000000000 |
| 0.4068321918785 | 0.0000000000000 | 0.0000000000000 |
| 0.4068321918785 | 0.0000000000000 | 0.0000000000000 |

TABLE II: List of $f_2$ for dihedral angles. Numbers in square brackets indicate the next digits for $n = 16$ (upper bound) and $n = 17$ (lower bound). Rational $1/n$ is used here and no interpolation of $a_{n,m}$ is used.

| $f_2$ |
|-------|
| 0 |
| 0.133462263587 |
| 0.133462263587 |
| 0.133462263587 |
| 0.133462263587 |
| 0.133462263587 |
| 0.133462263587 |
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| 0.133462263587 |
| 0.133462263587 |
| 0.133462263587 |
| 0.133462263587 |
| 0.133462263587 |

VI. MAXIMUM OF FREE ENERGY AND THE MONOMER-DIMER CONSTANT

It is well known that $f_2$ is a continuous concave function of $\alpha$ and at certain dimers, $f_2$ reaches its maximum at $\alpha = h_2$. However, there is no analytical knowledge of the location of the maximum and value ($f_2$) of the maximum for $\alpha > 1$. As shown in Appendix B, the maximum of $f_2$ is equal to the maximum of the monomer-dimer constant: $f_2 = n + 1$. Currently, the best value for $h_2$ is given in Ref. 12, which gives $h_2 = 0.6279897277$. It is well known that $f_2$ is the maximum of $f_2$ for $\alpha = h_2$. Therefore, we can assume that the value of $f_2$ for $\alpha = h_2$ is the maximum of $f_2$.

In this Section we use the same computational procedure described in the previous sections to locate accurately the value of $f_2$. Using rational dimer density $\alpha = p/q$ and choose appropriate $p$ and $q$, we can locate the maximum of $f_2$ using $\alpha = h_2$. As shown in Figure 7, we obtain

$$f_2(\alpha) = \frac{1}{n} \left( \frac{1}{n} \sum_{i=1}^{n} \cos \frac{i}{n+1} + \frac{1}{n} \sum_{i=1}^{n} \cos \frac{i}{n+1} \right)^{n+1}$$

(18)

The last column in Table I lists the values obtained from the numerical experiments in the column $n$ next to it. Again, as shown in the previous Section, the accuracy at $\alpha = 1$ is up to 11 or 12 decimal places for most of the values of $\alpha$.
TABLE III: The coefficients $c_0 (t_{\rho n}^\pm)$ for different $n$ and on lattice strips $l$ with free boundaries. The numbers in parentheses are the number of data points used in the fitting. The last column $n$ is from the exact expression Eq. (23) when $l = 1$. Rational $p$ is used here and no interpolation of $a_{\rho n} (\pm)$ is used.

| $l$ | $n$ | $c_0 (t_{\rho n}^\pm)$ |
|-----|-----|------------------------|
| 1/4 | 2  | 0.40186721888414 (101) |
| 1/2 | 3  | 0.40685058083319 (101) |
| 3/4 | 4  | 0.40186721888414 (101) |
| 1   | 5  | 0.40186721888414 (101) |

![Image 1](https://example.com/image1.png)

**Figure 1:** (Color online) The function of $f_2 (\rho)$ in the region of $19 \times 20$ and $9 \times 14$. All data points use rational $p$, so no interpolation is used. Then the data points at $n = 63812311$ of $n = 12$, 14, and 16 can be used to obtain an extrapolated value of $f_2 (\rho) = 0.6627989728336$, while the data points of $n = 13, 15, and 17$ give another extrapolation value $f_2 (\rho) = 0.6627989728341$. Together these two extrapolation values converge to $f_2 (\rho) = 0.662798972834$, with 11 correct digits.

