Higher order expansions for the entropy of a dimer or a monomer-dimer system on d-dimensional lattices

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Abstract

Recently an expansion as a power series in $1/d$ has been presented for the specific entropy of a complete dimer covering of a d-dimensional hypercubic lattice. This paper extends from 3 to 10 the number of terms known in the series. Likewise an expansion for the dimer-density p-dependent entropy of a monomer-dimer system involving a sum $\sum_k a_k(d)p^k$ has been recently offered. We herein extend the number of the known expansion coefficients from 6 to 20 for the hypercubic lattices of general dimensionality d and from 6 to 24 for the lattices of dimensionalities $d < 5$. We show that this extension can lead to accurate numerical estimates of the p-dependent entropy for lattices with dimension $d > 2$. The computations of this paper have led us to make the following marvelous conjecture: *In the case of the hypercubic lattices, all the expansion coefficients, $a_k(d)$, are positive!* This paper results from a simple melding of two disparate research programs: one computing to high orders the Mayer series coefficients of a dimer gas, the other studying the development of entropy from these coefficients. An effort is made to make the paper self-contained by including a review of the earlier works.

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I. INTRODUCTION AND RESULTS

The dimer problem arose in a thermodynamic study of diatomic molecules and was abstracted into one of the most basic and natural problems in both statistical mechanics[1–3] and combinatorial mathematics[4]. In more recent years, dimers found interesting applications also in information[5] and string theories[6,7].

Given a hyper-simple-cubic (hsc) lattice with number of sites N in d dimensions, the dimer problem loosely speaking is to count the number of different ways dimers (dominoes) may be laid down in the lattice (without overlapping) to completely cover it. Each dimer covers two nearest neighbor vertices. It is known that the number of such coverings is roughly $\exp(\lambda_d N)$ for some constant λ_d as N goes to infinity. In 1980 H.Minc[8] gave a proof of the asymptotic relation (asymptotic as $d \to \infty$)

$$\lambda_d \sim \frac{1}{2}\ln(2d) - \frac{1}{2} \tag{1}$$

In a series of papers[9–12], one of the authors, P.F., found a mathematical argument for a full asymptotic expansion

$$\lambda_d \sim \frac{1}{2}\ln(2d) - \frac{1}{2} + \frac{c_1}{d} + \frac{c_2}{d^2} + \cdots \tag{2}$$

and computed the first three terms in the Table I also making the conjecture that no further terms would be computed. He was very wrong! One of the results of the present paper is the set of coefficients from c_4 to c_{10} reported in Table I. Viewing the sequence of c_i, we are

TABLE I: Expansion coefficients c_n of the dimer entropy $\lambda_d \sim \frac{1}{2}\ln(2d) - \frac{1}{2} + \sum_n \frac{c_n}{d^n}$ in the case of the hyper-simple-cubic lattices.

c_1	1/8	c_6	20815/21504
c_2	5/96	c_7	9151/6144
c_3	5/64	c_8	39593/73728
c_4	237/1280	c_9	-645691/61440
c_5	349/768	c_{10}	-107753037/901120

certainly led to expect the sum in Eq.(2) to be asymptotic and not convergent.

If we consider covering by dimers of a fraction of the vertices denoted here by $p = 2\rho$ (where ρ is the dimer density per site and the vertices not covered by dimers are considered covered by monomers) and as above study the number of such coverings, we arrive similarly at a function $\lambda_d(p)$ where

$$\lambda_d(1) = \lambda_d \tag{3}$$

Another common notation for λ_d is $\tilde{h}_d$. One also studies

$$h_d = \max_{0 \le p \le 1} \lambda_d(p) \tag{4}$$

For $\lambda_d(p)$ Friedland et al.[5,13] proved the asymptotic relation (asymptotic as $d \to \infty$)

$$\lambda_d(p) = \frac{1}{2}(p\ln(2d) - p\ln(p) - 2(1-p)\ln(1-p) - p) \tag{5}$$

Both this equation and Eq.(1) may be viewed as the mean field approximations for the respective quantities. This was first mentioned in Ref.[12] and is briefly discussed at the end of Section III. By a similar development to that in Ref.[12] one of the authors, P.F. and Friedland[14] argued for an expansion

$$\lambda_d(p) = \frac{1}{2}(p\ln(2d) - p\ln(p) - 2(1-p)\ln(1-p) - p) + \sum_{k=2} a_k(d)p^k \tag{6}$$

where, setting $x(d) = \frac{1}{2d}$, those authors computed the following coefficients,

$a_2(d) = \frac{1}{4}x$
$a_3(d) = \frac{1}{12}x^2$
$a_4(d) = \frac{1}{24}x^2\,(-5x+3)$
$a_5(d) = \frac{1}{40}x^3\,(-39x+20)$
$a_6(d) = \frac{1}{60}x^3\,(-19x^2-30x+20)$

The main result of this paper is the extension of known values:

$a_7(d) = \frac{1}{84}x^4\,(1093x^2-1008x+231)$
$a_8(d) = \frac{1}{112}x^4\,(967x^3-35x^2-602x+189)$
$a_9(d) = \frac{1}{144}x^5\,(-66047x^3+68712x^2-23556x+2856)$
$a_{10}(d) = \frac{1}{180}x^5\,(-67721x^4+18495x^3+29565x^2-15405x+2232)$
$a_{11}(d) = \frac{1}{220}x^6\,(5456221x^4-6452710x^3+2752860x^2-524700x+39710)$
$a_{12}(d) = \frac{1}{264}x^6\,(887437x^5+2477970x^4-3847316x^3+1824724x^2-378004x+31130)$
$a_{13}(d) = \frac{1}{312}x^7(-614279535x^5+794742624x^4-392705664x^3+95702984x^2$
$-11868441x+621504)$
$a_{14}(d) = \frac{1}{364}x^7(678357525x^6-1192936836x^5+869146005x^4-339116960x^3+$
$75444460x^2-9220393x+497016)$
$a_{15}(d) = \frac{1}{420}x^8(89365899701x^6-124219633888x^5+68478916835x^4-19687487260x^3+$
$3185117250x^2-281248772x+10870055)$
$a_{16}(d) = \frac{1}{480}x^8(-206929670185x^7+330409603725x^6-221634792330x^5+83075676915x^4-$
$19146441210x^3+2751382878x^2-231206020x+8907885)$
$a_{17}(d) = \frac{1}{544}x^9(-16388790941183x^7+24197151077904x^6-14547689415128x^5+$
$4724677127184x^4-911997832372x^3+106422324240x^2-7073226040x+210678416)$
$a_{18}(d) = \frac{1}{612}x^9(55311212276891x^8-89669360611981x^7+61471303146642x^6$
$-23833002227449x^5+5824219780656x^4-933123781978x^3+97025317251x^2-6063514389x+$
$176829104)$
$a_{19}(d) = \frac{1}{684}x^{10}(3770925296332945x^8-5844092886538362x^7+3760855236979965x^6$
$-1340101438257204x^5+293876531465913x^4-41181769780866x^3+3649368222699x^2$
$-189574974180x+4489042410)$
$a_{20}(d) = \frac{1}{760}x^{10}(-16045042327489089x^9+26850617367263509x^8-19173445082939896x^7+$
$7825625528101485x^6-2044727194575071x^5+359651992720132x^4-43125672212794x^3$
$+3440152700645x^2-167626520550x+3849436062)$

For the hsc lattices of dimensionality $d < 5$ four more coefficients $a_k(d)$ are available. They are listed in Table II. In Ref.[14] it was conjectured that the series in Eq.(6) is convergent for $0 \leq p \leq 1$. Author P.F. in fact proved[15] that this series converges for small enough p.

We have checked that the $a_k(d)$ are positive for integer values of d with $k \leq 20$. Due to this and to the behavior of the roots of $a_k(d)$ (see Appendix), we are then led to make the conjecture that *the $a_k(d)$ are all positive for integer values of d in the case of the hsc lattices.*

TABLE II: Higher order expansion coefficients $a_k(d)$ of the dimer entropy $\lambda_d(p)$ on the hsc lattices of dimension $d < 5$.

$a_{21}(2)=$ 255640084561/923589767331840	$a_{21}(3)=$ 66223472491867/1023724363217633280	$a_{21}(4)=$ 15299547547784641/9684540638697514 59840
$a_{22}(2)=$ 50273131919/193514046488576	$a_{22}(3)=$ 1171503630290797/20269742391709138944	$a_{22}(4)=$ 117431629955187175/852239576205381284 6592
$a_{23}(2)=$ 4312434281365/17803292276948992	$a_{23}(3)=$ 6903357438819689/133201164288374341632	$a_{23}(4)=$ 902716034982108733/7467242001037626494 1568
$a_{24}(2)=$ 5789230773063/25895697857380352	$a_{24}(3)=$ 40662370356724697/871862166251177508864	$a_{24}(4)=$ 6949151047607061613/6516865746360110394 90048

It follows that the partial sums $\sum_{k\geq 2}^{r} a_k$ are positive for integer values of d for any r, so that the expansion Eq.(6) gives good approximations of $\lambda_d(1)$ also in low dimensions, unlike the expansion Eq.(2), which is numerically useful only for sufficiently large d. In the Appendix we shall further discuss this conjecture and shall return to the numerical approximations in Section IV.

It is interesting to point out some results of historic importance for the dimer problem. The exact value of λ_2 calculated by M.E. Fisher[1] and P.W. Kasteleyn[2] is given by the closed form expression

$$\lambda_2 \equiv \tilde{h}_2 = \frac{1}{\pi}(\frac{1}{1^2} - \frac{1}{3^2} + \frac{1}{5^2} - \frac{1}{7^2} \cdots) = G/\pi = 0.2915609040... \tag{7}$$

with G Catalan's constant. The technique used in the proof of this relation had great influence in the field of exactly soluble models.

The one-dimensional problem has an even more complete solution[13]

$$\lambda_1(p) = \frac{p}{2}\ln(2) - \frac{p}{2}\ln(p) - (1-p)\ln(1-p) - \frac{p}{2} + \sum_{k=2}^{\infty} \frac{(p/2)^k}{(k-1)k} \tag{8}$$

so that $\lambda_1(1) \equiv \tilde{h}_1 = 0$ and $h_1 = \ln\frac{1+\sqrt{5}}{2}$. Notice that in this simple case all the $a_k(1)$ are positive and rapidly vanishing as $k \to \infty$ so that the series converges for $0 \leq p \leq 1$.

Let us turn for the moment to consideration of a dimer gas on our d -dimensional lattice. The gas of dimers is taken as a "hard body" system. Between each two dimers there is a potential energy 0 if the dimers are disjoint and $+\infty$ if they overlap. For this gas we are interested in the coefficients in the Mayer series[16] $b_1(d), b_2(d), ...$

Both the formalism in Ref.[12] used to derive Eq.(2) and the formalism in Ref.[14] used to derive Eq.(6) take as inputs the $b_i(d)$ and have as outputs the c_i of Table I and the $a_k(d)$. Author P.F. did not have as good an algorithm for computing to high orders the $b_i(d)$ as in Ref.[17–19] and was not aware of the already existing lower-order expansions[20–22] for small lattice dimensionalities. This explains the many additional terms computed in Eq.(2) and Eq.(6) when the computations of Ref.[19] were used as inputs. In Sect.II, the technique used in Ref.[18,19] to compute the $b_i(d)$ is discussed. For the computations of the $a_i(d)$, $i = 1, 2, ...20$, one needed exactly the $b_i(d)$ for $1 \leq i \leq 20$, and $1 \leq d \leq 10$. (Interestingly these values in fact determine the $b_i(d)$, $1 \leq i \leq 20$, for all d. This will be shown in Section II and in an independent way in Section III.)

