Asymptotics of the monomer-dimer model on two-dimensional semi-infinite lattices

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By using the asymptotic theory of Pemantle and Wilson [R. Pemantle and M. C. Wilson, J. Comb. Theory, Ser. A 97, 129 (2002)], asymptotic expansions of the free energy of the monomer-dimer model on twodimensional semi-infinite $\infty \times n$ lattices in terms of dimer density are obtained for small values of *n*, at both high- and low-dimer-density limits. In the high-dimer-density limit, the theoretical results confirm the dependence of the free energy on the parity of *n*, a result obtained previously by computational methods by Y. Kong [Y. Kong, Phys. Rev. E 74, 061102 (2006); Phys. Rev. E 73, 016106 (2006); Phys. Rev. E 74, 011102 (2006)]. In the low-dimer-density limit, the free energy on a cylinder $\infty \times n$ lattice strip has exactly the same first *n* terms in the series expansion as that of an infinite $\infty \times \infty$ lattice.

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I. INTRODUCTION

One of the seminal achievements in statistical mechanics and combinatorial mathematics is the exact solution of the close-packed dimer model $[1-3]$ $[1-3]$ $[1-3]$. Shortly after the discovery of the exact solution to the close-packed dimer problem on rectangular lattices, it was found that the finite-size properties of the model depend on the parity of the lattice width $[4]$ $[4]$ $[4]$. More recently, this dependence on the parity of the lattice width was also discovered on other types of lattices when they are fully packed $[5,6]$ $[5,6]$ $[5,6]$ $[5,6]$. Logarithmic conformal field theory was used to explain this unusual finite-size behavior $\lceil 7 \rceil$ $\lceil 7 \rceil$ $\lceil 7 \rceil$.

For the more general monomer-dimer problem where there are vacancies (monomers) on the lattice, however, an exact solution is elusive despite years of investigation. Recently, in the investigation of the monomer-dimer model on two-dimensional rectangular lattices by computational methods, it was found that at the high-dimer-density limit, one of the correction terms of the free energy depends on the parity of the width of the lattice strip $\lceil 8-10 \rceil$ $\lceil 8-10 \rceil$ $\lceil 8-10 \rceil$. These results showed that for the monomer-dimer problem, the dependence of physical properties on the parity of the lattice width occurs not only at, but also below, the close-packed density.

For a two-dimensional $m \times n$ rectangular lattice, we define the dimer density ρ as $\rho = 2s/mn$, where *s* is the number of dimers. With this definition, a close-packed lattice will have $\rho = 1$. The grand canonical partition function of the monomer-dimer system in a $m \times n$ two-dimensional lattice is

$$
Z_{m,n}(x) = \sum_{s=0}^{N} a_{m,n}(s)x^s = \sum_{0 \le \rho \le 1} a_{m,n} \left(\frac{\rho mn}{2}\right) x^{\rho mn/2}, \quad (1)
$$

where $a_{m,n}(s)$ is the number of distinct ways to arrange *s* dimers on the $m \times n$ lattice, *x* is the activity of the dimer, and *N* is the maximum number of possible dimers on the lattice: $N = \lfloor mn/2 \rfloor$. The free energy per lattice site at a given dimer density ρ is defined as

$$
f_{m,n}(\rho) = \frac{1}{mn} \ln a_{m,n} \left(\frac{\rho mn}{2} \right).
$$

The free energy per lattice site on the semi-infinite lattice strip $\infty \times n$ is defined as

$$
f_{\infty,n}(\rho) = \lim_{m \to \infty} f_{m,n}(\rho).
$$

We use $f_{\infty,\infty}(\rho)$ to denote the free energy per lattice site on the infinite lattice:

$$
f_{\infty,\infty}(\rho) = \lim_{m,n \to \infty} f_{m,n}(\rho) = \lim_{n \to \infty} f_{\infty,n}(\rho).
$$

For a semi-infinite $\infty \times n$ lattice at the high-dimer-density limit as $\rho \rightarrow 1$, the computational method [[8](#page-12-6)] shows that the free energy $f_{\infty,n}(\rho)$ depends on the parity of the fixed lattice width *n* as $\rho \rightarrow 1$:

$$
f_{\infty,n}(\rho) \sim f_{\infty,n}^{\text{lattice}}(1) + \begin{cases} (1-\rho)\ln\frac{1}{1-\rho}, & n \text{ is odd,} \\ \frac{1}{2}(1-\rho)\ln\frac{1}{1-\rho}, & n \text{ is even,} \end{cases}
$$
 (2)

where $f_{\infty,n}^{\text{lattice}}(1)$ is the free energy of a close-packed lattice with width *n*, the exact expression of which is known and is dependent on the type of boundary conditions—i.e., cylinder versus free $[1,2]$ $[1,2]$ $[1,2]$ $[1,2]$. Here the free-boundary condition means tiling a rectangle and cylinder means dimers are allowed to wrap around in the direction of *n* from the left edge of the lattice to the right edge. A slightly more general expression, for a finite $m \times n$ lattice at the high-dimer-density limit as *Electronic address: matky@nus.edu.sg $\rho \rightarrow 1$ and $m \rightarrow \infty$, is given by [[8](#page-12-6)]

$$
f_{m,n}(\rho) \sim f_{\infty,n}^{\text{lattice}}(1) + \begin{cases} (1-\rho)\ln\frac{1}{1-\rho} & -\frac{1}{2mn}\ln m + \frac{1}{2mn}\ln\frac{1}{1-\rho}, & n \text{ is odd,} \\ \frac{1}{2}(1-\rho)\ln\frac{1}{1-\rho} & -\frac{1}{2mn}\ln m + \frac{1}{2mn}\ln\frac{1}{1-\rho}, & n \text{ is even.} \end{cases}
$$
(3)

For the coefficient of the term $(1-\rho)\ln\frac{1}{1-\rho}$ in the above expansion of the free energy $f_{\infty,n}(\rho)$, computational results gave values very close to 1 when *n* is odd and $1/2$ when *n* is even $[8]$ $[8]$ $[8]$. Although this numerical evidence strongly supports the dependence of the coefficient of the $(1-\rho)\ln\frac{1}{1-\rho}$ term on the parity of *n*, there are several reasons to be skeptical of this evidence. First, the sequence of *n* used in the computational studies was not very long. For cylinder lattices, the largest *n* used was 17. For lattices with free edges, the maximum value of $n=16$ was used. Second, at the high-dimerdensity limit, the convergent rate is the poorest and some heuristic weighting averages had to be used in the fitting procedure $\lceil 8 \rceil$ $\lceil 8 \rceil$ $\lceil 8 \rceil$.

In this report, we use the asymptotic theory of Pemantle and Wilson $\lceil 11,12 \rceil$ $\lceil 11,12 \rceil$ $\lceil 11,12 \rceil$ $\lceil 11,12 \rceil$ to get the asymptotics of the free energy $f_{\infty,n}(\rho)$ of $\infty \times n$ lattices. The asymptotics show that the coefficients of the $(1-\rho)\ln\frac{1}{1-\rho}$ term in the high-dimer-density expansion of $f_{\infty,n}(\rho)$ is exactly 1 when *n* is odd and 1/2 when *n* is even. Furthermore, the Pemantle-Wilson method is also used to investigate the low-dimer-density expansion of $f_{\infty,n}(\rho)$. By comparing $f_{\infty,n}(\rho)$ of a semi-infinite cylinder lattice with $f_{\infty,\infty}(\rho)$ of the infinite lattice, it is found that in the low-dimer-density limit, $f_{\infty,n}(\rho)$ has exactly the same first *n* terms as $f_{\infty,\infty}(\rho)$ in the expansion, up to the term of ρ^{n-1} . The difference between $f_{\infty,n}(\rho)$ and $f_{\infty,\infty}(\rho)$ starts with the term of ρ^n . Closed-form expressions can be obtained for the coefficients of the first two or probably three terms of the differ-ence [Eq. ([20](#page-8-0)) and Table [I](#page-2-0)]. These properties not only explain the fast convergence rate of the free energy on cylinder lattices when the dimer density is low, but also provide a quantitative indicator of the errors when the results of finitesize lattices are used to approximate the infinite lattice.