We can also get the same conclusion graphically from Figure 2. By inspecting the pattern of the data points of different values of $n$ in the inset of Figure 2, we notice that the difference between the data points of $n = 14$ and $n = 16$ is bigger than the difference between $n = 15$ and $n = 17$. This indicates that the true value of $f_2 (\rho)$ lies closer to the data point of $n = 17$ than the data point of $n = 16$. From Figure 3 we can quite sure that the 11-th digit of $f_2 (\rho)$ is 3 instead of 4, and the 12-th digit is probably 4, as indicated by the two extrapolation values mentioned above.

The value of $f_2 (\rho)$ is in excellent agreement with that reported in Ref. [22] which gives 9 correct digits (Friedland and Pelko also guess correctly the 10-th digit as 8). The value also agrees with that in Ref. [22] which gives 8 correct digits [22]. The value of $f_2 (\rho)$ is exactly that of $f_2 (\rho)$.
TABLE IV: The coefficient $c_0$ ($f_{1n}$) for different $n$ and on cylinder lattice strips $l$ around. The numbers in parentheses are the number of data points used in the fitting.

| $n$ | $c_0$ for $f_{1n}$ | $c_0$ for $f_{1n}$ | $c_0$ for $f_{1n}$ | $c_0$ for $f_{1n}$ |
|-----|-----------------|-----------------|-----------------|-----------------|
| 1   | 0.470643631091106 (880) | 0.47064363208559868 (880) | 0.470643632085629 (880) | 0.470643632497390 (880) |
| 2   | 0.683451694063943 (901) | 0.683451695019491 (901) | 0.683451695019538 (901) | 0.683451696930585 (901) |
| 3   | 0.65983910462378 (901) | 0.659839105636353 (901) | 0.659839105636492 (901) | 0.659839105492258 (901) |
| 4   | 0.66319985040839 (901) | 0.6631998508009 (901) | 0.6631998508009 (901) | 0.6631998508009 (901) |
| 5   | 0.662701144804059 (901) | 0.662701144804059 (901) | 0.662701144804059 (901) | 0.662701144804059 (901) |
| 6   | 0.662818978973677 (901) | 0.662818979809862 (901) | 0.66281897980987 (901) | 0.662818979809837 (901) |
| 7   | 0.662794693257766 (901) | 0.662794695287048 (901) | 0.662794695287048 (901) | 0.662794695287048 (901) |
| 8   | 0.66279924786632 (901) | 0.66279992478662 (901) | 0.66279992478662 (901) | 0.66279992478662 (901) |
| 9   | 0.6627987543959 (901) | 0.6627987543959 (901) | 0.6627987543959 (901) | 0.6627987543959 (901) |
| 10  | 0.66279923857733 (901) | 0.66279923857733 (901) | 0.66279923857733 (901) | 0.66279923857733 (901) |
| 11  | 0.66279927830871 (901) | 0.66279927830871 (901) | 0.66279927830871 (901) | 0.66279927830871 (901) |
| 12  | 0.6627957775594 (901) | 0.6627957775594 (901) | 0.6627957775594 (901) | 0.6627957775594 (901) |
| 13  | 0.662798972113453 (901) | 0.662798972113453 (901) | 0.662798972113453 (901) | 0.662798972113453 (901) |
| 14  | 0.662798973011805 (901) | 0.662798973011805 (901) | 0.662798973011805 (901) | 0.662798973011805 (901) |
| 15  | 0.66279897893030 (970) | 0.66279897893030 (970) | 0.66279897893030 (970) | 0.66279897893030 (970) |
| 16  | 0.662798972844882 (375) | 0.662798972844882 (375) | 0.662798972844882 (375) | 0.662798972844882 (375) |
| 17  | 0.662798972830869 (226) | 0.662798972830869 (226) | 0.662798972830869 (226) | 0.662798972830869 (226) |
TABLE V : Comparison with Baxter’s results. Numbers in square brackets indicate the next digits for n = 16 (upper bound) and n = 17 (lower bound).