In Sect.III the machines in Refs.[12] and [14] to calculate the c_i and $a_k(d)$ respectively, are discussed. But they are too technical to get deeply into all of the theory. Recently, in fact within the past year, P.F. found another route from the $b_i(d)$ to expansions for $\lambda_d(p)$, simple enough for us to completely describe it in this paper[23]. We close this Section by specializing[24] the expansion in Eq.(6) to $d = 2$, to see what such an expansion looks like

$$\lambda_2(p) \sim \frac{1}{2}(p\ln(4) - p\ln(p) - 2(1-p)\ln(1-p) - p) + 2(\frac{1}{2\cdot 1}(\frac{p}{4})^2 + \frac{1}{3\cdot 2}(\frac{p}{4})^3 + \frac{7}{4\cdot 3}(\frac{p}{4})^4 + \frac{41}{5\cdot 4}(\frac{p}{4})^5 \cdots \tag{9}$$

where this equation is determined by an infinite sequence of integers

$$1, 1, 7, 41, 181, 757, 3291, 14689, 64771, 276101, 1132693, 4490513, 17337685, ... \tag{10}$$

of which the first 23 integers are known from the calculations of this paper. It is very natural to try to find a pattern in the successive terms of this sequence so that a closed form expression for $\lambda_2(p)$ be realized, recalling that it exists for $\lambda_2 = \lambda_2(1)$.

Recently we came across an early paper by Rushbrooke, Scoins and Wakefield [25] computing by a somewhat different method the first six coefficients in Eq.(10) for the square lattice and the first five for other two-dimensional and three-dimensional lattices.

The rest of the paper is organized as follows. In Section II we recall how the Mayer expansion for the dimer problem is related to the high-temperature low-field expansion of an Ising system. Section III sketches how the expansion of Eq.(6) is derived from the Mayer series. In Section IV we show how simply the expansion Eq.(6) can lead to accurate estimates of the p-dependent entropy $\lambda_d(p)$. The Appendix contains additional comments on the positivity conjecture and lists of the coefficients appearing in some generalizations of Eq.(6) to lattices other than the hsc. We have included in the Appendix also a subsection on the graphical expansion procedure for the Ising model.

II. DIMERS AND THE ISING MODEL

It has long been known[1,2,20,21] that the number of ways to place s hard dimers onto a lattice can be evaluated up to a large s by computing, to the same order s and on the same lattice, the high-temperature (HT) and low-field series expansion of the free-energy of a spin-1/2 Ising model in the presence of a uniform magnetic field.

The dimer combinatorial problem can be simply formulated in the language of statistical mechanics. A set of dimers on a N-site lattice (N even) is described as a lattice-gas of molecules occupying nearest-neighbor sites subject to a non-overlap constraint, in terms of a macrocanonical partition function

$$\Xi_N(z) = 1 + \sum_{s=1}^{N/2} Z_s z^s = 1 + \sum_{s=1}^{N/2} g_N(s) z^s. \tag{11}$$

Due to the non-overlap constraint, Z_s, the canonical partition function for a fixed number s of dimers simply counts the allowed dimer configurations, so that $g_N(s)$ is precisely the number of ways of placing s dimers over the links of the lattice, and $z = \exp(\beta\mu)$ is the dimer activity. The chemical potential μ, namely the energy cost of adding one more dimer to the system, is zero whenever there is room on the lattice for adding one more dimer and infinite otherwise. Therefore the value of $\beta = 1/k_B T$ with T the temperature and k_B the Boltzmann constant, is irrelevant and can be fixed to unity. Thus $z = 1$ is the value of the activity describing the combinatorics of a monomer-dimer system i.e. of a dimer system that does not cover completely the lattice, while $z = \infty$ describes the complete coverings.

In the $N \to \infty$ (thermodynamical) limit one gets

$$\Xi(z) = \lim_{N\to\infty} [\Xi_N(z)]^{1/N} = 1 + \sum_{s=1}^{\infty} g(s) z^s \tag{12}$$

from which a "pressure" (or macrocanonical potential) can be defined in the usual way

$$P(z) = \ln(\Xi(z)) = \sum_{s=1}^{\infty} b_s z^s. \tag{13}$$

since $\beta = 1$. The dimer density per site ρ is expressed in terms of the pressure by

$$\rho(z) = z\frac{dP}{dz} = \sum_{s=1}^{\infty} s b_s z^s. \tag{14}$$

The series for $\rho(z)$ can be inverted to get z as a power series in the density and by substituting $z = z(\rho)$ in Eq. (13), P can be expressed as a power series in the density ρ, thus obtaining the virial expansion. Eqs.(13) and (14) are called the Mayer expansions of the dimer lattice-gas.

The specific entropy $s_d(p)$ of a dimer system of density ρ in d dimensions is

$$s_d(p)/k_B \equiv \lambda_d(p) = -\rho_d(z)\ln z + P_d(z) = \frac{1}{2}(p\ln(2d) - p\ln p) + O(p) \tag{15}$$

where the last expression arises by setting $z = z(p)$, and $\rho = p/2$, and observing that on the hsc lattices $z = \frac{p}{2d} + O(p^2)$. This structure was further specified in Ref.[5,13], as indicated in Eq.(19). One can also easily check that changing the variable from z to p, the point $z = 1$ corresponds to a stationary point of the entropy with respect to p, thus linking the definition given above of h_d in terms of $\lambda_d(p)$ with the definition used in Ref.[17] as $P(z)|_{z=1}$. We now couple the relation Eq.(15) with the expansions above for $P(p)$ and $z(p)$. We write

$$z = \frac{p}{2b_1}(1 + F(p)) \tag{16}$$

and then get from Eq. (15) and (16)

$$\lambda_d(p) = P(p) - \frac{p}{2}\ln(\frac{p}{2b_1}) - \frac{p}{2}\ln(1 + F(p)) \tag{17}$$

or

$$\lambda_d(p) = P(p) - \frac{p}{2}\ln(p) + \frac{p}{2}\ln(2d) - \frac{p}{2}\ln(1 + F(p)) \tag{18}$$

using $b_1 = d$. Referring to Eq.(6) we may put Eq. (18) in the form

$$\lambda_d(p) = \frac{1}{2}(p\ln(2d) - p\ln p - 2(1-p)\ln(1-p) - p) + \sum_{k=2}^{\infty} a_k p^k \tag{19}$$

when the a_k are suitably determined from the Mayer series coefficients in a straightforward manner.