The article is organized as follows. In Sec. II, the Pemantle-Wilson (PW) method for the asymptotics of multivariate generating functions is summarized. The starting point for the PW method is the multivariate generating function of the model under study, and in our case of the monomer-dimer model, the generating functions are bivariate. In Appendix A, the bivariate generating functions of monomer-dimer models in two-dimensional rectangular lattices are listed for small values of *n*. These generating functions are used as the input to the PW method in this article. In Sec. III, the asymptotic expansions of $f_{\infty,n}(\rho)$ at high dimer density are derived for some small values of *n*. The coefficients obtained for the $(1-\rho)\ln\frac{1}{1-\rho}$ term confirm the dependence on the parity of n , as shown in Eq. (3) (3) (3) . In Sec. IV, we discuss the asymptotic expansions of $f_{\infty,n}(\rho)$ at low dimer density.

II. PEMANTLE-WILSON METHOD FOR THE ASYMPTOTICS OF MULTIVARIATE GENERATING FUNCTIONS

To extract asymptotics from a sequence, it is usually useful to utilize its associated generating function. The method for extracting asymptotics from *univariate* generating functions is well known $|13|$ $|13|$ $|13|$. For multivariate generating functions, however, the techniques were "almost entirely missing" until the recent development of the Pemantle-Wilson method $\lceil 11,12 \rceil$ $\lceil 11,12 \rceil$ $\lceil 11,12 \rceil$ $\lceil 11,12 \rceil$. For combinatorial problems with known generating functions, the method can be applied in a systematic way. The theory applies to generating functions with multiple variables, and for the bivariate case that we are interested here, the generating function of two variables takes the form

$$
G(x,y) = \frac{F(x,y)}{H(x,y)} = \sum_{s,m=0}^{\infty} a_{sm} x^{s} y^{m},
$$
 (4)

where $F(x, y)$ and $H(x, y)$ are analytic and $H(0, 0) \neq 0$. In this case, the PW method gives the asymptotic expression as $([11],$ $([11],$ $([11],$ theorem 3.1)

$$
a_{sm} \sim \frac{F(x_0, y_0)}{\sqrt{2\pi}} x_0^{-s} y_0^{-m} \sqrt{\frac{-y_0 H_y(x_0, y_0)}{mQ(x_0, y_0)}}
$$
(5)

for $s, m \rightarrow \infty$, where (x_0, y_0) is the positive solution to the two equations

$$
H(x, y) = 0, \quad mx \frac{\partial H}{\partial x} = sy \frac{\partial H}{\partial y}
$$
(6)

and $Q(x, y)$ is defined as

$$
-(xH_x)(yH_y)^2 - (yH_y)(xH_x)^2
$$

$$
-x^2y^2[H_x^2H_{xx} + H_x^2H_{yy} - 2H_xH_yH_{xy}].
$$

Here H_x , H_y , etc., are partial derivatives $\partial H/\partial x$, $\partial H/\partial y$ and so on. If *H* is smooth (H, H_x) , and H_y never simultaneously vanish) and if $F(x_0, y_0)$ and $Q(x_0, y_0)$ are nonvanishing, then the convergence of Eq. ([5](#page-1-1)) is *uniform* when s/m and m/s are bounded. The uniform convergence is one of the advantages of the PW method over previous methods.

When the coefficients a_{sm} in Eq. ([4](#page-1-2)) are non-negative, as are the cases for most combinatorial problems including the monomer-dimer model discussed here, the existence of a positive solution (x_0, y_0) to Eq. ([6](#page-1-3)) is guaranteed by the nonnegativity of a_{sm} ([[12](#page-12-10)], theorem 3.14).

TABLE I. Coefficients of ρ^i in the series expansion of $f_{\infty,n}(\rho)$ of cylinder lattices at low dimer density. The term $-\frac{1}{2}\rho \ln(\rho)$, common to lattices of all sizes, is not shown. The last row for the infinite lattice $f_{\infty,\infty}(\rho)$ is taken from the series expansion, Eq. ([19](#page-8-1)). Terms of $f_{\infty,n}(\rho)$ that are equal to those of the infinite lattice are underlined.

\boldsymbol{n}	ρ	$-\rho^2$	$-\rho^3$	$-\rho^4$	$-\rho^5$	$-\rho^6$	$-\rho'$	$-\rho^8$
	$ln 2 + 1$	3/8	7/48	5/64	31/640	21/640	127/5376	255/14336
2	\bigcirc $\ln 2 + \frac{1}{2}$	13/32	115/768	419/6144	5491/163840	17489/983040	116687/11010048	423771/58720256
3	$\ln 2 + 1/2$	7/16	1/6	127/1536	1027/20480	8653/245760	17677/688128	2381/131072
$\overline{4}$	$\ln 2 + 1/2$	7/16	31/192	239/3072	461/10240	3569/122880	27325/1376256	7579/524288
5	$\ln 2 + 1/2$	7/16	31/192	121/1536	473/10240	941/30720	3791/172032	4375/262144
6	$\ln 2 + 1/2$	7/16	31/192	121/1536	471/10240	1243/40960	3707/172032	4177/262144
7	$\ln 2 + 1/2$	7/16	31/192	121/1536	471/10240	1867/61440	3719/172032	4215/262144
∞	$\ln 2 + 1/2$	7/16	31/192	121/1536	471/10240	1867/61440	7435/344064	4211/262144

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

$$
G_n(x,y) = \sum_{m=0}^{\infty} \sum_{s=0}^{mn/2} a_{m,n}(s) x^s y^m = \sum_{m=0}^{\infty} Z_{m,n}(x) y^m.
$$
 (7)

For the monomer-dimer model, as well as a large class of lattice models in statistical physics, the bivariate generating function $G(x, y)$ is always in the form of Eq. ([4](#page-1-2)), with $F(x, y)$ and $H(x, y)$ as polynomials in *x* and *y*. In fact, for the monomer-dimer model as well as other lattice models, we can get the generating function $G = F/H$ directly from the matrix M_n used in the recursive formula to calculate the partition functions $[8-10,14]$ $[8-10,14]$ $[8-10,14]$ $[8-10,14]$ $[8-10,14]$. More discussions on how the generating functions are calculated can be found in Appendix A.

The relation between the number of dimers, *s*, and the dimer density ρ is given by $s = \rho mn/2$. If we fix the dimer density ρ and substitute this relation into Eq. ([6](#page-1-3)), then we see that the solution (x_0, y_0) of Eq. ([6](#page-1-3)) depends only on ρ and *n*, and not on *m* or *s*

$$
H(x, y) = 0,
$$

\n
$$
x \frac{\partial H}{\partial x} = \frac{\rho n y}{2} \frac{\partial H}{\partial y}.
$$
 (8)

Substituting this solution $[x_0(n, \rho), y_0(n, \rho)]$ into Eq. ([5](#page-1-1)) we obtain, with *n* and ρ fixed as $m \rightarrow \infty$,

$$
f_{m,n}(\rho) \sim -\frac{1}{n} \ln(x_0^{\rho n/2} y_0) - \frac{1}{2} \frac{\ln m}{mn}
$$

+
$$
\frac{1}{mn} \ln \left(F(x_0, y_0) \sqrt{\frac{-y_0 H_y(x_0, y_0)}{2 \pi Q(x_0, y_0)}} \right).
$$
 (9)

From this asymptotic expansion we obtain the logarithmic correction term with coefficient of exactly $-1/2$ [the second term in Eq. (9) (9) (9) for both even and odd values of *n*. In fact, the PW asymptotic theory predicts that, as long as the conditions described above for Eq. (5) (5) (5) hold, there exists such a logarithmic correction term with a coefficient of −1/2 for a

large class of lattice models when the two variables involved are proportional—that is, when the models are at a fixed "density." For those lattice models which can be described by bivariate generating functions, this logarithmic correction term with a coefficient of $-1/2$ is universal when those models are at a fixed "density." For the monomer-dimer model, this proportional relation is for *s* and *m* with $s = \rho mn/2$.