| x    | f_1( ) | f_2( ) |
|------|--------|--------|
| 0.00 | 1.0    | 0.29(0.3) | 0.291557 |
| 0.02 | 0.994176 | 0.319(2.8) | 0.319463 |
| 0.05 | 0.936216 | 0.355(0.2) | 0.3551068 |
| 0.10 | 0.96456376 | 0.4047(5.8) | 0.404771005 |
| 0.20 | 0.924706050 | 0.4810(9.9) | 0.481088747 |
| 0.30 | 0.8846581140 | 0.536892(1.4) | 0.5368922350 |
| 0.40 | 0.8453815864 | 0.5782845(2.9) | 0.5782845477 |
| 0.50 | 0.8072764728 | 0.60881(3.4) | 0.6088143934 |
| 0.60 | 0.7705280966 | 0.63085609(6.8) | 0.6308560970 |
| 0.80 | 0.7013863228 | 0.655894637(3.5) | 0.6558946374 |
| 1.00 | 0.6381231092 | 0.6627989728(4.6) | 0.6627989726 |
| 1.50 | 0.5042632394 | 0.6349928930(8.9) | 0.634992920 |
| 2.00 | 0.4006451804 | 0.5776864722(2.7) | 0.577686472 |
| 2.50 | 0.3217824989 | 0.5140877358(6.4) | 0.514087737 |
| 3.00 | 0.2603068980 | 0.4528361791(2.9) | 0.4528361790 |
| 3.50 | 0.2134739146 | 0.3973878949(1.3) | 0.3973878949 |
| 4.00 | 0.1771543204 | 0.3499573614(3.0) | 0.3499573615 |
| 4.50 | 0.1486988909 | 0.3088705099(2.6) | 0.3088705306 |
| 5.00 | 0.126162903820 | 0.273811439807(1.2) | 0.2738114398 |

FIG. 5: (Color online) Fitting result for f_1( ) as ! 1.

VIII. HIGH DIMER DENSITY NEAR CLOSE PACKING

It is well known that phase transition for the onom er model only occurs at = 1 [4]. Since the close-packed dimer system is at the critical point, it is interesting to investigate the behavior of the model when ! 1. Using the similar computational procedure outlined before, the following results are obtained at high dimer density (lattice):

\[
\begin{align*}
&f_{1,\text{ave}}(x) = f_{1,\text{lattice}}(x) + \frac{1}{2} (1 - \frac{1}{2} \ln(1 - x)) \quad n \text{ odd} \\
&f_{1,\text{ave}}(x) = f_{1,\text{lattice}}(x) + \frac{1}{2} (1 - \frac{1}{2} \ln(1 + x)) \quad n \text{ even}
\end{align*}
\]

(22)

where \(f_{1,\text{lattice}}(x)\) is the free energy of close-packed lattice with width \(n\), and is given, based on the boundary condition, by Eq. 22 (cylinder lattices) or Eq. 23 (lattices with free boundary condition). Eq. 22 for \(n = 1\) is verified from the exact result as shown in Eq. 25. The result is also consistent for other values of \(n\) by using the Pemantle and Wilson asymptotic methods for multivariate generating function, as described in Section III. For space limitation these consistent results are not presented in this paper.

The dependence of the asymptotic form of \(f_{1,\text{ave}}(x)\) on the parity of the lattice width \(n\) shown in Eq. 22 reminds us of the results reported previously for the onom er model with \(n\) odd number of onom er sites [29], in which the coefficient of the logarithmic correction term of the free energy depends on the parity of the lattice width \(n\). These two results are consistent with each other. If we substitute the relation \(v = (1 - x)m\) into Eq. 22, we will get the logarithmic correction term with coefficient \(v\) for odd \(n\), and \(v=2\) for even \(n\). More discussions about this asymptotic form will be found in Section IX (Eq. 24).