The Mayer coefficients $b_s(d)$ are simply obtained from the HT expansion of the free-energy for the Ising model. To illustrate the relationship between the Ising and the dimer problems, recall the "primitive"[26] method of HT and low-field graphical expansion for the partition function $Z_N(\beta, h) = \sum_{m\geq 0}\sum_{l=m}^{L_{max}} \gamma_N(2m, l)\tanh(h)^{2m}\tanh(\beta)^l$ of a spin-1/2 Ising model on a lattice of N sites. Here $\beta = 1/k_BT$ denotes the inverse temperature and $h = \beta H$ with H the uniform external magnetic field. The expansion coefficient $\gamma_N(2s, s)$ counts all possible lattice configurations of graphs represented by precisely s disconnected edges placed onto disjoint links of the lattice and therefore coincides with the quantity $g_N(s)$ in Eq.(12). The procedure of forming the specific free-energy $f_N(\beta,h) = \frac{1}{N}\ln Z_N$ and then taking the thermodynamical limit, exactly parallels[21] the procedure leading to Eq.(13), so that one concludes that from the expansion $f(\beta,h) = \sum_{m\geq 0}\sum_{l=m}^{L_{max}} f_{2m,l}\tanh(h)^{2m}\tanh(\beta)^l$, the Mayer expansion coefficients can be read as $b_s = f_{2s,s}$.

Let us now recall that recently a significant extension, of the HT series for several models in the Ising universality class, including the conventional spin-1/2 model, has been obtained for a sequence of bipartite lattices, in particular the hsc lattices of spatial dimensionality $1 \leq d \leq 10$ and the hyper-body-centered-cubic (hbcc) of any dimensionality (at least in principle, because the only way in which dimension enters is in the power of the embedding number, and the time it takes to preform the computation for the hbcc lattices varies very slowly with the dimension; in practice only results for $d \leq 7$ have been obtained). It is also convenient, at this point, to give some simple details on these calculations. It is most convenient to use[18,19] the classical linked-cluster method[27] of graphical expansion. At each HT order l, the series coefficients are expressed as the sum of an appropriate class of l-edge graphs. Each graph contributes a ratio of two integers: the "free-embedding-number" and the symmetry-number of the graph, times a product of "bare vertex-functions" associated to the vertices of the graph and depending on the magnetic field. The embedding-number counts the number of distinct ways (per site of the underlying lattice) in which the graph can be placed onto the lattice with each vertex assigned to a site and each edge to a link. This number depends on the topology of the graph and on the dimensionality d of the lattice. The important property is that, in the case of the hsc lattices (but not for the hbcc lattices!), for a generic graph with l edges, the embedding-number is a polynomial in d of degree l at most. The symmetry-number counts the automorphisms of the graph and depends only on the topology of the graph. The great advantage of the linked-cluster method comes from the recognition that the huge variety of graphs that contribute at relatively high orders of expansion to the computation of a physical quantity, e.g. the magnetization, can be obtained by combining simpler graphs in a smaller class[27], thus making possible to trade the computational complexity for algebraic complexity.

From the field-dependent free-energy, one can compute all its field-derivatives usually called (higher) susceptibilities. It is clear at this point that, on the hsc lattices, the computation of these quantities through the 10th order, can be extended to a generic d, by a simple interpolation of the series coefficients using the computation on a sequence of hsc lattices of dimensionalities $1 \leq d \leq 10$ and based on the fact that the lth order expansion coefficient is a simple polynomial[28] of degree l in d (with zero constant term). Actually much more than this can be done. One can observe[19] that the knowledge of the free-energy gives access to the HT expansions of the successive derivatives of the magnetic field with respect to the magnetization $\partial^{2p+1}h/\partial\mathcal{M}^{2p+1}$, for $p = 0, 1...$ and that these quantities are expressed only in terms of connected graphs having no articulation-vertex, i.e. no vertex whose deletion would disconnect the graph. What is decisive for our aims is the fact that the embedding-number onto a hsc lattice of an l-edge graph in this class is a polynomial in d of degree $\lfloor l/2 \rfloor$ at most[28]. Here $\lfloor l/2 \rfloor$ denotes the integer part of $l/2$. Therefore, in spite of the fact that the HT expansion coefficients of the (higher)-susceptibilities at order l are polynomials in d of degree l, the susceptibilities can be simply expressed in terms of the successive derivatives of the magnetic field with respect to the magnetization which, at the same expansion order, are polynomials in d of degree $\lfloor l/2 \rfloor$ only. Thus, one can conclude that the exact dependence on d of the HT coefficients of the higher susceptibilities can actually be determined up to order

20, using only a sequence of hsc lattices of dimensionalities $1 \leq d \leq 10$, by an interpolation in d of the series coefficients!

Let us finally stress that the elements of the coefficients matrix $f_{2m,l}$ of the HT and low-field expansion for the free-energy of the spin-1/2 Ising model can be linearly expressed in terms of the expansion coefficients of the susceptibilities and therefore they also are polynomials in d of degree l. This property holds in particular for the Mayer coefficients $b_s(d) = f_{2s,s}(d)$ of the dimer gas. More details concerning the graphical expansion procedure can be found in Subsect. C of the Appendix.