When the dimer density ρ and the lattice width n are fixed, the first term of Eq. (9) (9) (9) is a constant and does not depend on *m*. We identify it as $f_{\infty,n}(\rho)$:

$$
f_{\infty,n}(\rho) = -\frac{1}{n} \ln(x_0^{\rho n/2} y_0).
$$
 (10)

In theory, as long as the bivariate generating function $G(x, y)$ or its denominator $H(x, y)$ is known, (x_0, y_0) could be solved from the system of equations ([8](#page-2-2)) and $f_{\infty,n}(\rho)$ could be obtained from Eq. ([10](#page-2-3)). In practice, however, only very small values of *n* can be handled this way. When $n=1$, the generating function is given by (Appendix A)

$$
G = \frac{F}{H} = \frac{1}{1 - y - xy^2}.
$$

Here $F=1$ and $H=1-y-xy^2$. The derivatives of *H* are H_x $=-y^2$ and $H_y=-1-2x$. Let us first check whether the conditions of Eq. (5) (5) (5) hold. The numerator *F* equals 1, which never vanishes. To check the smoothness of *H*, we check that *H*, H_x , and H_y never simultaneously vanish. We can use the Gröbner basis techniques to verify this. For example, the following MAPLE 8 command can be used (the syntax of the command differs sightly among different MAPLE versions):

$$
g basis([H, H_x, H_y], \quad tdeg(y, x)).
$$

The command returns $[1]$ $[1]$ $[1]$, indicating that the intersection of the three equations $(H, H_x, \text{ and } H_y)$ is empty. To compute x_0 and y_0 , Eqs. (8) (8) (8) for this case become

$$
1 - y - xy^2 = 0,
$$

FIG. 1. (Color online) The positive solutions to Eq. (8) (8) (8) for $n=1, \ldots, 6$ of cylinder lattices (from top to bottom). The five connected lines are the solutions at $\rho = 0.3$, 0.4, 0.5, 0.6, and 0.7 (from left to right).

$$
-xy^2 = -\frac{\rho y}{2}(1 - 2xy).
$$
 (11)

These equations are easy enough to solve by hand. Alternatively, the Gröbner basis computation can be used. For example, the above equation can be solved by using the MAPLE 8 command

$$
g basis([H, x * H_x - \rho * y/2 * H_y], \quad \text{plex}(y, x)).
$$

The command computes the reduced, minimal Gröbner basis in pure lexicographic term ordering and in this case gives two first-order elimination polynomials for *x* and *y*: $[-(2-\rho)y+2(1-\rho), 4(1-\rho)^2x-2\rho(1-\rho)],$ which lead to the unique solution

$$
x_0 = \frac{\rho(2-\rho)}{4(1-\rho)^2}
$$
, $y_0 = \frac{2(1-\rho)}{2-p}$.

Substituting the solution into Eq. (10) (10) (10) yields

$$
f_{\infty,1}(\rho) = \left(1 - \frac{\rho}{2}\right) \ln\left(1 - \frac{\rho}{2}\right) - \frac{\rho}{2} \ln \frac{\rho}{2} - (1 - \rho) \ln(1 - \rho).
$$

This expression is exact for $0 \le \rho \le 1$ [Eq. (B4) of Ref. [[8](#page-12-6)]]. To check that *Q* does not vanish for $0 < \rho < 1$, we use the Gröbner basis computation again to verify that *Q* and the two equations in Eqs. (11) (11) (11) never simultaneously vanish. This is confirmed by the MAPLE 8 command

$$
g basis([\mathcal{Q}, H, x \ast H_x - \rho \ast y/2 \ast H_y], \quad tdeg(y, x));
$$

which returns $[1]$ $[1]$ $[1]$. In fact, the MAPLE 8 command

normalf(
$$
Q
$$
,[H , $x * H_x - \rho * y/2 * H_y$], $\text{plex}(y, x)$);

gives a reduced form of the polynomial *Q* modulo the ideal of $[H, xH_x - \rho yH_y/2]$ as $Q = y(1-y)$, from which the closed form of Q as a function of ρ can be obtained as

FIG. 2. (Color online) The values of $F(x_0, y_0)$ (the numerator of the generating function) as a function of dimer density ρ ($0 < \rho < 1$) for *n* $= 1, \ldots, 6$ of cylinder lattices. On the left top corner of the plot around $(0,1)$, the curves for *n* $= 1, \ldots, 6$ are from top to bottom.

FIG. 3. (Color online) The values of $Q(x_0, y_0)$ as a function of dimer density ρ ($0 < \rho < 1$) for $n = 1, \ldots, 6$ of cylinder lattices. On the left bottom corner of the plot around $(0,0)$, the curves for *n* $= 1, \ldots, 6$ are from bottom to top.

$$
Q(\rho) = \frac{2\rho(1-\rho)}{(2-\rho)^2}.
$$

 $32(1 - \rho)^3 x^4 + 144(1 - \rho)^3 x^3 + 4(1 - \rho)(10\rho^2 - 20\rho + 3)x^2$ $+ 4(2 - \rho)$ $(3\rho^2 - 3\rho + 1)$ $x - \rho(1 - \rho)$ $(2 - \rho)$ $= 0.$ (12)

From this closed form of *Q* it is evident that *Q* does not vanish for $0 < \rho < 1$.

When $n=2$, for both the cylinder lattice and the lattice with free boundaries, $H(x, y)$ is a cubic polynomial in both x and *y* (Appendix A). To solve Eqs. ([8](#page-2-2)) using the Gröbner basis, the MAPLE 8 command

 $g_{\text{basis}}([H, x * \text{diff}(H, x) - \rho * y * \text{diff}(H, y)], \text{plex}(y, x));$

yields two polynomials which are the reduced, minimal Gröbner basis in lexicographic term ordering. The first of the two polynomials is the elimination polynomial for *x*. For the

cylinder lattice, x_0 satisfies the quartic equation

+
$$
4(2-\rho)(3\rho^2 - 3\rho + 1)x - \rho(1-\rho)(2-\rho) = 0.
$$
 (12)

After x_0 is solved, y_0 can be solved as a rational function in ρ and x_0 by setting the second basis polynomial returned by gbasis command to zero as

$$
y_0 = \frac{w(x_0, \rho)}{v(\rho)},
$$
\n(13)

where

$$
w(x_0, \rho) = -32(1 - \rho)^3 (45\rho^2 - 83\rho + 21)x_0^3
$$

- 16(1 - \rho)^3 (413\rho^2 - 776\rho + 210)x_0^2
- 4(1 - \rho)(572\rho^4 - 2446\rho^3 + 3437\rho^2 - 1873\rho
+ 429)x_0 + 300\rho^5 - 1552\rho^4 + 2812\rho^3 - 2182\rho^2

FIG. 4. (Color online) Free energy $f_{\infty,n}(\rho)$ of cylinder lattices calculated using Eq. (10) (10) (10) for *n* $= 1, \ldots, 6$ for $0 \leq \rho \leq 1$. From bottom to top, *n* $= 1, 3, 5, 6, 4,$ and 2. The values at $\rho = 1$ are cal-culated using the exact solution, Eq. ([17](#page-6-0)). For each *n*, $f_{\infty,n}(0) = 0$.

 $+ 744p - 54$

and

$$
v(\rho) = (1 - \rho)(2 - \rho)(43\rho^{3} - 123\rho^{2} + 90\rho - 27).
$$

The same procedures outlined above for $n=1$ can also be used to verify that *H* is smooth and *F* and *Q* do not vanish for $0 < \rho < 1$.

The solution for $n=2$ can be simplified if we substitute $x = z/y$. After the substitution, the denominator of the generating function becomes

$$
H = 1 - y - (3 + y)z + z2 + z3.
$$
 (14)

The Gröbner basis in lexicographic term ordering of the two polynomials in Eq. (8) (8) (8) after the substitution now consists of two polynomials in *z* and *y*. The elimination polynomial for \bar{z} is still a quartic polynomial, but simpler than that for \bar{x} [Eq. (12) (12) (12) :

$$
(2 - \rho)z^4 + 2(2 - \rho)z^3 + 2(1 - 2\rho)z^2 - 2(2 - \rho)z + \rho = 0.
$$
\n(15)

The solution of *y* in terms of z_0 is now given by

$$
y_0 = \frac{-(2-\rho)z_0^3 - z_0^2 + 3\rho z_0 + 1 - 2\rho}{1-\rho}.
$$
 (16)

Although when $n=2$ closed-form expressions could be written down for x_0 (z_0) and y_0 [and hence $f_{\infty,2}(\rho)$] as functions of ρ , the long expressions are not very informative. We can, however, obtain highly accurate numerical results from Eqs. (15) (15) (15) and (16) (16) (16) [or Eqs. (12) (12) (12) and (13) (13) (13)] for the $n=2$ cylinder lattice for different values of ρ . For example, when $\rho = 1/2$, we can solve x_0 and y_0 numerically from Eqs. ([12](#page-4-0)) and ([13](#page-4-1)) as $x_0 = 0.389\,620\,618\,156\,217\,959$ and $y_0 = 0.442\,004\,100\,446\,556\,690$, which leads to $f_{\infty,2}(\frac{1}{2})$ = 0.643 863 506 776 659 088.