We also investigate the behavior of \(f_2( )\) (for n on site) as \(v=1\). Since \(f_{1,n}( )\) does not converge fast enough as \(v=1\) (Table I), we use weighted average of \(f_1,n( )\) and \(f_1,n( )\) as an approximation of \(f_2( )\). The weights are calculated from the exact results at \(v=1\). Fitting these data to the following function

\[
f_2( ) = G = \frac{1}{2} (1 - \frac{1}{2} \ln(1 - x) + b_1(1))
\]

(23)

we obtain 1.69775 and \(b_1 = 0.427832\). No other reasonable form of functions other than Eq. 24 gives better fitting. Including a term of \(1/v\) in Eq. 24 leads to only slight changes in the values of \(b_1\) and \(b_2\). The data and the fitting result are shown in Figure 5.

Using the equivalence between statistical ensembles discussed in Appendix A, we can relate our results with Gauß’s series expansions [1]. Plugging \(f_2( )\) as in Eq. 24 into \(f( ) + \frac{1}{2} \ln(b)\) (see Eq. 10), giving weight with respect to, and solving for, we obtain the average dimer density (\(x\)) at the activity \(x\). Expressing \(x\) as a function of \(\beta\), we have

\[
x = \frac{e^{2\beta}}{(1 - \frac{1}{2} \ln(1 - x))}
\]

This is in the same form of Eq. (3.7) of Gauß [3]. If we put in the values of \(b_1\) and \(b_2\), we can estimate the amplitude \(A = \exp(2\beta) = 0.4308\). Gauß obtains through series expansions \(1.73 = 4\) and \(A = 0.8030\) 4, and conjectures that \(\beta = 7.4\). Our results support the same functional form, and the numerical values are close to those obtained by Gauß’s series analysis. As for the conjectured value of \(\beta\), the current data seem to indicate a value lower than 7.4. In fact, the data presented here as well as theoretical arguments not shown here indicate that \(\beta = 5.3\). More discussion on this constant can be found in the next Section.
IX. DISCUSSION

In Section II we show by computational methods that there is a logarithmic correction term in the free energy with a coefficient of \( l = 1.2 \). By introducing the newly developed Pen antle and Wilson asymptotic method, we give a theoretical explanation of this term. We also demonstrate that this term is not unique to the monomer-dimer model. Many statistical lattice models can be cast in the form of bivariate (or multivariate) generating functions, and when the two variables are proportional to each other so that the system is at a fixed "density", we will expect such a universal logarithmic correction term with coefficient of 1 = 2. We anticipate many applications of this asymptotic method in statistical physics in the future.

The Pen antle and Wilson asymptotic method not only gives a nice explanation of the logarithmic correction term and its coefficient found by computational means, but also gives exact numerical values of \( f_{1,m} \) for all \( m \) (the width of the lattice strips). These exact values can be used to check the accuracy of the computational method, as already mentioned in Section II. In Section III we discuss how this can be done. The denominator \( H(x,y) \) of the bivariate generating functions is derived from the characteristic function of the matrix \( M_n \), and the size of \( M_n \) is given by \( u_n(n) \) in Section II for cylinder lattices, and in Ref. \([28]\) for lattices with free boundaries. For small \( n \), the size of \( M_n \) is small enough so that the characteristic function can be calculated symbolically. As \( n \) increases, however, the size of \( M_n \) increases exponentially: \( u_n(17) = 4112 \) for cylinder lattice when \( n = 17 \), and \( u_n(16) = 32896 \) when \( n = 16 \). It is currently in practice to calculate the characteristic functions symbolically from matrices of such sizes to get \( H(x,y) \) of the corresponding bivariate generating functions, so the Pen antle and Wilson method cannot be applied when the width of the lattice \( n \) becomes larger. Even when \( H(x,y) \) is available, it is of the order of thousands or higher, which will lead to instabilities in the numerical calculations. The computational method utilized here, however, can still give important and accurate data in these situations.