III. DERIVATION OF EXPANSIONS

As mentioned in the introduction we have a second route for deriving $\lambda_d(p)$ and λ_d expansions. The key initial step is the computation of the quantity $\tilde{J}_i(d)$ from the quantities $b_i(d)$. The $\tilde{J}_i(d)$ depend on the set of $b_n(d)$ with $n \leq i$. The computations are given in Ref. [29] as follows

$$\tilde{J}_1 = 0.$$

We first find $\tilde{J}_r^L$, with $\tilde{J}_1^L = 0$, and from $r = 2$ on, inductively defined by

$$\tilde{J}_r^L = \frac{1}{L}\Big\{S_r - (exp(L\sum_{i=1}^{r-1} \tilde{J}_i^L x^i))|_r\Big\} \tag{20}$$

where

$$S_r = \sum_{p=0}^{r} \Big\{(exp(L\sum_i b_i(\frac{x}{2d})^i))|_p \frac{1}{(r-p)!}(\frac{-1}{2(L-1)})^{r-p}\frac{(L-2p)!}{(L-2r)!}\Big\}. \tag{21}$$

The symbol | with the subscript j indicates the jth coefficient in the formal power series in x. The $\tilde{J}_r$ are determined from the $\tilde{J}_r^L$ by taking L to infinity. We may also inductively go from the $\tilde{J}_i$ to the b_i by the same formulae.

This set of relations was first implicitly used in Ref.[12], but not explicitly written down there. Just as the $b_i(d)$ are the cluster expansion coefficients of a dimer gas, the $\tilde{J}_i(d)$ are the cluster expansion coefficients of a certain polymer gas[12] and these coefficients of the two gases are related by the development surrounding eqs. (20) and (21). This is a clean calculation that requires no hard proof. The $\tilde{J}_i(d)$ can be proved[10] to be of the form

$$\tilde{J}_s(d) = \frac{c_{s,r}}{d^r} + \frac{c_{s,r+1}}{d^{r+1}} + ... + \frac{c_{s,s-1}}{d^{s-1}} \tag{22}$$

with $r \geq s/2$.

Whereas our first development was basically for each d individually, we will see as with this last equation that the dependence on d is in the nitty-gritty of this second development. The present treatment allows us to get results relating the series for different d's. As an example, suppose we know the $\tilde{J}_i(d)$ for $1 \leq d \leq 10$, $i \leq 20$. Then one may derive $\tilde{J}_i(d)$ for $i \leq 20$ and all d! (One has enough information to compute all the $c_{s,r}$ for $i \leq 20$.) The same statement holds for the $b_i(d)$ since one may go between the set of $b_i(d)$ with $i < n$ and the set of $\tilde{J}_i(d)$ with $i < n$ as mentioned above.

So far all the results dealt with in this section have been true and rigorously proven. We now turn to the further development, certainly true but for which we do not yet have a rigorous proof. We work for a given d and take as known the $\tilde{J}_i(d)$ (which as above could be calculated from the $b_i(d)$). We then compute $\alpha_i(d)$ by iterations, from $\alpha_i = 0$, of

$$\alpha_k = \big(\tilde{J}_k p^k\big)\frac{1}{(1-2\sum_{i=2} i\alpha_i)^{2k}}\big(1-2\sum_{i=2} i\alpha_i/p\big)^k. \tag{23}$$

Then $\lambda_d(p)$ is given by

$$\lambda_d(p) = Q_1 + Q_2 \tag{24}$$

$$Q_1 = \frac{1}{2}(p\ln(2d) - p\ln p - 2(1-p)\ln(1-p) - p) \tag{25}$$

$$Q_2 = \sum_{i=2}\alpha_i - \sum_{k=2}\frac{1}{k}\Big(2\sum_{i=2} i\alpha_i\Big)^k + \frac{1}{2}p\sum_{k=2}\frac{1}{k}\Big(2\sum_{i=2} i\alpha_i/p\Big)^k. \tag{26}$$

Q_2 may be developed as a power series in p

$$Q_2 = \sum_2^\infty a_k(d)p^k \tag{27}$$

where $a_k(d)$ is a polynomial in power of $\frac{1}{d}$ with powers satisfying $k/2 \le r < k$ (as the powers in Eq. (22)), see Refs. [14] or [15]. So for example if we know $a_k(d)$ for $k \le 20$ and $d \le 10$, then we can deduce $a_k(d)$ for $k \le 20$ and all d. To determine a_k only the values of $a_k(d)$, $d = 1, .., \lfloor k/2 \rfloor$ are needed, the remaining $10 - \lfloor k/2 \rfloor$ values were used to give consistency checks for each $k < 20$. This is a consistency check on both the computation of the $b_i(d)$ and of the theory, since as we mentioned above the development of Eq.(23)-Eq.(27) has not been yet made rigorous.

We can deduce the series for λ_d, Eq. (2) above, basically by setting $p = 1$ in Eq.(24). It is important to note for this that each power of $\frac{1}{d}$ gets a contribution from only a finite number of $a_k(d)$. Specifically $1/d^s$ get contributions from those $a_k(d)$ for which $k/2 \le s < k$. For example if we know $a_k(d)$ for $k \le 20$, then we can deduce the terms in λ_d up to $1/d^{10}$.

To get at the theory (of the formal argument leading to eqs.(24)-(27), our second development of the $\lambda_d(p)$ and λ_d expansions), we recommend to the reader starting by reading Ref.[12], a three page paper, or Section 5 of Ref.[14]. We now give a slightly hand waving capsule summary of the introductory portion of this theory up to the derivation of the mean field formulae Eq.(1) and (5) above.

