# Dimer statistics on a Bethe lattice

A. B. Harris[a] and Michael Cohen
*Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104*

(Received 19 April 2006; accepted 26 September 2006; published online 13 November 2006)

We discuss the exact solutions of various models of the statistics of dimer coverings of a Bethe lattice. We reproduce the well-known exact result for noninteracting hard-core dimers by both a very simple geometrical argument and a general algebraic formulation for lattice statistical problems. The algebraic formulation enables us to discuss loop corrections for finite dimensional lattices. For the Bethe lattice we also obtain the exact solution when either (a) the dimers interact via a short-range interaction or (b) the underlying lattice is anisotropic. We give the exact solution for a special limit of dimers on a Bethe lattice in a quenched random potential in which we consider the maximal covering of dimers on random clusters at site occupation probability $p$. Surprisingly the partition function for "maximal coverage" on the Bethe lattice is identical to that for the statistics of branched polymers when the activity for a monomer unit is set equal to $-p$. Finally we give an exact solution for the number of residual vacancies when hard-core dimers are randomly deposited on a one dimensional lattice. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2364501]

## I. INTRODUCTION

The statistics of covering a lattice with monomers or dimers has a long and continuing history in condensed matter physics. Recently there has been a revival of interest in this topic in connection with a number of seemingly unrelated problems such as quantum fluctuations in Heisenberg antiferromagnets,[1] stability and dynamics in granular systems,[2] phase transitions in certain complex fluids,[3] dynamics of catalysis on surfaces,[4] and the biophysics of membranes.[5] Accordingly, we have been led to revisit this problem with the goals of (a) drastically simplifying the derivation of existing approximations and (b) providing a framework within which the more modern techniques of statistical mechanics can be applied.

The first studies of the statistics of dimer coverings of a lattice were carried out more than 50 years ago,[6–8] obtaining results analogous to those of the Bethe approximation[9–11] for the Ising and Heisenberg models. At that time, the relation of this approximation scheme to the structure of the Cayley tree (a recursive "lattice," an example of which, with coordination number $q$, is shown in Fig. 1) was apparently not known. It was later recognized by Sykes,[12] who apparently first coined the term "Bethe lattice," that the Bethe approximation was to be associated with local properties evaluated near the center of the tree, in order to avoid surface effects which, for $d$-dimensional hypercubic lattices, are unphysical. The pathological effects of the anomalously large surface were later studied by several authors in the 1970s,[13–16] but, as was clear from the work of Fisher and Gaunt in 1964,[17] it was the results for local properties at the center of the infinite tree which could be connected to those of hypercubic lattices in the limit $d \to \infty$. They obtained expansions in powers of $1/d$ for the coefficients of series expansions in the coupling constant. However, it was later shown by the renormalization group[18] that the critical exponents for typical lattice models were those of mean field theory for $d > 4$.

Most of the results of this paper will be obtained for the Bethe lattice. We implement the Bethe lattice condition either by explicitly considering sites far from the boundary or, alternatively, by using a formulation appropriate to periodic lattices and then introducing approximations which become exact when the lattice does not support any loops.[19] By initially treating a periodic lattice we eliminate anomalous surface effects. We are thus assured that our results are characteristic of the interior of the tree and should be associated with what is now commonly called a Bethe lattice.[20]

Of course, an important aim is to treat real $d$-dimensional lattices. To this end there have been a number of papers dealing with series expansions for the problem of dimer or monomer-dimer coverings of a lattice. Nagle[21] in 1966 developed a series expansion in powers of the dimer activity $z$ for a number of two- and three-dimensional lattices. Longer series were later obtained by Gaunt[22] who exploited the relation between the dimer problem and the Ising model in a field. Alternative formulations, based on the generalization of the Mayer cluster expansion[23] by Rushbrooke and Scoins,[24] have also been given.[25] More recently Brazhnik and Freed[26] have given a formulation suitable not only for dimers but also for more complicated entities. Here we treat the cases of both noninteracting and interacting dimers. We first address these problems using a simple intuitive geometrical approach. Then we adopt an algebraic approach based on a transformation introduced by Shapir[27] which enables us to develop an expansion for a $d$-dimensional lattice in which the leading term is the exact result for the Bethe lattice of the same coordination number $q$. For noninteracting dimers corrections are obtained in powers of $1/q$ and the activity $z$, similar to the result of Nagle.[21]

Briefly this paper is organized as follows. In Sec. II we

[a]Electronic mail: harris@physics.upenn.edu

 © 2006 American Institute of Physics

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

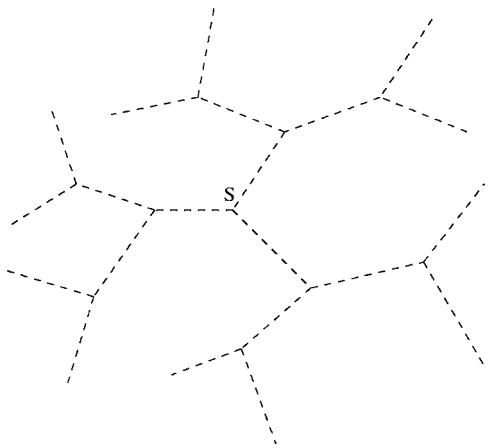


FIG. 1. A Cayley tree with coordination number $q=3$. The tree consists of three generations of bonds starting from the seed site, $S$.