Previously we demonstrated that when the monomer number \( v \) or the dimer number \( s \) are xed, there is also a logarithmic correction term in the free energy \([28,29]\). When the number of dimers is \( xed \) (low dimer density \( \text{lim} \)), the coefficient of this term equals to the number of dimers. When the number of monomer onomers is \( xed \) (high dimer density \( \text{lim} \)), the coefficient, however, depends on the parity of the lattice width \( n \): it equals to \( v \) when \( n \) is odd, and \( v=2 \) when \( n \) is even. In this high dimer density \( \text{lim} \), as \( m = 1, \) dimer density \( \text{lim} \). In this paper we focus on the situation where the dimer density is \( xed \), and nd that again there is a logarithmic correction term, but this time its coefficient equals to \( 1=2 \) and does not depend on the parity of the lattice width. Why does the dependence of the coefficient on the parity of the lattice width disappear as dimer density \( \text{lim} \)?

This seemingly paradoxical phenomenon can be explained as follows. When the number of monomer onomers \( v \) is \( xed \) and as \( m = 1 \), if we can put \( v = (1 \text{mod } n) \) into Eq. \((11)\), then the term of \( (1 \text{mod } n) \) leads to a term of \( v \text{mod } m = (v \text{mod } n) \) when \( n \) is odd, and a term of \( v \text{mod } m = (2m \text{mod } n) \) when \( n \) is even. At the same time, the logarithmic correction term with \( l = 1 \) as coefficient \( (\text{lim } m = 2m \text{mod } n) \), the second term in Eq. \((11)\), gets canceled out by the a term of \( n(\text{mod } n = (2m \text{mod } n) \) from the third term in Eq. \((11)\) as \( m = 1 \) and \( 1 \). Putting Eqs. \((11)\) and \((2)\) together, we have for \( n \) even, \( m = 1 \) and \( 1 \),

\[
f_{1,m}(1) = f_{1,m}^{\text{lattice}}(1) + \left( \frac{1}{2} \right) \ln(1) + \left( \frac{1}{2} \right) \ln(1)
\]

result, however, seems to be closer to \( G \)'s result \([32]\). It should be recognized that, as pointed out previously \([33,34]\), as well as in the present work, the convergence is poorest when the dimer density is near close packing. On the other hand, theoretical calculations undertaken (not shown here due to space limitation) indeed indicate that this coefficient of \( (1 \text{mod } n) \) is \( \text{lim} \) for the in nine lattice is \( 5=6 \), or equivalently, \( 5=3 \).

It is well known that there is a one to one correspondence between the Ising model in a rectangular lattice with zero magnetic field and a fully packed dimer model in a decorated lattice \([22,23]\). By using a similar method \([24]\), it has been shown that the Ising model in a non-zero magnetic field, a well-known unsolved problem in sta-
A statistical mechanics, can be mapped to a macroscopic state model with density $< 1$. The investigation of the macroscopic state model near close packing is of interest within this context.

As mentioned in Section V, several authors have applied exact theoretical methods to analyze the macroscopic state model (see, for example, Ref. [3]). In such studies, the macroscopic state problem is expressed as a many-body effective theory. For close-packed dimers model, the expression is a free energy theory with quadratic action, which is exactly solvable as expected. For general macroscopic state model, the expression is an interacting effective theory with a quartic interaction term, and self-consistent Hartree approximation is used to prove the Feynman rules to derive the series expansions. The transforms that are obtained using these methods (such as Eq. (B.1), which is similar to Eq. (2.1)), make the series expansions converge in the full range of the dimer activity. The accuracy of these calculations, however, is not comparable to the accuracy of the computational method reported here, possibly due to the limited length of the series expansion.

**Appendix A: Equivalence of Statistical Ensembles**

Throughout the paper our focus is on the functions $f_{m,n}(\cdot)$, $F_{1,m}(\cdot)$, or $f_{2}(\cdot)$ at a given dimer density. These functions are in essence properties of the canonical ensemble. In this Appendix we make the connection between $f_{2}(\cdot)$ and the functions of $(x)$ and $h_{2}(x)$ as defined in Eqs. (A.1) and (A.2), which are properties of the grand canonical ensemble. The results are used in Section V, III, to compare the results of near close packing dimer density with Gaunt’s series analysis, and in Section VI, II, to compare our results with those of Baxter, whose calculations are carried out in terms of $(x)$ and $h_{2}(x)$.