We work on a periodic d-dimensional lattice with number of sites N. A "difunction" is a translation invariant periodic function on pairs of distinct vertices. We associate to dimers the difunction f, that is 1 if the pair of vertices are nearest neighbors and 0 otherwise. We call a sequence $X_1, X_2, ...$ of pN distinct vertices a "p-sequence". We let $\sum$ denote the sum over all p-sequences. We note that the number of distinct dimer coverings that cover a fraction p of the vertices can be represented as

$$\frac{1}{2^{(pN/2)}}\frac{1}{(pN/2)!}\sum\prod_{\substack{i=1\\ i\ \text{odd}}}^{pN} f(X_i, X_{i+1}). \tag{28}$$

The numerical factors before the sum divide by the number of different p-sequences that correspond to the same choice of dimers. The sum is over $\frac{N!}{((1-p)N)!}$ p-sequences.

We let f_0 be the difunction of constant value $(\frac{2d}{N-1})$. f and f_0 have the same "normalization" in the sense that, if one fixes its first component and sums over the second, one gets the same answer for both functions. Replacing f in Eq.(28) by f_0 and using the Stirling formula gives the mean field answer

$$\exp \lambda_{mf} N$$

for the number of our dimer covers, where λ_{mf} is as in Eq. (5).

We write

$$f = f_0 + \mathcal{V} \tag{29}$$

with

$$\mathcal{V} = f - f_0. \tag{30}$$

Expansions in powers of $\mathcal{V}$ may be converted into the expansions of this paper.

IV. NUMERICAL ESTIMATES

It is interesting at this point to get some feeling about the accuracy of the estimates of h_d and $\tilde{h}_d \equiv \lambda_d(1)$ that can be obtained from the expression Eq.(6) for $\lambda_d(p)$ when a sufficiently large number of coefficients $a_k(d)$ is known. For the evaluation of both h_d and $\tilde{h}_d$ a first orientation comes from truncating the expansion $\sum_{k=2}^{\infty} a_k(d)p^k$ at the order $k = r$ and plotting the result vs. some power of $1/r$. Let us first consider the quantity $\tilde{h}_d$. Assume that the series converges for $p = 1$ and that the coefficients $a_k(d)$ are all positive, then its successive truncations must provide an increasing sequence of lower bounds of the limit. Actually, we can check that the approximation of truncating the expansion at the highest known order is always consistent with the known upper bounds. However in the case of $d = 2$ and $d = 3$ the values thus obtained, i.e. $\tilde{h}_2 = 0.2865..$ and $\tilde{h}_3 = 0.44916..$ respectively, appear to be still too small. Therefore one should properly extrapolate the sequences $(S_r) = \frac{1}{2}(\ln(2d) - 1) + \sum_2^r a_k(d)$ of the truncated expressions. Of course, the best way to do this depends on the behavior of the sequences. It is very encouraging to notice that for all values of d, the sequences are smooth and their behavior is well approximated by the simple Ansatz $S_r = a + b/r^{\alpha}$ and so one has $a \approx \tilde{h}_d$. This procedure is very successful. We observe that α increases with d and ranges from $\alpha \approx 1$ for $d = 2$ to $\alpha \approx 2.6$ for $d = 6$. In dimensionality $d = 2$, this Ansatz gives a good fit of the last 4 - 10 terms of the sequence and the extrapolated value $a = 0.2915(20)$ agrees with the exactly known value $\tilde{h}_2 = 0.291560...$ in Eq.(7), within the estimated error. The uncertainty we have written is very conservative, although somewhat arbitrary. It is obtained allowing for the spread of values resulting from small variations of the exponent α in the functional form used for fitting or from a comparison with other extrapolations obtained for example evaluating the series $\sum_{k=2}^{r} a_k(d)p^k$ for $p = 1$, by Padé or differential approximants[30] and adding the result to the expression $\frac{1}{2}(\ln(2d) - 1)$. Analogously, for $d = 3$ the sequence (S_r) is well fitted by the Ansatz$a + b/n^{1.3}$ and leads to the estimate $\tilde{h}_3 = 0.4499(2)$. This value is not far from the estimate $\tilde{h}_3 = 0.4479$ obtained by a MonteCarlo calculation[31] or from $\tilde{h}_3 = 0.453(1)$ obtained[32] extrapolating a much shorter expansion, and it is also completely consistent with the bounds[8,13,33,34] $0.440075842 \leq \tilde{h}_3 \leq 0.4575469308$.

Proceeding along the same lines, we can determine the values of $\tilde{h}_d$ for any value of d. We notice that the apparent precision of the results improves rapidly as d grows, while the differences between the extrapolated values and the highest order truncations of the series (as well as the estimated uncertainties) decrease rapidly. The final estimates are always completely consistent with the known bounds. Our estimates of $\lambda_d(1)$ for $d = 2, ..., 8$ are reported in table III. Notice that evaluations of these quantities appear very rarely[35] in the literature.

The computation of h_d requires only a quite short comment. Unsurprisingly, the sequences of truncated expansions $\sum_{k=2}^{r} a_k(d)p^k$ evaluated for $p < 1$ show a faster convergence than for $p = 1$. The estimates of h_d thus obtained agree well, within their uncertainties, with those already listed in Table VII of Ref.[17] which have been obtained resumming via Padé approximants the expansion of $P(z)$ for $z = 1$. Therefore the reader is referred to this source.

TABLE III: Our estimates of $\tilde{h}_d = \lambda_d(1)$ for the (hyper)-simple-cubic lattices of dimensions $d = 2, 3, ...8$ with the rigorous lower and upper bounds[14] defined by $(1/2)\ln(2d) - 1/2 \le \lambda_d(1) \le \ln((2d)!)/4d$. While these rigorous bounds are valid for all d, for $d = 2$ we have simply reported the known exact value and for $d = 3$ we have reported the tighter bounds from Refs.[8,13,33,34]. The non-rigorous lower bounds are simply obtained assuming the validity of the positivity conjecture for the coefficients $a_k(d)$ and truncating our expansions at the highest available order.