For the $n=3$ cylinder lattice, in order to solve x_0 (or y_0), we have to solve a polynomial equation with a degree of 10 after using the Gröbner basis technique to get the elimination polynomial. When ρ is not so close to 1, reliable numerical solutions can be obtained. For example, when $\rho = 1/2$, x_0 and *y*⁰ can be solved as 0.441 361 340 073 863 149 and 0.277 272 018 269 763 844, respectively, leading to $f_{\infty,3}(\frac{1}{2})$ = 0.632 058 256 526 951 594. These "exact" numerical values can be used to check the results obtained previously by the computational methods (Table [I,](#page-2-0) Ref. [[8](#page-12-6)]). This procedure confirms the conclusion that the computational methods used previously give results of $f_{\infty,n}(\rho)$ with up to 12 and 13 correct digits.

Although we do not have a rigorous proof that the conditions for the PW method $[Eq. (5)]$ $[Eq. (5)]$ $[Eq. (5)]$ hold for a general value of *n*, numerical evidence strongly supports that the conditions are satisfied for all values of *n*. We verified these conditions for $n = 1, \ldots, 6$, and some of the numerical results are shown in Figs. $1-3$. In Fig. [1,](#page-3-0) the positive "minimal" (see discussion below) solutions (x_0, y_0) to Eq. ([8](#page-2-2)) are shown for different values of ρ . In Figs. [2](#page-3-1) and [3,](#page-4-2) F and Q are shown as a function of ρ , respectively. The values were calculated using MAPLE 8. High-precision calculations (with the number of

digits as 100) were used in order to obtain stable numerical results. For $n = 1, ..., 4$, the values of (x_0, y_0) were calculated from the Gröbner basis and the values of *G* and *Q* were calculated using normalized polynomials. For $n=5$ and n = 6, the Gröbner basis computation took too long to finish. Instead of using a Gröbner basis computation, Eq. ([8](#page-2-2)) was solved directly with a numerical method (fsolve in MAPLE 8) and the results were checked against those obtained from the Gröbner basis elimination polynomials at a few values of ρ . Consistent results were verified for the two methods.

As mentioned above, the existence of positive solutions of (x_0, y_0) is guaranteed by the non-negative values of $a_{m,n}(s)$. These solutions, however, are not necessarily unique. There are multiple branches of $H=0$ in the first quadrant. Although in general there are multiple positive solutions to Eq. (8) (8) (8) , the PW theory states that, when the coefficient $a_{m,n}(s) \ge 0$, only the solutions of (x_0, y_0) that lie on the southwest facing part of the graph (that is, the *minimal* point in the first quadrant) contribute to the asymptotics $(12]$ $(12]$ $(12]$, corollary 3.16). The solutions (x_0, y_0) shown in Fig. [1](#page-3-0) are these "minimal" points. From Fig. [1](#page-3-0) it is evident that at the low-dimer-density limit when $\rho \rightarrow 0$, $x_0 \rightarrow 0$ and $y_0 \rightarrow 1$. At the high-dimer-density limit when $\rho \rightarrow 1$, $x_0 \rightarrow \infty$ and $y_0 \rightarrow 0$.

From Figs. [2](#page-3-1) and [3](#page-4-2) we see that *F* does not vanish in the region of $0 \le \rho \le 1$. For *Q*, the only zeros are at $\rho = 0$ and $\rho=1$.

The dependence on the parity of *n* for (x_0, y_0) , $F(\rho)$, and $Q(\rho)$ is also evident in these figures. In Fig. [1](#page-3-0) the connected lines at fixed ρ show a zigzag pattern. In Fig. [2,](#page-3-1) *F* is a convex function in $0 \leq \rho \leq 1$ for odd *n* (when *n* > 1) and a monotonically decreasing function in $0 \leq \rho \leq 1$ for even *n*. In Fig. [3,](#page-4-2) the curves of *Q* have quite different behaviors for odd and even values of *n* as $\rho \rightarrow 1$.

Figure [4](#page-4-3) shows the free energy $f_{\infty,n}(\rho)$ of cylinder lattices for $n=1,\ldots,6$. The free energy $f_{\infty,n}(\rho)$ is calculated using Eq. ([10](#page-2-3)). From the figure we see that $f_{\infty,n}(\rho)$ converges quickly to $f_{\infty,\infty}(\rho)$ when ρ is not very close to $\rho = 1$. The details of these plots near the maximum of $f_{\infty,n}(\rho)$, calculated with the computational method for *n* up to 17, are shown in Figs. $1-4$ in Ref. [[8](#page-12-6)].

For longer *n*, it becomes increasingly difficult to solve the system of polynomial equations ([8](#page-2-2)). Even numerical solutions become highly unstable, especially at high dimer density. In the following we investigate the series expansions of the free energy for lattice strips $\infty \times n$ for small values of *n*. Since the behaviors of the solution x_0 and y_0 , and hence the asymptotics of the free energy $f_{\infty,n}(\rho)$, are quite different at the high- and low-dimer-density limits, we discuss the two cases separately.

III. ASYMPTOTICS AT THE HIGH-DIMER-DENSITY LIMIT

For clarity we define $u=1-\rho$. At the high-dimer-density limit when $u \rightarrow 0$, numerical calculations show that for both odd and even *n*, $x_0 \rightarrow \infty$ and $y_0 \rightarrow 0$ (Fig. [1](#page-3-0)). If we expand $1/x_0$ and y_0 as series of *u*, from Eq. ([8](#page-2-2)) it is found that $1/x_0$ and y_0 have different leading terms in the series expansion

for odd and even *n*. For odd *n*, the leading term of $1/x_0$ is u^2 and the leading term of y_0 is u^n . For even *n*, the leading terms of $1/x_0$ and y_0 are *u* and $u^{n/2}$, respectively:

$$
\frac{1}{x_0} = \sum_{i=2}^{\infty} a_i u^i, \quad y_0 = \sum_{i=n}^{\infty} b_i u^i \quad \text{when } n \text{ is odd,}
$$
\n
$$
\frac{1}{x_0} = \sum_{i=1}^{\infty} a_i u^i, \quad y_0 = \sum_{i=n/2}^{\infty} b_i u^i \quad \text{when } n \text{ is even.}
$$

These differences in the leading terms of the series expansions of $1/x_0$ and y_0 lead directly to the different coefficients of *u* ln *u* in $f_{\infty,n}(1-u)$ for odd and even *n*. By using Eq. ([10](#page-2-3)) we obtain for odd *n*, as $u \rightarrow 0$,

$$
f_{\infty,n}(1-u) \sim \frac{1-u}{2} \ln(a_2 u^2 + a_3 u^3 + \cdots)
$$

$$
-\frac{1}{n} \ln(b_n u^n + b_{n+1} u^{n+1} + \cdots)
$$

$$
= \left[\frac{\ln a_2}{2} - \frac{\ln b_n}{n}\right] - u \ln u
$$

$$
+ \left[\frac{a_3}{2a_2} - \frac{b_{n+1}}{nb_n} - \frac{\ln a_2}{2}\right] u + \cdots
$$

and for even *n*, as $u \rightarrow 0$,

$$
f_{\infty,n}(1-u) \sim \frac{1-u}{2} \ln(a_1 u + a_2 u^2 + \cdots)
$$

$$
-\frac{1}{n} \ln(b_{n/2} u^{n/2} + b_{n/2+1} u^{n/2+1} + \cdots)
$$

$$
= \left[\frac{\ln a_1}{2} - \frac{\ln b_{n/2}}{n}\right] - \frac{1}{2} u \ln u
$$

$$
+ \left[\frac{a_2}{2a_1} - \frac{b_{n/2+1}}{nb_{n/2}} - \frac{\ln a_1}{2}\right] u + \cdots
$$

The difference in the coefficients of *u* ln *u* in $f_{\infty,n}(1-u)$ comes directly from the different leading terms of $1/x_0$ for odd and even *n*.