Suppose at $\phi = 1$, the sum and $a_{m,n}(\cdot) = 0$ in Eq. (A.1) reaches its maximum. By using the standard thermodynamic equivalence between different statistical ensembles [32, Chap. 4], we have

$$h_{2}(x) = \lim_{m,n \to 1} \ln \frac{Z_{m,n}(x)}{F_{m,n}} = \lim_{m,n \to 1} \left( \ln a_{m,n}(\cdot) + \frac{1}{m+n} \right) = f_{2}(\cdot) + \frac{1}{2} \ln x.$$  \hspace{1cm} (A.1)

In other words, if we define $F_{2}(\cdot,x) = f_{2}(\cdot) + \frac{1}{2} \ln x$, then

$$h_{2}(x) = \max_{0,1} (f_{2}(\cdot) + \frac{1}{2} \ln x) = \max_{0,1} F_{2}(\cdot,x).$$  \hspace{1cm} (A.2)

As a special case, the macroscopic state constant is the maximum of the function $f_{2}(\cdot)$ by setting $x = 1$

$$h_{2} = \max_{0,1} f_{2}(\cdot) = f_{2}(\cdot).$$  \hspace{1cm} (A.3)

The connection for the average dimer coverage can also be obtained by using Eqs. (2) and (A.3), as

$$(x) = \lim_{m,n \to 1} m \cdot n \cdot (x) = \lim_{m,n \to 1} \frac{1}{m} \frac{1}{n} \ln \frac{Z_{m,n}(x)}{\ln x} = (x)$$  \hspace{1cm} (A.4)

with the understanding that $f_{2}(\cdot,x) = f_{2}(\cdot) + \frac{1}{2} \ln x$, not $f_{2}(\cdot)$, reaches its maximum. Substituting Eq. (A.4) into Eq. (A.1), we obtain

$$h_{2}(x) = f_{2}(\cdot,x) + \frac{(x)}{2} \ln x.$$  \hspace{1cm} (A.5)

In Section V, the excellent agreement of our result of $f_{2}(\cdot)$ with the result on $h_{2}$ of Friedland and Peled [12] has already been demonstrated. In Ref. 13, what is calculated is actually $h_{2}$. Eq. (A.3) makes it possible to compare our result with that of Friedland and Peled. Eq. (A.5) is proved as a theorem for the macroscopic state problem in Ref. 12 as Theorem 4.1.

Since there is an analytical solution to the one-dimensional lattice case, Eqs. (A.1) and (A.5) can be compared for the one-dimensional lattice by explicit calculations, as shown in Appendix B.

**Appendix B: Explicit Results for One-Dimensional Lattice**

In this Appendix we summarize some exact results for the one-dimensional lattice ($n = 1$) which are useful to compare and check the results for lattices with $n > 1$. When $n = 1$, the problem is a special case of the so-called "parking problem" in one-dimensional lattice in which a k-mer covers k consecutive lattice sites in a non-overlapping way. Various methods exist which lead to closed form solutions to the general case of interacting k-mers (for example, see Refs. [33, 41]). For the macroscopic state model, $k = 2$ and there is no interaction between the dimers. The number of ways to put $s$ dimers in the one-lattice is known as

$$a_{n,1}(s) = \frac{m}{s}.$$  \hspace{1cm} (B.1)

From this expression, in the next subsection we derive the asymptotic expression of the free energy by using the traditional method. As an illustration, later we also give an explicit demonstration of Feynman and Wilson's asymptotic method as it is applied to the bivariate generating function.
1. Canonical ensemble