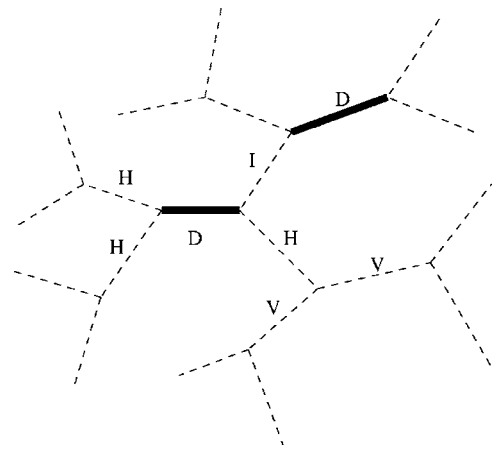


FIG. 2. Classification of bonds in a lattice partially covered by dimers. As indicated in the text $D$ labels a dimer, $V$ a dimer vacancy, $I$ an interacting bond, and $H$ a half bond.

present a simple geometrical derivation of the Bethe approximation for the statistics of distributing hard-core (but otherwise noninteracting) dimers on a lattice. We also give an alternative algebraic derivation of this result which enables us to generate loop corrections for the case of a $d$-dimensional periodic lattice. We also briefly consider noninteracting dimers on an anisotropic lattice. In Sec. III we consider a model which includes dimer-dimer interactions. We derive the Bethe approximation (which is exact on the Bethe lattice) for this model by both the geometrical and algebraic approaches. The exact solution of a model in the special limit of quenched randomness in which each cluster of randomly occupied sites is maximally covered by noninteracting dimers is given in Sec. IV. In Sec. V we consider a model of random deposition of hard-core dimers in one dimension. We give an exact result for the fraction of sites which remain vacant after deposition is completed. Finally, our conclusions are summarized in Sec. VI. In a future paper we will generalize our approach to treat the statistics of entities more complicated than dimers.

## II. NONINTERACTING DIMERS ON A BETHE LATTICE

### A. Geometrical derivation of the exact result

Here we will develop a formula for $\rho$, the average number of dimers per edge on a lattice in terms of the dimer chemical potential $\mu$, or preferably in terms of the parameter $z \equiv e^{\beta\mu}$, where $\beta = 1/(kT)$. (Interactions between dimers and the underlying lattice as well as internal degrees of freedom of the dimer are easily included by a redefinition of $z$.) We will give what we believe to be the simplest possible "geometric" derivation of the well-known[6–8] "Bethe approximation," which has been shown[5] to be surprisingly accurate for some two-dimensional lattices, and which is exact when applied to the Bethe lattice. We assume that only dimers can be adsorbed on the lattice, and that they can be adsorbed only as lying dimers (i.e., an adsorbed dimer covers two lattice sites). In the present section we will assume that there are no interactions between adsorbed dimers except for the hard-core restriction that two dimers cannot touch the same site. It is easy to generalize this treatment to deal with the two-component lattice and also to include the possibility of adsorption of standing dimers and monomers.[28]

As stated in the Introduction, we initially deal with a periodic $d$-dimensional lattice and will obtain the results for the Bethe lattice by introducing an approximation which is exact when the lattice is treelike (i.e., it contains no loops). As a starting point of this discussion we introduce the (unnormalized) probability that there are $N_D$ dimers on the lattice, $W_N(N_D)z^{N_D}$, where $W_N(N_D)$ is the number of distinct configurations of $N_D$ dimers on a lattice of $N$ sites. The equation of state for this dimer system is the relation between $z$ and $\bar{N}_D/N$, where $\bar{N}_D$ is the average value of $N_D$. In the Bethe approximation[6–8]

$$z = \frac{2}{q}\frac{\bar{N}_D}{N}\left(1 - \frac{2\bar{N}_D}{qN}\right)\left(1 - \frac{2\bar{N}_D}{N}\right)^{-2}, \tag{1}$$

where $q$ is number of sites which are nearest neighbors of a given site. To emphasize that this result applies to a Bethe lattice we express it in terms of densities such as $\rho \equiv 2\bar{N}_D/(qN)$, the fraction of bonds (a bond is an edge connecting two sites) covered by a dimer or $q\rho$, the fraction of sites which are covered by a dimer. Stated alternatively, $\rho$ is the probability that a given bond is covered by a dimer and $q\rho$ is the probability that a given site is covered. In terms of these variables the equation of state is

$$z = \rho(1-\rho)(1-q\rho)^{-2} \tag{2}$$

or, equivalently,

$$\rho = \frac{1 + 2qz - \sqrt{1 + 4\sigma z}}{2(1 + q^2 z)}, \tag{3}$$

where $\sigma = q - 1$.