For $n=4$,

$$
f_{\infty,4}(1-u) \sim -\frac{1}{4}\ln(2-\sqrt{3}) - \frac{1}{2}u\ln u + \frac{1}{2}\left[1-\ln\left(\frac{102}{23}-\frac{54}{23}\sqrt{3}\right)\right]u - \left[\frac{1008}{529}+\frac{149}{1058}\sqrt{3}\right]u^2 - \left[\frac{6535949}{839523}-\frac{2581941}{559682}\sqrt{3}\right]u^3.
$$

For *n*=5,

$$
f_{\infty,5}(1-u) \sim \frac{1}{5} \ln \frac{\sqrt{5} + \sqrt{41} + \sqrt{15 - 2\sqrt{5}} + \sqrt{5 + 2\sqrt{5}}}{4} - u \ln u + \left[1 + \frac{1}{2} \ln \frac{849 + 44\sqrt{205} + 12\sqrt{6215 + 422\sqrt{205}}}{20500}\right]u.
$$

B. Lattices with free boundaries

The asymptotic expansions of $f_{\infty,n}(\rho)$ in lattices with free boundaries at high dimer density are listed below for *n* $= 1, \ldots, 4$ $= 1, \ldots, 4$ $= 1, \ldots, 4$. For lattices with free boundaries, the constant term of $f_{\infty,n}(\rho)$ is given by the exact expression [1]

Some explicit expressions of $f_{\infty,n}(\rho)$ for cylinder lattices and lattices with free boundaries are listed in the following.

A. Cylinder lattices

The asymptotic expansions of $f_{\infty,n}(\rho)$ in cylinder lattices at high dimer density are listed below for $n=1, \ldots, 5$. For cylinder lattices, the constant term of $f_{\infty,n}(\rho)$ is given by the exact expression $\lceil 1 \rceil$ $\lceil 1 \rceil$ $\lceil 1 \rceil$

$$
f_{\infty,n}(1) = \frac{1}{n} \ln \prod_{i=1}^{n/2} \left[\sin \frac{(2i-1)\pi}{n} + \left(1 + \sin^2 \frac{(2i-1)\pi}{n} \right)^{1/2} \right],\tag{17}
$$

which can be used to check the constant terms in the following results.

As $u \rightarrow 0$, for $n=1$,

$$
f_{\infty,1}(1-u) \sim -u \ln u - (\ln 2 - 1)u - \sum_{i=1}^{\infty} \frac{u^{2i+1}}{2i(2i+1)}.
$$

For *n*=2,

$$
f_{\infty,2}(1-u) \sim \frac{1}{2}\ln(1+\sqrt{2}) - \frac{1}{2}u\ln u + \frac{1}{2}[1-\ln(4-2\sqrt{2})]u
$$

$$
-\left[\frac{1}{2} + \frac{1}{8}\sqrt{2}\right]u^2 - \left[\frac{1}{3} - \frac{1}{8}\sqrt{2}\right]u^3
$$

$$
-\left[\frac{1}{3} - \frac{67}{192}\sqrt{2}\right]u^4 - \left[\frac{9}{10} - \frac{45}{64}\sqrt{2}\right]u^5.
$$

For *n*=3,

$$
f_{\infty,3}(1-u) \sim \frac{1}{6} \ln \left(\frac{5}{2} + \frac{1}{2} \sqrt{21} \right) - u \ln u
$$

+
$$
\left[1 - \frac{1}{2} \ln \left(\frac{6300}{289} - \frac{1008}{289} \sqrt{21} \right) \right] u
$$

-
$$
\left[\frac{96}{289} - \frac{200}{2023} \sqrt{21} \right] u^2
$$

-
$$
\left[\frac{1975875}{167042} - \frac{1368324}{584647} \sqrt{21} \right] u^3.
$$

$$
f_{\infty,n}^{\text{fb}}(1) = \frac{1}{n} \ln \left\{ \prod_{i=1}^{n/2} \left[\cos \frac{i\pi}{n+1} + \left(1 + \cos^2 \frac{i\pi}{n+1} \right)^{1/2} \right] \right\},\right\}
$$

which can be used to check the constant terms of the following results.

For $n = 2$,

$$
f_{\infty,2}^{\text{fb}}(1-u) \sim \frac{1}{2} \ln\left(\frac{1}{2} + \frac{1}{2}\sqrt{5}\right) - \frac{1}{2}u \ln u + \frac{1}{2}\left[1 - \ln(5 - 2\sqrt{5})\right]u - \left[1 + \frac{1}{20}\sqrt{5}\right]u^2 + \left[\frac{2}{5}\sqrt{5} - \frac{13}{12}\right]u^3 + \left[-\frac{8}{3} + \frac{1073}{600}\sqrt{5}\right]u^4 + \left[\frac{162}{25}\sqrt{5} - \frac{561}{40}\right]u^5.
$$

For $n=3$,

$$
f_{\infty,3}^{fb}(1-u) \sim \frac{1}{6} \ln(2+\sqrt{3}) - u \ln u + \left[1 + \ln\left(\frac{1}{36}\sqrt{6} + \frac{1}{6}\sqrt{2}\right)\right]u + \left[\frac{103}{121}\sqrt{3} + \frac{240}{121}\right]u^2 - \left[\frac{112740}{14641}\sqrt{3} + \frac{806673}{29282}\right]u^3 + \left[\frac{369777941}{1771561}\sqrt{3} + \frac{492403464}{1771561}\right]u^4.
$$

For $n=4$,

$$
f_{\infty,4}^{fb}(1-u) \sim \frac{1}{4} \ln \frac{\sqrt{5} + 1 + \sqrt{22 + 2\sqrt{5}}}{4} + \frac{1}{4} \ln \frac{\sqrt{5} - 1 + \sqrt{22 - 2\sqrt{5}}}{4} - \frac{1}{2}u \ln u + \left[\frac{1}{2} + \frac{1}{2} \ln \frac{341801}{2} - \frac{1}{2} \ln(545403 + 81734\sqrt{29}) \right] - 4\sqrt{27680943526 + 5123717738\sqrt{29}} \bigg] u.
$$

IV. ASYMPTOTICS AT THE LOW-DIMER-DENSITY LIMIT

Unlike the high-dimer-density case, at low dimer density when $\rho \rightarrow 0$, numerical calculations show that x_0 approaches zero and y_0 approaches 1 for both odd and even values of *n*. Case-by-case calculations show that the leading term of x_0 is $a_1 \rho$ and the leading term of y_0 is $1+b_1 \rho$. The series expansions of x_0 and y_0 thus have the forms

$$
x_0 = \sum_{i=1}^{\infty} a_i \rho^i
$$
, $y_0 = 1 + \sum_{i=1}^{\infty} b_i \rho^i$.

From Eq. ([10](#page-2-3)), as $\rho \rightarrow 0$, the general form of the free energy at the low dimer density is

$$
f_{\infty,n}(\rho) \sim -\frac{\rho \ln \rho}{2} - \left[\frac{\ln a_1}{2} + \frac{b_1}{2} \right] \rho - \left[\frac{a_2}{2a_1} + \frac{b_2}{n} - \frac{b_1^2}{2n} \right] \rho^2 + \cdots
$$

For both odd and even values of *n*, at low dimer density the coefficient of the logarithmic term ρ ln ρ is −1/2, consistent with previous results obtained by computational methods $[10]$ $[10]$ $[10]$. This coefficient comes directly from the fact that the leading term in the series expansion of x_0 is $a_1\rho$.

The asymptotic expansions of free energy in cylinder lattices at low dimer density show an interesting property: for lattice strips $\infty \times n$ with a width of *n*, the first *n* terms in the series expansion of $f_{\infty,n}(\rho)$ are exactly the same as the first *n*

terms in the series expansion of $f_{\infty,\infty}(\rho)$, the free energy of the infinite lattice. In order to compare the free energy in semi-infinite $\infty \times n$ lattice strips with that of an infinite ∞ $\times \infty$ lattice, in the following section the series of Gaunt [[15](#page-12-13)] is used to derive the series of $f_{\infty,\infty}(\rho)$. The series expansion of free energy for lattices with free boundaries at the lowdimer-density limit is listed in Appendix B.

A. Free energy for an infinite lattice

Gaunt gave a series expansion of the dimer activity *x* as a function of the number density t (Ref. [[15](#page-12-13)], column 2 of Table 2):

$$
x(t) = t + 7t2 + 40t3 + 206t4 + 1000t5 + 4678t6 + 21336t7
$$

+ 95514t⁸ + 421472t⁹ + 1838680t¹⁰ + 7947692t¹¹
+ 34097202t¹² + 145387044t¹³ + 616771148t¹⁴
+ 2605407492t¹⁵ + ... (18)

Here $t = \theta/4$, where θ is the average number of sites covered by dimers when grand canonical ensembles are considered $\lceil 8 \rceil$ $\lceil 8 \rceil$ $\lceil 8 \rceil$.