	Lower Bound	Non-rig. L.B.	Our Estimate	Upper Bound
$\lambda_2(1)$	0.29156090	0.286521	0.2915(20)	0.291560905
$\lambda_3(1)$	0.44007584	0.449164	0.4499(2)	0.457546931
$\lambda_4(1)$	0.53972077	0.576517	0.57666(3)	0.662787682
$\lambda_5(1)$	0.65129254	0.679434	0.67949(2)	0.755220629
$\lambda_6(1)$	0.74245332	0.765301	0.765315(2)	0.832800604
$\lambda_7(1)$	0.81952866	0.838785	0.838789(1)	0.899686471
$\lambda_8(1)$	0.88629436	0.902947	0.902949(1)	0.958495629

A. Series expansion for h_d for d large

As d goes to infinity, h_d tends to $\tilde{h}_d$. One can compute the rate with which the former approaches the latter performing an expansion in $\frac{1}{\sqrt{d}}$.

To compute h_d one looks for a stationary point of Eq.(6). Putting $y = 1/\sqrt{2d}$, the stationarity equation can be written as

$$(1 - p_{st})^2 - p_{st}y^2 \exp(-2\sum_{k=2} ka_k p_{st}^{k-1}) = 0 \tag{31}$$

This equation can be solved for large d. Knowing a_k up to $k = 20$, one can solve iteratively the equation up to the order y^{42}. Here we shall report only the first few terms

$$p_{st} = 1 - y + \frac{1}{2}y^2 + \frac{3}{8}y^3 - y^4 + \frac{201}{128}y^5 - \frac{5}{2}y^6 + \frac{7003}{1024}y^7 - 22y^8 + ... \tag{32}$$

At the second order in y, it agrees with the value of p_{st} associated to the lower bound for h_d found in[5,13]

$$p_{st} = \frac{4d + 1 - \sqrt{8d + 1}}{4d} \tag{33}$$

Substituting Eq.(32) into Eq.(6), one gets

$$h_d - \tilde{h}_d = y - \frac{1}{4}y^2 - \frac{11}{24}y^3 + ... \tag{34}$$

$$h_d = \frac{1}{2}(\ln 2d - 1) + \frac{1}{\sqrt{2d}} - \frac{11}{48\sqrt{2d^3}} + O(d^{-2}) \tag{35}$$

in which we wrote only the first three terms out of the 40 terms we computed. Using 40 terms, this series expansion agrees with the difference $h_d - \tilde{h}_d$ computed numerically up to $2 \cdot 10^{-6}$ for $d = 7$, 10^{-15} for $d = 20$. From $d = 40$ up to $d = 9000$ the precision is only 10^{-16}. Probably the reason for this is that as d increases the point of maximum p_{st} moves closer to 1, decreasing the precision.

The terms given in Eq.(35) give h_d with error less than $3 \cdot 10^{-3}$ for $7 \leq d < 100$ and $2 \cdot 10^{-5}$ for $100 \leq d < 10000$.

In particular from Eq.(32) and Eq.(34) one gets

$$\lim_{d\to\infty} \frac{h_d - \tilde{h}_d}{p_{st}(d) - 1} = -1 \tag{36}$$

V. APPENDIX

A. The conjecture that the coefficients a_k are positive in the case of the hsc lattices

We proved that the coefficients $a_k(d)$ are positive integers for $k \leq 20$ and $d \geq 1$ by locating in the complex d-plane their real roots, and counting the complex ones to make sure that none is missing. It is interesting to note that for $1 < d < 2$ or for $2 < d < 3$ the $a_k(d)$ can be negative, and that there are roots approaching 1 and 2 as k gets large. As we have already noticed, based on the conjecture that the a_k are positive, the computed values of a_k provide a lower bound of λ_d. For $d = 2$ in the case of h_d, this lower bound 0.662798966, is smaller than the estimate 0.662798972(1) obtained in Ref.[17] by Padé approximants. For $d \geq 3$ these lower bounds reproduce within the error the Padé estimates of Ref.[17].

TABLE IV: Real roots of $a_k(d)$ for $k \geq 10$

$k = 10$	-0.65502486055142554	0.99997855862379883	
$k = 11$	1.0000010707811947	1.6603775954637132	
$k = 12$	-0.12473442164710268	1.0000008060184913	1.5835444714309055
$k = 13$	0.99999998817575145		
$k = 14$	1.0000000363954472	1.628126162558255	
$k = 15$	1.000000000099149	1.9594209128425236	
$k = 16$	0.99999999993591589		
$k = 17$	0.99999999999934955	2.0071302031011769	2.4952449117198663
$k = 18$	1.0000000000002549	1.9889667170409254	
$k = 19$	1.0000000000000033	1.9993853767904753	
$k = 20$	0.99999999999999901	2.0009898597900763	2.6230186617839066

B. Generalization of the positivity conjecture to other bipartite lattices

There is some evidence that the positivity conjecture can be extended to other bipartite lattices. Let us recall what is known on other lattices. λ_d has been computed from the Mayer coefficients b_n on other lattices using the formula

$$\lambda_d = -\frac{1}{2}p\ln(\frac{p}{q}) - (1-p)\ln(1-p) - \frac{p}{2} + \frac{q}{2}\sum_{k=2} \frac{C_k(\frac{p}{q})^k}{k(k-1)} \tag{37}$$

with q the lattice coordination number. The notation $a_k = \frac{q}{2}\frac{C_k/q^k}{k(k-1)}$ extends that used for the hypercubic case.

Let us now report the available data for other bipartite lattices.