For this discussion it is convenient to define some terminology to describe configurations of dimers on a lattice. In Fig. 2 we show a small section of a lattice where one sees occupied bonds ($D$) on which dimers are placed and unoccupied bonds, which can be of three types depending on whether or not the two sites of the bond are covered by dimers. If both sites of an unoccupied bond are uncovered,

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

the bond is called a "dimer vacancy," ($V$). If both sites of the unoccupied bond are covered, the bond is called (in anticipation of Sec. III where we allow dimer-dimer interactions) an "interacting bond" ($I$), and if only one site of the unoccupied bond is covered, the bond is called a "half bond" ($H$). We first observe that in the thermodynamic limit the average and most probable values of $N_D$ differ negligibly. Thus we may say that the average number of dimers $\bar{N}_D$ is the value of $N_D$ for which the probability $W_N(N_D)z^{N_D}$ is maximal. The condition that this quantity be stationary is

$$\frac{W_N(\bar{N}_D+1)}{W_N(\bar{N}_D)} = \frac{1}{z}. \tag{4}$$

Consider the left-hand side of this equation. From any configuration of $N_D$ dimers we can obtain a configuration of $N_D+1$ dimers by placing an additional dimer on a dimer vacancy. The number of new configurations obtained by placing a dimer on one of the $N_V$ dimer vacancies of each configuration of $N_D$ dimers is thus $\bar{N}_V W_N(N_D)$, where $\bar{N}_V$ is the average number of dimer vacancies for configurations having $N_D$ dimers. However, we note that in this new set of configurations each configuration occurs $N_D+1$ times because each dimer in the new configuration could have been the one newly added. So[29]

$$\frac{W_N(N_D+1)}{W_N(N_D)} = \frac{\bar{N}_V}{N_D+1}, \tag{5}$$

where we will replace $N_D+1$ by $N_D$ in the thermodynamic limit. Applying this for the most probable value of $N_D$ gives the simple result[5]

$$\frac{\bar{N}_V}{\bar{N}_D} = \frac{1}{z}. \tag{6}$$

If we introduce the density of dimer vacancies $\rho_V$ by $\rho_V = \bar{N}_V/N_B$, where $N_B$ is the total number of bonds, then this may be written as

$$\frac{\rho_V}{\rho} = \frac{1}{z}. \tag{7}$$

Note that $\rho$ (or $\rho_V$) is defined to be the total number of dimer (or dimer vacancies) divided by the total number of bonds. These quantities can also be defined locally for a subsystem of bonds. It is not obvious that when $\rho$ and $\rho_V$ are replaced by their local versions, Eq. (7) will still hold. Indeed, for the Ising model on a Cayley tree in an applied field, the total magnetization divided by the total number of sites is not the same as the local magnetization of a single site near the center of the tree. We now argue that $\rho_V/\rho$ does *not* depend on position within the tree. Consider two subsystems[30] $S_1$ and $S_2$ which consist of $N_1$ and $N_2$ bonds, respectively, where $N_1$ and $N_2$ are both large compared to 1 (so that we do not need to worry about discreteness effects). Suppose $\rho_V/\rho$ assumes *different* values within these two subsystems. Then, if we move a dimer from subsystem $S_1$ to subsystem $S_2$, the ratio of the number of configurations $W$ before moving the dimer to that, $W'$, after moving the dimer is

$$\frac{W}{W'} = \frac{\rho_{V1}\rho_2}{\rho_{V2}\rho_1}, \tag{8}$$

where the subscripts identify the subsystem in question. We may view the $\rho_{Vn}$ for subsystem $S_n$ as being order parameters. In order that $W_N(N_D)$ actually be maximal with respect to variation of these order parameters, it must be stationary with respect to moving a dimer. So $W/W'=1$, which implies that $\rho_V/\rho$ is the same for all large subsystems. Thus Eq. (7), which initially involved the ratio of global properties, is actually valid when interpreted as a relation between local quantities.

We now express $\rho_V$ as an explicit function of $\rho$ in a region far from the boundary, so that Eq. (7) yields the equation of state we seek. If $A$ and $B$ are nearest neighboring sites, then

$$\begin{aligned}\rho_V &= P(\text{sites } A \text{ and } B \text{ are vacant})\\ &= P(A \text{ is vacant})\\ &\quad \times P(B \text{ is vacant, given that } A \text{ is vacant})\\ &= (1-q\rho)\times P(B \text{ is vacant, given that } A \text{ is vacant}).\end{aligned} \tag{9}$$

Here the symbol $P(\,)$ denotes the probability of the event inside the parentheses. The basic probability space consists of all configurations of dimers on the lattice. The (unnormalized) probability assigned to a configuration is $z^{N_D}$, where $N_D$ is the number of dimers in the configuration. Equivalently, we could limit our probability space to the set of configurations containing exactly $N_D$ dimers, with all configurations equiprobable. The conditional probability [the last factor in the last line of Eq. (9)] is denoted $P(B \text{ vacant}|A \text{ vacant})$ and is, by definition, equal to $P(B \text{ vacant and } A \text{ vacant})/P(A \text{ vacant})$. More generally, for any two events $E_1$ and $E_2$

$$P(E_2|E_1) = P(E_2 \text{ and } E_1)/P(E_1). \tag{10}$$

We now invoke the approximation in which we replace the factor $P(B \text{ vacant}|A \text{ vacant})$ in Eq. (9) by $P(B \text{ vacant}|\text{bond } AB \text{ unoccupied})$. This replacement ignores the possibility that at most one of the other bonds touching site $A$ might be occupied and thereby might indirectly affect whether site $B$ is occupied or not. Of course this possible inaccuracy can only arise if there is some indirect path from site $A$ to site $B$ not going through the bond $AB$. Since this approximation (which we will refer to as the *tree decoupling*) is exact for the Bethe lattice it leads to the Bethe approximation. Thus

$$\rho_V = (1-q\rho)\times P(B \text{ is vacant}|\text{bond } AB \text{ is unoccupied}). \tag{11}$$