The functions $f_{m,n}(\rho)$, $f_{\infty,n}(\rho)$, and $f_{\infty,\infty}(\rho)$ considered so far are at a given dimer density ρ , so they are in essence properties of canonical ensembles, where the number of molecules of interest (in our case the dimers) is fixed. The dimer activity x and the average dimer coverage $\theta = 4t$ in Eq. ([18](#page-7-0)), however, are the properties of grand canonical ensembles,

where the activity of the molecules is fixed and the number of molecules can fluctuate. The relation between the canonical ensemble and the grand canonical ensemble in a general setting is discussed in many standard statistical mechanics textbooks, and for the monomer-dimer model in particular, a short discussion can be found in Appendix A of Ref. $[8]$ $[8]$ $[8]$. For a given dimer activity *x*, the average dimer coverage $\theta(x)$ equals the value of ρ where the function

$$
g(\rho) = f_{\infty,\infty}(\rho) + \frac{\rho}{2} \ln x
$$

reaches its maximum. It is well known that $f_{\infty,\infty}(\rho)$ (as well as free-energy functions for other dimensions) is a continuous concave function of ρ [[16](#page-12-14)]. Taking the derivative of $g(\rho)$ with respect to ρ and substituting θ for ρ , we obtain the relation of θ and *x*:

$$
\frac{\partial f_{\infty,\infty}(\theta)}{\partial \theta} + \frac{1}{2} \ln x = 0.
$$

Since we know x as a function of θ from Eq. ([18](#page-7-0)), the above equation can be integrated to obtain $f_{\infty,\infty}(\rho)$ (after changing θ back to dimer density ρ :

$$
f_{\infty,\infty}(\rho) = -\frac{1}{2} \int \ln \left[x \left(\frac{\rho}{4} \right) \right] d\rho + C,
$$

where the constant *C* can be evaluated with $f_{\infty,\infty}(0) = 0$. From this relation and the series in Eq. (18) (18) (18) we can obtain the series expression for the free energy of the infinite lattice:

$$
f_{\infty,\infty}(\rho) = -\frac{1}{2}\rho \ln(\rho) + \left[\frac{1}{2} + \ln(2)\right]\rho - \frac{7}{16}\rho^2 - \frac{31}{192}\rho^3
$$

$$
-\frac{121}{1536}\rho^4 - \frac{471}{10240}\rho^5 - \frac{1867}{61440}\rho^6 - \frac{7435}{344064}\rho^7
$$

$$
-\frac{4211}{262144}\rho^8 - \frac{116383}{9437184}\rho^9 - \frac{459517}{47185920}\rho^{10}
$$

$$
-\frac{1821051}{230686720}\rho^{11} - \frac{7255915}{1107296256}\rho^{12}
$$

$$
-\frac{9687973}{1744830464}\rho^{13} - \frac{16697149}{3489660928}\rho^{14}
$$

$$
-\frac{157001097}{37580963840}\rho^{15} + \cdots
$$
 (19)

B. Cylinder lattices

The coefficients of ρ^i in the series expansion of $f_{\infty,n}(\rho)$ of cylinder lattices at low dimer density are listed in Table [I](#page-2-0) for $n=1, \ldots, 7$. The term $-\frac{1}{2}\rho \ln(\rho)$, which is common to lattices of all sizes, is not included in the table. Also listed in the last row of the table are the coefficients for the infinite lattice [Eq. (19) (19) (19)]. It is evident from the table that for lattice strips $\infty \times n$ with a width of *n*, the first *n* terms of $f_{\infty,n}(\rho)$ [including the term of $-\frac{1}{2}\rho \ln(\rho)$ is exactly the same as those of $f_{\infty,\infty}(\rho)$ of the infinite lattice. For example, the lattice strip $\infty \times 7$ has

the first seven terms identical to those of the infinite lattice, up to the term of ρ^6 . This nice property gives a quantitative estimate of the error when we use the values of finite lattices to approximate the properties of the infinite lattice. It also explains why the sequence of the free energy in cylinder lattices converges so fast, especially when ρ is small [[8](#page-12-6)].

The term of ρ^n in $f_{\infty,n}(\rho)$ is the first term that differs from the series expansion of $f_{\infty,\infty}(\rho)$. The difference between the coefficients of ρ^n in $f_{\infty,n}(\rho)$ and $f_{\infty,\infty}(\rho)$ shows a regular pattern: starting from *n*=2, the differences are $\frac{1}{32}$, $-\frac{1}{192}$, $\frac{1}{1024}$, $-\frac{1}{5120}$, $\frac{1}{24576}$, $-\frac{1}{114688}$,.... For example, for *n*=2, $-\frac{13}{32} - (-\frac{7}{16}) = \frac{1}{32}$. The closed form of this alternating sequence clearly is $\frac{(-1)^n}{n4^n}$.

The difference between the coefficients of ρ^{n+1} , the second term that differs between finite and infinite lattices, also shows a regular pattern. Starting from $n=3$, the sequence is $-\frac{1}{256}, \frac{1}{1024}, -\frac{1}{4096}, \frac{1}{16384}, -\frac{1}{65536}, \dots$ It is obvious that the sequence takes the closed form expression $\frac{(-1)^n}{4 \times 4^n}$.

There is also a pattern for the third term (ρ^{n+2}) that differs between $f_{\infty,n}(\rho)$ and $f_{\infty,\infty}(\rho)$. Starting from $n=4$, the differences are $-\frac{3569}{122880} - \left(-\frac{1867}{61440}\right) = \frac{11}{2^{13}}, \quad -\frac{3791}{172032} - \left(-\frac{7435}{344064}\right) = -\frac{14}{2^{15}},$ $-\frac{4177}{262144} - \left(-\frac{4211}{262144}\right) = \frac{17}{2^{17}}, \dots$ The limited number of data points in Table [I](#page-2-0) suggests that it might take a closed form of $(-1)^n$ 4*n* $\frac{3n-1}{2^5}$. Due to the limited number of data points, currently it is not clear whether the differences of higher-degree terms can also be written in simple closed forms.

From the closed-form expressions of these three dominant terms that differ between finite and infinite lattices at low dimer density, we see that

$$
f_{\infty,\infty}(\rho) \sim f_{\infty,n}(\rho) - \frac{(-1)^n}{4^n} \left(\frac{\rho^n}{n} + \frac{\rho^{n+1}}{2^2} + \frac{(3n-1)\rho^{n+2}}{2^5} \right) + O(\rho^{n+3}),
$$
\n(20)

with the understanding that the first correction term ρ^n is for $n \ge 2$, the second correction term ρ^{n+1} is for $n \ge 3$, and the third correction term ρ^{n+2} is for $n \ge 4$.

The coefficients of ρ^i in the series expansion of x_0 and −(ln *y*₀)/*n* are also listed in Tables [II](#page-10-0) and [III.](#page-11-0) From the tables we can see that for cylinder lattice strips $\infty \times n$, x_0 and $(\ln y_0)/n$ share the same first *n*−1 terms with their corresponding series expansions of the infinite lattice.

APPENDIX A: BIVARIATE GENERATING FUNCTIONS OF MONOMER-DIMER MODELS IN TWO-DIMENSIONAL PLANAR LATTICES

1. Calculation of the generating functions

The bivariate generating functions of monomer-dimer models can be derived directly from the matrices M_n which are used in the computational studies $[8-10,14]$ $[8-10,14]$ $[8-10,14]$ $[8-10,14]$ $[8-10,14]$. The general method is described in Eqs. (10) – (15) of Ref. $[14]$ $[14]$ $[14]$, and the detailed method for monomer-dimer model is described on pp. 2–3 of Ref. $[9]$ $[9]$ $[9]$, where an explicit example of the matrix

 M_3 for lattices with free boundaries is included.¹ For *d*-dimensional lattices, the general method applies to the family of lattices which are generated by expanding the lattice in one dimension while keeping the remaining *d*− 1 dimensions fixed. For example, a two-dimensional rectangular $m \times n$ lattice can be considered to be built up by starting with a one-dimensional lattice with *n* sites and expanding row by row in the *m* direction. Similarly, a two-dimensional cylinder lattice with $m \times n$ sites is made up of *m* rows of onedimensional circular lattices, each with *n* sites. As shown before $[9,14]$ $[9,14]$ $[9,14]$ $[9,14]$, for the monomer-dimer problem the partition function of a lattice with width of *n* is determined by the configurations of dimers on two adjacent rows of the lattice $(in the *m* direction).$ The relation is captured in the following recurrence equation involving a square matrix $M_n(x)$:

$$
\Omega_m(x) = M_n(x)\Omega_{m-1}(x). \tag{A1}
$$

Here the vector Ω_m is made up of various partition functions for the $m \times n$ lattice, including $Z_{m,n}(x, y)$ of Eq. ([1](#page-0-1)), the partition function that we are interested in, as well as other *contracted* partition functions for the cases where some of the lattice sites in the last two rows of lattice strip are kept in certain fixed configurations $[9,14]$ $[9,14]$ $[9,14]$ $[9,14]$. The partition functions of the latter kind are ignored in this paper. The detailed algorithm for constructing the matrix $M_n(x)$ is given on p. 2 of $Ref. [9]$ $Ref. [9]$ $Ref. [9]$.