In the case of the tetrahedral lattice ($q = 4$), taking the Mayer coefficients b_n from Ref.[21,22] we obtain the following set of coefficients C_k

$1, 1, 1, 1, 31, 253, 1261, 4897, 16201, 49501, 161239, 643969, 3006823, 14104861, 60942421, 237903169, 854124745, 2955594097$

For the bcc lattice, the b_n for $n \leq 24$ have been computed in Ref.[17] for $d = 3, 4, 5, 6, 7$. The coefficients C_k computed from them are all positive. In Table V we list the coefficients $C_k(d)$ for hbcc lattices of dimensionalities $d = 3, 4, 5$. The coordination-number is $q = 2^d$.

For the hexagonal lattice[36], the coefficients C_k are

$1, 1, 1, 1, 11, 85$

Let us now turn to the case of non-bipartite lattices.

For the triangular lattice ($q = 6$) the coefficients up to C_6 are listed in Ref.[36], while higher-order ones are obtained from Ref.[21]

$1, -3, -11, 1, 91, 141, -1651, -16143, -87329, -295063, -72533, 8092033, 76819835$

For the fcc lattice ($q = 12$), from Ref.[21] we obtain:

$1, -7, 19, 41, -779, 3557, 46327, 118529, -557909$

These data imply that the positivity conjecture for the C_k has to be restricted to bipartite lattices.

On a Bethe lattice[37,38] the entropy is given by Eq.(37) with $C_k = 1$ for all k. Notice that on any lattice $C_k = 1$ for $k < r$, where r is the length of the smallest nontrivial loop on the lattice, because the diagrams contributing to such C_k can't tell the difference between the given lattice and a Bethe lattice of the same coordination number.

A stronger form of the positivity conjecture is that $C_k \geq 1$ for bipartite lattices.

C. Graphical expansion procedure for the Ising model

For simplicity, the whole graphical expansion procedure can be split into three steps. First, one has to list all graphs entering into the calculation up to the maximum order L_{max} of expansion. To begin with, one forms the simple, topologically distinct one-vertex-irreducible graphs with $l \leq L_{max}$ edges. One can further restrict to the subset of the bipartite graphs, since only these can be embedded onto the bipartite hsc or hbcc lattices. This is the only memory intensive part of the procedure, because there are many graphs[18,19,39] (approximately $3 \cdot 10^5$ graphs at order 20, and over $5 \cdot 10^7$ at order 24, but it took only a few hours. In a second step, the lattice embedding-numbers and the symmetry-numbers of these graphs are computed, one vertex of these graphs is "marked" in all possible ways and

TABLE V: The coefficients $C_k(d)$ in Eq.(37) with $k = 2, ..., 24$ for the (hyper)-body-centered-cubic lattices of dimensionalities $d = 3, 4, 5$.

	$d = 3$	$d = 4$	$d = 5$
C_2	1	1	1
C_3	1	1	1
C_4	37	151	541
C_5	241	1001	3601
C_6	1651	21241	290851
C_7	13861	276445	4136581
C_8	109873	4138275	185447641
C_9	850465	61222177	3766174561
C_{10}	6620401	903139171	134478272521
C_{11}	51657541	13527055301	3251891481301
C_{12}	403327651	201952069177	105463232417731
C_{13}	3151118881	3041256137921	2794164743354401
C_{14}	24647038963	45839858214697	86840903677417891
C_{15}	192950685061	69396577375846	2421252466929163141
C_{16}	1510882839217	10530703348244851	73870429278903327001
C_{17}	11833222518145	160247978490447425	2123026721471921771521
C_{18}	92728596423613	2444106838568935375	64306694719829414761621
C_{19}	727194198560401	37359234126615235321	1883895461127373802533921
C_{20}	5707071682914097	572176086489368008851	56961277210166888567226841
C_{21}	44820667959807601	8779078842662089743601	1690242630478526669835704401
C_{22}	352227866459521537	134925544759538198882283	51146624643545703193238849401
C_{23}	2769671081569110445	2076868645293925124133493	1531526780518608097927545101821
C_{24}	21790699297032926587	32014374542692855556562921	46435767644223061358549293433371

the graphs are "decorated" to have also multiple lines. This is the subset of the graphs from which the expansion of the magnetization can be reconstructed.

In the case of hsc lattices of high dimensionality, the most time-consuming part of this procedure is the computation of the embedding-number for each graph. In the case of the hbcc lattices the timings are much smaller and very slowly dependent on d, but unfortunately the expansion coefficients are not polynomials in d. One begins by appropriately ordering the graph vertices, and then the first of them is placed at the lattice origin. The possible positions of the second vertex can be counted exploiting the symmetries of the hypercube. After fixing the first two points of the embedding, the possible positions of the remaining vertices are restricted to relatively few configurations by the constraints given by the distances from the first two points and the count can go on in a relatively easy way. On the hsc lattices, the timings for computing the magnetization expansion of the d-dimensional Ising model at order L_{max} increase exponentially with the order of expansion and the lattice dimensionality d: roughly as $O(5.5^{L_{max}} 2.5^d)$. In particular, the computation for the 10-dimensional Ising model at order 20 took 42 days of single-core time on a quad-core desktop computer with a CPU-clock frequency of $2.8GHz$. Actually, less time was used since the calculation was appropriately distributed on the four cores of the computer. Using more extensive computer resources, it would be possible to compute only a few more orders, for not too high lattice dimensionalities.

The next step implements the algebraic "vertex-renormalization", namely the procedure of reconstruction[27] of the magnetization from the one-vertex-irreducible graphs having a single marked vertex. By integrating the magnetization exactly with respect to the field one finally obtains the free-energy in terms of the bare vertices (up to a standard constant of integration). This step of the calculation is based on codes written in the Python language and is fast. The free-energy thus computed is model independent: eventually one has to specialize the precise form of the bare vertex-functions to the particular model of interest.

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