The probability that a particular bond is unoccupied is $1-\rho$, so that

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

$$P(B \text{ vacant}|\text{bond } AB \text{ unoccupied}) = \frac{P(B \text{ vacant and bond } AB \text{ unoccupied})}{P(\text{bond } AB \text{ unoccupied})} = \frac{P(B \text{ vacant and bond } AB \text{ unoccupied})}{(1-\rho)}. \quad (12)$$

If $B$ is vacant, the bond $AB$ must be unoccupied; therefore the numerator of Eq. (12) is just $P(B \text{ vacant}) = 1 - q\rho$. Thus

$$\rho_V = (1-q\rho)^2/(1-\rho), \quad (13)$$

which, in combination with Eq. (7), leads to Eq. (2). We have not succeeded in constructing a simple argument to estimate the magnitude of the difference between $P(B \text{ vacant}|A \text{ vacant})$ and $P(B \text{ vacant}|\text{bond } AB \text{ unoccupied})$ for $d$-dimensional lattices. Qualitatively, the important point is that, within the family of configurations in which bond $AB$ is unoccupied, the probability that site $B$ be vacant is not significantly influenced by the presence of a dimer on (at most) one of the other bonds emanating from $A$.

In Appendix C we present a simple calculation of the major correction to the tree approximation on a planar triangular lattice. However, the calculation is not the first term in a systematic series and is not easily extended to the square lattice. In the next section we will present a formalism which enables one to systematically generate corrections to the tree approximation.

### B. Solution by construction of an effective Hamiltonian

We now apply a technique introduced previously[31] in order to treat here the nonthermal statistical problem of constructing a generating function for covering a lattice with 0, 1, 2, etc., hard-core dimers. We wish to identify this generating function with a partition function, $Z$ of the form $Z = \mathrm{Tr}\exp(-\beta\mathcal{H})$, where $\mathcal{H}$ can then be interpreted as the Hamiltonian for the statistical problem.

The first step in this program is obviously to construct the effective Hamiltonian. This can be done by writing[27]

$$e^{-\beta\mathcal{H}} = e^{\Sigma_{\langle ij\rangle} z s_i s_j}, \quad (14)$$

where $\langle ij\rangle$ indicates that the sum is over pairs of nearest neighbors. For the expansion of the partition function in powers of $z$ to count all possible dimer configurations, where $z$ is the dimer activity, the following *trace rules* are imposed on the operators $s_i$:

$$\mathrm{Tr}_i\, s_i^n = C_n, \quad n = 0, 1, \ldots, \quad (15)$$

where $\mathrm{Tr}_i$ indicates a trace over states of site $i$ and we set $C_0 = C_1 = 1$ and $C_n = 0$ for $n > 1$. It is not actually necessary to explicitly construct such an operator because the only property of these operators we need in order to construct the partition function is the trace rules of Eq. (15). We see that the fact that the trace of two or more operators at the same site vanishes implements exactly the hard-core constraint for dimers. Thus the partition function $Z = \mathrm{Tr}\exp(-\beta\mathcal{H})$ will indeed give the grand partition function for dimers as a function of their chemical potential $\mu$,

$$Z = \sum_{\mathcal{C}} e^{\beta\mu n(\mathcal{C})}, \quad (16)$$

where the sum is over all configurations $\mathcal{C}$ of dimers and $n(\mathcal{C})$ is the number of dimers present in the configuration $\mathcal{C}$. From $Z$ we can get the fraction of sites covered by dimers $\rho$ as a function of the dimer chemical potential via

$$\rho \equiv \frac{2\bar{N}_D}{Nq} = \frac{2}{Nq\beta}\frac{\partial \ln Z}{\partial \mu} = \frac{2}{Nq}\frac{d\ln Z}{d\ln z}. \quad (17)$$

Since the "spin operators" $s_i$ commute with one another, we have a mapping of the athermal problem of dimers on a lattice into a statistical mechanical problem involving classical spins with a given Hamiltonian.