From the explicit expression of Eq. (B2) we can get the asymptotic expression of the free energy by using Stirling formula when $0 < 1$:

$$ f_{m \lambda} (\lambda) = \frac{\ln a_{m \lambda} (\lambda)}{m} = f_{1 \lambda} (\lambda) + \frac{1}{2m} \ln \frac{2^m}{1} - \frac{1}{2m} \ln \frac{2}{(1^\lambda)} $$

$$ + \sum_{j=1}^{m} \frac{1}{2} \frac{2^j}{j} \frac{(B_{2j})^2}{(1^j)} \frac{1}{2j+1} \begin{array}{c} \frac{1}{2j+1} \frac{1}{2} \frac{2^j}{j} \frac{(B_{2j})^2}{(1^j)} \frac{1}{2j+1} \end{array} $$

$$ = f_{1 \lambda} (\lambda) + \frac{1}{2m} \ln (m+1) + \frac{1}{2m} \ln \frac{2}{(1^\lambda)} $$

$$ + \sum_{j=1}^{m} \frac{1}{2} \frac{2^j}{j} \frac{(B_{2j})^2}{(1^j)} \frac{1}{2j+1} \begin{array}{c} \frac{1}{2j+1} \frac{1}{2} \frac{2^j}{j} \frac{(B_{2j})^2}{(1^j)} \frac{1}{2j+1} \end{array} $$

$$ = f_{1 \lambda} (\lambda) + \frac{1}{2m} \ln (m+1) + \frac{1}{2m} \ln \frac{2}{(1^\lambda)} $$

$$ + \sum_{j=1}^{m} \frac{1}{2} \frac{2^j}{j} \frac{(B_{2j})^2}{(1^j)} \frac{1}{2j+1} \begin{array}{c} \frac{1}{2j+1} \frac{1}{2} \frac{2^j}{j} \frac{(B_{2j})^2}{(1^j)} \frac{1}{2j+1} \end{array} + \frac{1}{2} \frac{2^j}{j} \frac{(B_{2j})^2}{(1^j)} \frac{1}{2j+1} \begin{array}{c} \frac{1}{2j+1} \frac{1}{2} \frac{2^j}{j} \frac{(B_{2j})^2}{(1^j)} \frac{1}{2j+1} \end{array} $$

(4.3)

where

$$ f_{1 \lambda} (\lambda) = (\frac{1}{2} \ln (\frac{1}{2}) - \frac{1}{2} \ln \frac{1}{2} (1^\lambda) \ln (1) $$

(4.4)

and $B_{2j}$ are the Bernoulli numbers.

From Eqs. (B2) or (B3) it is evident that for $n = 1$, the coefficient of the logarithmic correction term is $\lambda^2$ for $0 < 1$.

The asymptotic expression of $f_{1 \lambda} (\lambda)$ (Eq. (B4)) at $\lambda = 1$ is given by

$$ f_{1 \lambda} (\lambda) = (\frac{1}{2} \ln (\frac{1}{2}) - \frac{1}{2} \ln \frac{1}{2} (1^\lambda) \ln (1) $$

(5)

From this asymptotic expression we can see that the coefficient of $\ln (1^\lambda) \ln (1)$ is exactly 1, as in Eq. (B1) for odd values of $n$. By combining Eqs. (B2) and (B3) together we can meet Eq. (B4) for $n = 1$ at high density limit $m\lambda$.

2. Grand canonical ensemble

In this section we calculate various quantities associated with the grand canonical ensemble. The grand canonical partition function (Eq. (10)) is

$$ Z_{m \lambda} (\lambda) = \sum_{n=0}^{\infty} x^n s^n $$

To get a closed form of $Z_{m \lambda} (\lambda)$, we use the WZ method (Wiener-Zeilberger) [12] to get the following recurrence of $Z_{m \lambda} (\lambda)$

$$ xZ_{m \lambda} (\lambda) + Z_{m+1 \lambda} (\lambda) = 0; $$

from which we obtain the closed form solution as

$$ Z_{m \lambda} (\lambda) = \frac{1}{1 + 4x} m + 1 $$

(6)

$$ Z_{m \lambda} (\lambda) = \frac{1}{1 + 4x} m + 1 $$

(6)