Let us denote the size of the matrix $M_n(x)$ as $w \times w$. The exact formulas of *w* are given in Refs. $\lceil 8,10 \rceil$ $\lceil 8,10 \rceil$ $\lceil 8,10 \rceil$ $\lceil 8,10 \rceil$ for cylinder lattices and lattices with free boundaries, respectively. If the characteristic function of $M_n(x)$ is

$$
|\lambda I - M_n(x)| = a_0(x)\lambda^w + a_1(x)\lambda^{w-1} + \dots + a_w(x),
$$
\n(A2)

then all the partition functions that make up the vector Ω_m obey the same recurrence $[14]$ $[14]$ $[14]$

$$
a_0 Z_{m,n} + a_1 Z_{m-1,n} + \cdots + a_w Z_{m-w,n} = 0, \quad m \ge w. \tag{A3}
$$

The close relation between a recurrence like Eq. $(A3)$ $(A3)$ $(A3)$ and its rational generating function $G(x, y) = \sum_{m \ge 0} Z_{m,n}(x) y^m$ is well known. If we multiply Eq. ([A3](#page-9-0)) by y^m for $m \geq w$ and multiply $\sum_{j=0}^{m} a_j Z_{m-j,n}(x)$ by y^m for $0 \le m \le w$, then we have [for clarity Z_m is used here for $Z_{m,n}(x)$

$$
a_0Z_0 = a_0Z_0
$$

\n
$$
a_0Z_1y + a_1Z_0y = (a_0Z_1 + a_1Z_0)y
$$

\n...
\n
$$
a_0Z_{w-1}y^{w-1} + a_1Z_{w-2}y^{w-1} + \cdots + a_{w-1}Z_0y^{w-1} = (a_0Z_{w-1} + \cdots + a_{w-1}Z_0)y^{w-1},
$$

\n
$$
a_0Z_{w}y^w + a_1Z_{w-1}y^w + \cdots + a_{w-1}Z_1y^w + a_wZ_0y^w = 0,
$$

\n
$$
a_0Z_{w+1}y^{w+1} + a_1Z_wy^{w+1} + \cdots + a_{w-1}Z_2y^{w+1} + a_wZ_1y^{w+1} = 0,
$$

\n...
\n
$$
= 0.
$$

The sum of each column on the left-hand side gives a term $a_i y^i G(x, y)$ for $0 \le i \le w$,

$$
(a_0 + a_1y + \dots + a_0y^w)G = a_0Z_0 + (a_0Z_1 + a_1Z_0)y + \dots + (a_0Z_{w-1} + \dots + a_{w-1}Z_0)y^{w-1},
$$

which leads to the rational generating function $G(x, y)$:

$$
G(x,y) = \frac{a_0 Z_0 + (a_0 Z_1 + a_1 Z_0)y + \dots + (a_0 Z_{w-1} + \dots + a_{w-1} Z_0)y^{w-1}}{a_0 + a_1 y + \dots + a_w y^w}.
$$
 (A4)

From Eqs. $(A1)$ $(A1)$ $(A1)$, $(A2)$ $(A2)$ $(A2)$, and $(A4)$ $(A4)$ $(A4)$ we can calculate the rational generating function $G(x, y) = F(x, y) / H(x, y)$ as follows: once the matrix M_n is constructed, the denominator $H(x, y)$ can be obtained directly from the characteristic function of M_n [Eq. $(A2)$ $(A2)$ $(A2)$]. From Eq. $(A1)$ $(A1)$ $(A1)$, Ω_m , and hence $Z_{m,n}$ as the first element of Ω_m , can be calculated recursively for $m=1,2,...$, with $\Omega_0 = [1, 0, \dots, 0]^t$ as the initial value. From Eq. ([A4](#page-9-3)), the numerator $F(x, y)$ can then be calculated using the first *w* values of $Z_{m,n}(x, y)$ $(m=0, 1, \ldots, w-1)$ and the coefficients $a_i(x)$ of the denominator $H(x, y)$:

$$
H_n(x,y) = \sum_{i=0}^{w} a_i(x) y^i, \quad F_n(x,y) = \sum_{i=0}^{w-1} \left[\sum_{j=0}^{i} a_j(x) Z_{i-j,n}(x) \right] y^i.
$$

For completeness we list $M_n(x)$ and $G(x, y)$ for small values of *n* in this Appendix. The cylinder lattices and lattices with free edges are listed separately. The variable *x* is associated with the number of dimers, *s*, and the variable *y* is associated with the length of the lattice, *m*, as defined in Eq. $(7).$ $(7).$ $(7).$

¹In that matrix the horizontal and vertical dimer activities are assumed to take different values of *x* and *y*. In this paper we assume they have the same value *x*.

TABLE II. The coefficients in the series expansion of x_0 for cylinder lattice strips $\infty \times n$ at low dimer density. Terms that are equal to those of the infinite lattice are underlined.

\boldsymbol{n}	ρ	ρ^2	n^3	ρ^4	$\boldsymbol{\rho}$	ρ^6		ρ^8
	1/2	3/4		5/4	3/2	7/4	\overline{c}	9/4
2	1/4	13/32	71/128	1393/2048	6353/8192	55073/65536	230343/262144	7519577/8388608
3	1/4	7/16	81/128	423/512	4179/4096	9993/8192	23341/16384	854147/524288
$\overline{4}$	1/4	7/16	5/8	411/512	497/512	289/256	20917/16384	370861/262144
5	1/4	7/16	5/8	103/128	2001/2048	9369/8192	42803/32768	192145/131072
6	1/4	7/16	5/8	103/128	125/128	9355/8192	21329/16384	190871/131072
7	1/4	7/16	5/8	103/128	125/128	2339/2048	42673/32768	191043/131072
∞	1/4	7/16	5/8	103/128	125/128	2339/2048		

When $n=1$, there is no distinction between the two boundary conditions:

$$
M_1 = \begin{bmatrix} 1 & x \\ 1 & 0 \end{bmatrix}, \quad G_1 = \frac{1}{1 - y - xy^2}.
$$

2. Cylinder lattices

For *n*=2,

$$
M_2^c = \begin{bmatrix} 1 + 2x & 2x & x^2 \\ 1 & x & 0 \\ 1 & 0 & 0 \end{bmatrix},
$$

$$
G_2^c = \frac{1 - xy}{1 - (1 + 3x)y + x(x - 1)y^2 + x^3y^3}.
$$

For $n=3$,

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

$$
G_3^c = \frac{1 - 2yx - y^2x^3}{x^6y^4 - x^3(x-1)y^3 - x(1+3x+5x^2)y^2 - (5x+1)y+1}.
$$

For *n*=4,

$$
M_4^c = \begin{bmatrix} 1 + 4x + 2x^2 & 4x + 8x^2 & 4x^2 + 4x^3 & 2x^2 & 4x^3 & x^4 \\ 1 + 2x & 3x + 2x^2 & 2x^2 & x^2 & x^3 & 0 \\ 1 + x & 2x & x^2 & 0 & 0 & 0 \\ 1 & 2x & 0 & x^2 & 0 & 0 \\ 1 & x & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}
$$

and $G_4^c = F_4/H_4$, where

$$
F_4 = -x^8y^4 + 3x^5y^3 + 4x^4y^2 - x(3+4x)y + 1
$$

and

$$
H_4 = x^{12}y^6 - x^8(-x + 2x^2 + 1)y^5 - x^5(6x^2 + 2x + 1 + 9x^3)y^4
$$

+ 2x³(13x² + 5x + 1 + 4x³)y³ + x(-6x - 1 + 7x³ - 6x²)y²
– (x + 1)(6x + 1)y + 1.
For $n=5$, $G_5^c = F_5/H_5$, where
 $F_5 = -x^{15}y^6 + 2x^{11}(-2 + x)y^5 + x^8(8x^2 + 2 + 11x)y^4$
+ 2x⁵(7x² + 3 + 8x)y³ - x³(2 - x + 8x²)y² - 2x(2 + 5x)y
+ 1

and

$$
H_5 = x^{20}y^8 + x^{15}(3x^2 - x + 1)y^7 - x^{11}(19x^4 + 11x^3 + 7x^2 + 2x
$$

+ 1)y⁶ - x⁸(2x⁴ + 65x³ + 39x² + 11x + 2)y⁵ + x⁵(41x⁵
+ 95x⁴ + 39x³ - 9x² - 6x - 1)y⁴ + x³(34x⁴ + 85x³ + 69x²
+ 19x + 2)y³ - x(19x⁴ + 19x³ + 27x² + 10x + 1)y²
– (15x² + 9x + 1)y + 1.