Now we use this mapping to (a) construct the exact solution for the partition function for a Bethe lattice and (b) generate series expansions for finite dimensional lattices. To do that we develop a perturbation theory for a periodic lattice in which the leading term contains the sum of all contributions from tree diagrams. For this purpose we write $Z = \mathrm{Tr}\,\Pi_{\langle ij\rangle} f_{ij}$, where $f_{ij} = 1 + z s_i s_j$ [the trace rules allow us to linearize the exponential in Eq. (14)] or equivalently

$$Z = \mathrm{Tr}\left\{\left[\prod_i g_i^q\right]\left[\prod_{\langle ij\rangle}\frac{f_{ij}}{g_i g_j}\right]\right\}, \quad (18)$$

where $g$ can be chosen arbitrarily. We evaluate this perturbatively as

$$Z = \mathrm{Tr}\left\{\left[\prod_i g_i^q\right]\left[\prod_{\langle ij\rangle} 1 + \lambda V_{ij}\right]\right\}, \quad (19)$$

where $V_{ij} = f_{ij}/(g_i g_j) - 1$. We expand in powers of $\lambda$ which we set equal to unity at the end. Each term in this expansion which involves at least one power of $\lambda$ can be associated with a diagram in which the factor $V_{ij}$ is associated with a line connecting sites $i$ and $j$. We now choose $g$ so that diagrams having at least one line which is connected to only a single site ($j$) give zero contribution. Since all diagrams on a Bethe lattice have at least one free end, this choice of $g$ will lead to an exact evaluation of the partition function for a Bethe lattice and will enable us to generate loop corrections for $d$-dimensional lattices. The condition we implement is that

$$\mathrm{Tr}_j(g_j^q V_{ij}) = 0, \quad (20)$$

which can be written in the form

$$g_i = \frac{\mathrm{Tr}_j(f_{ij} g_j^\sigma)}{\mathrm{Tr}_j\, g_j^q}, \quad (21)$$

where $\sigma = q - 1$. This is a nonlinear equation for the function $g_j$, but in view of the trace rules it is easily solved. From the form of $f_{ij}$ one sees that $g_i$ has to be of the form

$$g_i = A + B s_i. \quad (22)$$

By substituting this form into Eq. (21),

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

$$A + Bs_i = \frac{\mathrm{Tr}_j[(1 + zs_is_j)(A + Bs_j)^\sigma]}{\mathrm{Tr}_j(A + Bs_j)^q}. \tag{23}$$

Using the trace rules we rewrite the right-hand side of this equation so that

$$A + Bs_i = \frac{A^\sigma + \sigma A^{\sigma-1}B + s_i(zA^\sigma)}{A^q + qA^\sigma B}. \tag{24}$$

This gives rise to the two equations

$$A = \frac{A^\sigma + \sigma A^{\sigma-1}B}{A^q + qA^\sigma B} = \frac{A + \sigma B}{A^2 + qAB}, \tag{25}$$

$$B = \frac{zA^\sigma}{A^q + qA^\sigma B} = \frac{z}{A + qB}. \tag{26}$$

We may solve Eq. (25) for $B$ as

$$B = \frac{A^3 - A}{\sigma - qA^2}. \tag{27}$$

Substituting this into Eq. (26) leads to

$$A^4(1 + q^2z) - A^2(2q\sigma z + 1) + z\sigma^2 = 0. \tag{28}$$

Thus

$$A^2 = \frac{2qz\sigma + 1 + \sqrt{1 + 4z\sigma}}{2(1 + q^2z)}. \tag{29}$$

(We chose the positive sign before the square root to ensure that $A \to 1$ as $z \to 0$.) Then for the Bethe lattice we have the exact result

$$Z^{1/N} = \mathrm{Tr}_i\, g_i^q = \mathrm{Tr}_i\, [A + Bs_i]^q = A^q + qBA^\sigma. \tag{30}$$

After some algebra it can be shown that when this result is inserted into Eq. (17) we recover the result of Eq. (3).

Unfortunately, this formalism leads to an expansion of the partition function $Z$, whereas for $d$-dimensional lattices, we would prefer to have an expansion for the free energy per site, $F=(1/N)\ln Z$. For that purpose we consider an expansion of the quantity $Z^n$, which in the limit $n \to 0$ is $1 + n \ln Z = 1 + nNF$. To obtain $Z^n$ we introduce the $n$-replicated Hamiltonian

$$e^{-\beta\mathcal{H}_n} = \prod_{\alpha=1}^{n} \prod_{\langle ij \rangle} [1 + zs_{i\alpha}s_{j\alpha}], \tag{31}$$

where $s_{i\alpha}$ and $s_{i\beta}$ are independent operators for $\alpha \neq \beta$ and for each replica index $s_{i\alpha}$ obeys the same trace rules as in Eq. (15). Usually replicas are introduced to perform the quenched average (over $\ln Z$) for random problems in which case the averaging leads to interactions between different replicas. Here we introduce replicas simply to facilitate construction of an expansion of $\ln Z$ and there are no interactions between different replicas. The partition function, $Z_{\mathrm{rep}}$, associated with the replicated Hamiltonian is

$$Z_{\mathrm{rep}} \equiv \mathrm{Tr}\, e^{-\beta\mathcal{H}_n} = Z^n. \tag{32}$$