where

$$ p_{1 \lambda} = \frac{1}{1 + 4x} $$

To calculate $\lambda$ using Eq. (6), we need to evaluate the sum

$$ \sum_{s=0}^{\infty} x^s s^n $$

A again by using WZ method, we obtain the following recurrence for $S (m)$

$$ (m + 2) x S (m) + (m + 1) S (m + 1) = 0; $$

To solve this recurrence, we use the generating function of $S (m)$: $G_s (z) = \sum_{m=0}^{\infty} S (m) z^m$, and get $G_s (z)$ from the recurrence as

$$ G_s (z) = \sum_{m=0}^{\infty} x^m s^n $$

From $G_s (z)$ a closed form expression of $S (m)$ can be found as

$$ S (m) = \sum_{m=0}^{\infty} x^m s^n $$

(7)

$$ S (m) = \sum_{m=0}^{\infty} x^m s^n $$

(7)

Substituting Eqs. (6) and (7) into Eq. (26), we obtain

$$ 1 (\lambda) = \frac{1}{1 + 4x} $$

(8)
Using Eq. (B.9) we can calculate $h_1(x)$ as

$$h_1(x) = \lim_{m \to 1} \frac{\ln Z_{m,1}(x)}{m} = \ln \left( 1 + \frac{p}{1 + 4x} \right)$$  \hspace{1cm} (B.10)

It is known that there are multiple methods to solve the one-dimensional lattice model. For example, transforming matrix methods can also be used [22]. In this case, the transformation matrix is

$$T_1 = \begin{pmatrix} 0 & x \\ 1 & 1 \end{pmatrix}$$

whose eigenvalues are $\lambda_1 = 0$, $\lambda_2 = 1 + \frac{p}{1 + 4x}$. As $m \to 1$, $Z_{m,1}(x) \to \ln x$, so we obtain $h_1(x)$ as Eq. (B.9). From $1(x) = 2 \ln 1 = \ln x$ we obtain Eq. B.8.

3. Equivalence of statistical ensembles

The confirmation of the equivalence of ensembles for the special case of $x = 1$ (Eq. A.9) has been done in Ref. [22]. Here we carry out the explicit calculations for the general case of arbitrary interaction $x$.

If we take the derivative of function $F_1(x; y) = f_1(x) + \ln y$, where $f_1(x) = f_1(y) = f_1(x)$ is given in Eq. (B.9), solve for $y$, and retain only the solution in $[0; 1]$, we have

$$y = 1 + \frac{1}{1 + 4x}$$

which is the same as Eq. (B.8). If we put the value of $F_1(x; y)$, we obtain the maximum of $F_1(x; y)$:

$$\max (f_1(x) + \ln y) = \ln \left( 1 + \frac{p}{1 + 4x} \right) = h_1(x)$$  \hspace{1cm} (B.11)

4. Application of Pemantle and Wilson asymptotic method to the bivariate generating function

The bivariate generating function of Eq. (B.13) can also be obtained in multiple ways, for example by direct summation of Eq. (B.13) or by using the characteristic function of $M_1$, or by using Eq. (23) of Ref. [22] (by setting the interaction parameter $= 1$ and the size of $m$ as $2$), to get

$$F_1(x; y) = \frac{1}{1 + xy^2}$$  \hspace{1cm} (B.12)

Here $G(x; y) = 1$ and $H(x; y) = 1 + xy^2$. Solving the two equations in $x$, we get $x_0(y_0)$ as $x_0(s) = s(m = 2s)$; $y_0 = (m = 2s)$. Substituting $x_0(y_0)$ into Eq. (B.11) we obtain

$$a_m = \frac{1}{2} (m + 2s)^{m + 1} (m + 2s)^{m + 2s} s^{1 + 2s}$$

By putting $s = m = 2$, the first three terms of $a_n(a_n)$ are recovered, including the term of logarithmic corrections $\ln m = (2m)$. Higher order terms can also be obtained if more terms of the asymptotic expressions are used [22].
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