3. Lattices with free boundaries

For *n*=2,

$$
M_2^{\text{fb}} = \begin{bmatrix} 1 + x & 2x & x^2 \\ 1 & x & 0 \\ 1 & 0 & 0 \end{bmatrix},
$$

$$
G_2^{\text{fb}} = \frac{1 - xy}{x^3 y^3 - xy^2 - (2x + 1)y + 1}.
$$

For *n*=3,

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

and $G_3^{\text{fb}} = F_3^{\text{fb}} / H_3^{\text{fb}}$, where

TABLE III. The coefficients in the series expansion of $-\ln(y_0)/n$ for cylinder lattice strips $\infty \times n$ at low dimer density. Terms that are equal to those of the infinite lattice are underlined.

\boldsymbol{n}	ρ	ρ^2	ρ^3	ρ^4	ρ^5	ρ^6		
	1/2	3/8	7/24	15/64	31/160	21/128	127/896	255/2048
2	1/2	13/32	115/384	419/2048	5491/40960	17489/196608	116687/1835008	423771/8388608
3	1/2	7/16	1/3	127/512	1027/5120	8653/49152	17677/114688	16667/131072
$\overline{4}$	1/2	7/16	31/96	239/1024	461/2560	3569/24576	27325/229376	53053/524288
5	1/2	7/16	31/96	121/512	473/2560	941/6144	3791/28672	30625/262144
6	1/2	7/16	31/96	121/512	471/2560	1243/8192	3707/28672	29239/262144
7	1/2	7/16	31/96	121/512	471/2560	1867/12288	3719/28672	29505/262144
∞	1/2	7/16	31/96	121/512	471/2560	1867/12288		

$$
F_3^{\text{fb}} = x^6 y^4 + x^4 y^3 - 2x^2 (1+x) y^2 - xy + 1
$$

and

$$
H_3^{\text{fb}} = -x^9y^6 + x^6(x - 1)y^5 + x^4(5x^2 + 3x + 2)y^4
$$

+
$$
x^2(2x + 1)(x - 1)y^3 - x(1 + x)(5x + 2)y^2
$$

-
$$
(1 + 3x)y + 1.
$$

For $n=4$, $G_4^{\text{fb}} = F_4^{\text{fb}} / H_4^{\text{fb}}$, with

$$
F_4^{fb} = x^{14}y^7 - 2x^{11}y^6 - x^8(3x + 5x^2 + 3)y^5 + x^6(2x + 3)(1 + x)y^4 + x^4(2x + 3)(1 + 3x)y^3 - 3x^2(1 + 3x + x^2)y^2 - 2x(1 + x)y + 1
$$

and

$$
H_4^{fb} = -x^{18}y^9 + x^{14}(-x + x^2 + 1)y^8 + x^{11}(2 + 9x^3 + 3x + 9x^2)y^7
$$

\n
$$
-x^8(19x^3 - 1 + 6x^2 + 5x^4)y^6 - x^6(29x^2 + 3 + 14x + 24x^3 + 21x^4)y^5 + x^4(41x^2 + 40x^3 + 9x^4 + 18x + 3)y^4 + x^2(4x^2 - 1 - 4x + 15x^4 + 27x^3)y^3 - x(5x^3 + 2 + 21x^2 + 13x)y^2
$$

\n
$$
+ (-1 - 3x^2 - 5x)y + 1.
$$

APPENDIX B: LATTICES WITH FREE BOUNDARIES AT THE LOW-DIMER-DENSITY LIMIT

The series expansions of x_0 , y_0 , $\ln(y_0)/n$, and $f_{\infty,n}(\rho)$ for lattices with free boundaries at low dimer density are listed below for $n=2$, 3, and 4. From these expressions we can see that, unlike cylinder lattices, none of the coefficients equals the coefficients of the infinite lattice. The only exception is the coefficient of ρ in $(\ln y_0)/n$, which is always equal to −1/2 for each value of *n*. The cylinder lattices have the same coefficient.

For *n*=2,

$$
x_0 = \frac{1}{3}\rho + \frac{5}{9}\rho^2 + \frac{7}{9}\rho^3 + \frac{239}{243}\rho^4 + \frac{851}{729}\rho^5 + \frac{2909}{2187}\rho^6 + \cdots,
$$

$$
y_0 = 1 - \rho - \frac{1}{3}\rho^2 + \frac{1}{27}\rho^3 + \frac{4}{27}\rho^4 + \frac{28}{243}\rho^5 + \frac{35}{729}\rho^6 + \cdots,
$$

$$
\frac{1}{2}\ln y_0 = -\frac{1}{2}\rho - \frac{5}{12}\rho^2 - \frac{17}{54}\rho^3 - \frac{49}{216}\rho^4 - \frac{403}{2430}\rho^5 - \frac{125}{972}\rho^6 + \cdots,
$$

$$
f_{\infty,2} = \frac{1}{2} (\ln 3 + 1) - \frac{1}{2} \rho \ln \rho - \frac{5}{12} \rho^2 - \frac{17}{108} \rho^3 - \frac{49}{648} \rho^4 - \frac{403}{9720} \rho^5 - \frac{25}{972} \rho^6 + \cdots
$$

For *n*=3,

$$
x_0 = \frac{3}{10}\rho + \frac{261}{500}\rho^2 + \frac{9207}{12500}\rho^3 + \frac{116397}{125000}\rho^4 + \frac{34826031}{31250000}\rho^5 + \frac{2021574591}{1562500000}\rho^6 + \cdots,
$$

$$
y_0 = 1 - \frac{3}{2}\rho - \frac{9}{50}\rho^2 + \frac{567}{1250}\rho^3 + \frac{17253}{50000}\rho^4 + \frac{311769}{12500000}\rho^5 - \frac{28341333}{312500000}\rho^6 + \cdots,
$$

$$
\frac{1}{3} \ln y_0 = -\frac{1}{2} \rho - \frac{87}{200} \rho^2 - \frac{1569}{5000} \rho^3 - \frac{44091}{200000} \rho^4 - \frac{2208627}{12500000} \rho^5 - \frac{192832569}{1250000000} \rho^6 + \cdots,
$$

$$
f_{\infty,3} = \frac{1}{2} \left(\ln \frac{10}{3} + 1 \right) - \frac{1}{2} \rho \ln \rho - \frac{87}{200} \rho^2 - \frac{1569}{10000} \rho^3 - \frac{14697}{200000} \rho^4 - \frac{2208627}{50000000} \rho^5 - \frac{192832569}{6250000000} \rho^6 + \cdots
$$

For
$$
n=4
$$
,
\n
$$
x_0 = \frac{2}{7}\rho + \frac{172}{343}\rho^2 + \frac{11888}{16807}\rho^3 + \frac{738720}{823543}\rho^4 + \frac{6219872}{5764801}\rho^5 + \frac{354308800}{282475249}\rho^6 + \cdots,
$$
\n
$$
y_0 = 1 - 2\rho + \frac{12}{49}\rho^2 + \frac{2232}{2401}\rho^3 + \frac{34848}{117649}\rho^4 - \frac{206848}{823543}\rho^5 - \frac{8375104}{40353607}\rho^6 + \cdots,
$$

$$
\frac{1}{4}\ln y_0 = -\frac{1}{2}\rho - \frac{43}{98}\rho^2 - \frac{2246}{7203}\rho^3 - \frac{26323}{117649}\rho^4 - \frac{750184}{4117715}\rho^5 - \frac{18361592}{121060821}\rho^6 + \cdots,
$$

$$
f_{\infty,4} = \frac{1}{2} \left(\ln \frac{7}{2} + 1 \right) - \frac{1}{2} \rho \ln \rho - \frac{43}{98} \rho^2 - \frac{1123}{7203} \rho^3 - \frac{26323}{352947} \rho^4 - \frac{187546}{4117715} \rho^5 - \frac{18361592}{605304105} \rho^6 + \dots + .
$$

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