Thus we solve Eq. (21) with $f_{ij} = \Pi_\alpha(1 + zs_{i\alpha}s_{j\alpha})$. Because different replicas are independent of one another, the solution to Eq. (21) is of the form

$$g_i = C\prod_{\alpha=1}^{n} [1 + Ds_{i\alpha}] \equiv C\hat{g}_i. \tag{33}$$

Because we need the partition function $Z_{\mathrm{rep}}$ to order $n$,[32] we must evaluate $C$ up to linear order in $n$ but $D$ can be evaluated for $n=0$ because it always appears in connection with a sum over replica indices which give a factor of $n$. The terms in $g_i$ in Eq. (21) independent of $s_{i\alpha}$ give

$$C = \mathrm{Tr}_j\, C^\sigma \hat{g}_j^\sigma / \mathrm{Tr}_j\, C^q \hat{g}_j^q \tag{34}$$

or

$$C^2 = \mathrm{Tr}_j\, \hat{g}_j^\sigma / \mathrm{Tr}_j\, \hat{g}_j^q = (1 + \sigma D)^n/(1 + qD)^n, \tag{35}$$

which to linear order in $n$ gives

$$C = 1 + \frac{n}{2} \ln\left(\frac{1 + \sigma D}{1 + qD}\right). \tag{36}$$

The terms in $g_i$ in Eq. (21) linear in $s_{i\alpha}$ give

$$CD = \frac{z\, \mathrm{Tr}_j\, C^\sigma s_{j\alpha} \Pi_\beta (1 + Ds_{j\beta})^\sigma}{\mathrm{Tr}_j\, C^q \Pi_\beta (1 + Ds_{j\beta})^q}. \tag{37}$$

For $n=0$ this is

$$D = z(1 + \sigma D)^{-1}, \tag{38}$$

which gives

$$D = \frac{-1 + r}{2\sigma}, \tag{39}$$

where $r \equiv \sqrt{1 + 4\sigma z}$.

Then the first term in the expansion of $F$ is

$$F = \frac{d}{dn}[\mathrm{Tr}_j(C\hat{g}_j)^q]_{n=0} = \frac{q}{2} \ln\left(\frac{1 + \sigma D}{1 + qD}\right) + \ln(1 + qD). \tag{40}$$

After some algebra one can show that when this is substituted into Eq. (17) we recover Eq. (2).

### C. Loop corrections

Here we consider the expansion in powers of $V_{ij} \equiv f_{ij}/(g_ig_j) - 1$. Our first objective is to show that contributions to $Z_{\mathrm{rep}}$ from disconnected diagrams are of order $n^2$ or higher and hence can be dropped. To see this we write

$$V_{ij} = C^{-2}\prod_\alpha ([1 + zs_{i\alpha}s_{j\alpha}][1 - Ds_{i\alpha}][1 - Ds_{j\alpha}]) - 1. \tag{41}$$

The contribution to $Z_{\mathrm{rep}}$ from a disconnected diagram is simply the product of the contributions from each connected component. We now argue that the contribution to $Z_{\mathrm{rep}}$ from a single connected diagram is of order $n$. Note that $V_{ij}$ is a multinomial in the $s_\alpha$'s whose constant term is proportional to $n$. Thus the contribution to $Z_{\mathrm{rep}}$ will get at least one factor of $n$, either from the constant term in a $V_{ij}$, or from a sum over replica indices from terms in a $V_{ij}$ involving an $s$ operator. Thus using the $n \to 0$ limit of the replica formalism we have eliminated unlinked diagrams.

Now we consider the leading loop corrections to $Z^n$. These come from the smallest loops that can be drawn on the

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

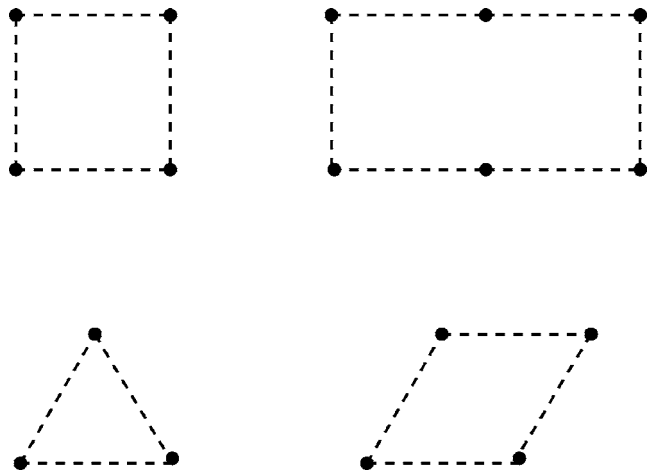

FIG. 3. Leading loop corrections to $Z^n$ for the hypercubic lattice (top) and for the plane triangular lattice (bottom).

lattice. In Fig. 3 we show these loops for both the $d$-dimensional hypercubic lattice and the plane triangular lattice. Here we will explicitly evaluate only the corrections from the smallest possible loop diagrams.

We will now show that this expansion involves evaluating a modified dimer partition function for diagrams with no free ends. The contribution to the replica partition function from such a diagram $\Gamma$ is given by

$$\delta Z_{\text{rep}}(\Gamma) = \text{Tr}\left\{\prod_{i\in\Gamma} g_i^q \prod_{\langle ij\rangle\in\Gamma}\left(\frac{f_{ij}}{g_i g_j} - 1\right)\right\} = n\,\delta F(\Gamma) + \mathcal{O}(n^2). \tag{42}$$

The notation $i\in\Gamma$ means that the site $i$ is a site covered by at least one bond of $\Gamma$. We do not change the result for $\delta F(\Gamma)$ if we divide this by a quantity which differs from unity by terms of order $n$. So, for later convenience we write

$$\delta Z_{\text{rep}}(\Gamma) = \frac{\text{Tr}\{\Pi_{i\in\Gamma} g_i^q \Pi_{\langle ij\rangle\in\Gamma}(f_{ij}/g_i g_j - 1)\}}{\text{Tr}\,\Pi_{i\in\Gamma} g_i^q}. \tag{43}$$

We now expand the product over bonds, into its $2^{N_B(\Gamma)}$ terms, where $N_B(\Gamma)$ is the number of bonds in the set $\Gamma$. In so doing note that when considered as a multinomial series in $\{s_{i\alpha}\}$, each term has the limiting value unity as $n\to 0$ (but the sum of all $2^{N_B}$ terms is zero in this limit). Since we are interested in the limit $n\to 0$, we consider $d\delta Z_{\text{rep}}(\Gamma)/dn$ (evaluated at $n=0$) and write

$$\frac{d\delta Z_{\text{rep}}(\Gamma)}{dn} = \sum_{\gamma\in\Gamma}(-1)^{N_B(\Gamma)-N_B(\gamma)} G(\gamma), \tag{44}$$

where the sum is over the $2^{N_B(\Gamma)}-1$ nonempty subsets $\gamma$ of $\Gamma$, including $\gamma=\Gamma$. (The term corresponding to the empty set is unity and therefore drops out when differentiated with respect to $n$.) Here

$$G(\gamma) = \frac{d}{dn}\left[\frac{\text{Tr}\Pi_{i\in\gamma} g_i^q \Pi_{\langle ij\rangle\in\gamma}(f_{ij}/g_i g_j)}{\text{Tr}\Pi_{i\in\gamma} g_i^q}\right]. \tag{45}$$

Because we divided by the factor in the denominator, it is no longer necessary to involve sites in $\Gamma$ which are not in $\gamma$. The subtractions of subdiagrams indicated in Eq. (44) define the cumulant operation (indicated by a subscript $c$), so we write

$$\delta F(\Gamma) = G_c(\Gamma), \tag{46}$$

where $G_c(\Gamma)$ is the right-hand side of Eq. (44). This representation is not very efficient because it contains $2^{N_B(\Gamma)}-1$ terms, many of which are either zero or are identical to one another. The following equivalent recursive definition is more convenient:

$$G_c(\gamma) = G(\gamma) - \sum_{\gamma'\in\gamma}{}' G_c(\gamma'), \tag{47}$$

where the prime indicates that in the sum over subsets $\gamma'$ we do not include $\gamma'=\gamma$. For the smallest loop on a hypercubic lattice, namely, a square of four bonds, there are no nonzero subtractions and $G_c(\gamma)$ is equal to its "bare" value $G(\gamma)$. More generally Eq. (47) has many fewer terms than Eq. (44) and furthermore, all the cumulants of the subdiagrams will have been previously calculated in a lower order calculation. So, to implement the cumulant subtraction we only need to subtract the cumulant contributions of subgraphs with no free ends.

It remains to discuss the calculation of $G(\gamma)$. We take

$$g_i = C\prod_\alpha(1+Ds_{i\alpha}) \equiv C\prod_\alpha \hat{g}_{i\alpha} \tag{48}$$

and

$$f_{ij} = \prod_\alpha(1+zs_{i\alpha}s_{j\alpha}) \equiv \prod_\alpha f_{ij;\alpha}. \tag{49}$$

Then

$$G(\gamma) = \frac{d}{dn}\left[\frac{C^{-2N_B(\gamma)}\Pi_\alpha \text{Tr}\Pi_{i\in\gamma}\hat{g}_{i\alpha}^q \Pi_{\langle ij\rangle\in\gamma}(f_{ij;\alpha}/\hat{g}_{i\alpha}\hat{g}_{j\alpha})}{\Pi_\alpha \text{Tr}\Pi_{i\in\gamma}\hat{g}_{i\alpha}^q}\right] = \frac{d}{dn}[C^{-2N_B(\gamma)}(1+qD)^{-N_s(\gamma)n}Q(\gamma)^n], \tag{50}$$

where $N_s(\gamma)$ is the number of sites in $\gamma$ and $Q(\gamma)$ is a partition function for the graph $\gamma$,

$$Q(\gamma) = \text{Tr}\left[\prod_{i\in\gamma}(1+Ds_i)^q \prod_{\langle ij\rangle\in\gamma}\frac{1+zs_is_j}{(1+Ds_i)(1+Ds_j)}\right] = \text{Tr}\left[\prod_{i\in\gamma}(1+Ds_i)^{q-q_i(\gamma)}\prod_{\langle ij\rangle\in\gamma}(1+zs_is_j)\right], \tag{51}$$

where $q_i(\gamma)$ is the number of sites neighboring to $i$ which are connected to $i$ by a bond in $\gamma$. Because of the trace rules, the product over sites mimics a site-dependent monomer activity $z_i \equiv 1+[q-q_i(\gamma)]D$ and we therefore have

$$Q(\gamma) = \left[\prod_{i\in\gamma} z_i\right]\hat{Q}(\gamma; z_{ij} = z/(z_iz_j)), \tag{52}$$

where $\hat{Q}$ is the grand partition function for the set of bonds $\gamma$ in which the bond $\langle ij\rangle$ has the bond-dependent activity $z_{ij} \equiv z/(z_iz_j)$,

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

$$\hat{Q}(\gamma;\{z_{ij}\}) = \mathrm{Tr} \prod_{\langle ij\rangle \in \gamma} (1 + z_{ij} s_i s_j). \tag{53}$$

Thus the renormalized free energy associated with a diagram with no free ends is only slightly more complicated than its unrenormalized ($g_i=1$) value. To summarize,

$$G(\gamma) = -N_s(\gamma)\ln(1+qD) + N_B(\gamma)\ln\left(\frac{1+qD}{1+\sigma D}\right) + \sum_{i\in\gamma} \ln(1+[q-q_i(\gamma)]D) + \ln \hat{Q}(\gamma;\{z_{ij}\}). \tag{54}$$

It is a remarkable fact that for a diagram $\gamma$ with no loops, $G(\gamma)$ vanishes and this forms a nice check of computer programs used to evaluate $G(\gamma)$ for an arbitrary diagram. (This is easy to check for small diagrams.) Furthermore, for a diagram with loops and which has a free end, $G(\gamma)$ does *not* vanish, but its cumulant $G_c(\gamma)$ *does* vanish. (This is also a nice check of computer programs.)

For the hypercubic lattice we consider the leading correction from a square of four nearest neighbor bonds, $\gamma$. So we use Eq. (54) with $q=4$ and $q_i(\gamma)=2$, so that $z_{ij}=z/(1+2D)^2$. Then $\hat{Q}(\gamma)=1+4z_{ij}+2z_{ij}^2$ and

$$\begin{aligned} G(\gamma) &= 4\ln(1+2D) - 4\ln(1+4D) + 4\ln\left(\frac{1+4D}{1+3D}\right) + \ln\left[1 + \frac{4z}{(1+2D)^2} + \frac{2z^2}{(1+2D)^4}\right] \\ &= -4\ln(1+3D) + \ln\left[(1+2D)^4 + 4z(1+2D)^2 + 2z^2\right]. \end{aligned} \tag{55}$$

Now use $1+3D=z/D$ from Eq. (38), so that

$$\begin{aligned} G(\gamma) &= \ln\left[\left(1-\frac{D^2}{z}\right)^4 + 4\frac{D^2}{z}\left(1-\frac{D^2}{z}\right)^2 + 2\frac{D^4}{z^2}\right] \\ &= \ln\left[1+\frac{D^8}{z^4}\right]. \end{aligned} \tag{56}$$

For $z$, small $D$ is proportional to $z$ and this diagram gives a contribution to the free energy of order $z^4$. Since there are $d(d-1)/2$ squares per site, the perturbative contribution to the free energy per site is

$$\delta F = \frac{1}{2}d(d-1)\ln\left[1+\frac{D^8}{z^4}\right]. \tag{57}$$

The dimer density then follows using Eq. (17) and the results are given in Table I for a square lattice.

We now identify the expansion parameters in this formulation. It is clear that the free energy, $F$, is obtained as a sum of contributions associated with diagrams having no free ends, the smallest of which are shown in Fig. 3. This development will lead to an evaluation of $F$ as a power series in the activity,

$$F = \sum_n F_n z^n. \tag{58}$$

From Eq. (40) we see that for the Bethe lattice and for large $qF_n \sim q^n/n$. We assert that the contributions to $F_n$ from a diagram $\gamma$ [which we denote $\delta F(\gamma)$] are of order

$$\delta F_n(\gamma)/F_n \sim q^{-r(\gamma)}, \tag{59}$$

where $r(\gamma)$ is an integer which increases with the size and complexity of the diagram. For instance, for a square of four bonds Eq. (57) indicates that $r=2$ and for a loop of $2n$ bonds a similar result shows that $r=n$. So our diagrammatic formulation generates corrections in inverse powers of $q$. Furthermore, if one expands $f_{ij}$ and $g_i$ in powers of $z$, one sees that $V_{ij}$ is of order $z$. This means that a diagram $\gamma$ with $N_B(\gamma)$ bonds contributes to $F(q)$ at order $z^{N_B(\gamma)}$ *and higher*. So our formulation involves the two expansion parameters $z$ and $1/q$.

An entirely analogous calculation gives the leading loop correction for the triangular lattice from triangles as

$$\delta F = N_T \ln\left[1-\frac{D^6}{z^3}\right], \tag{60}$$

where $N_T=2$ is the number of triangles per site. Thus we see that the leading correction to the Bethe lattice result has the opposite sign for triangular lattices as compared to hypercubic lattices. The results based on Eq. (60) are given in Table II.

The present development appears to be related to that of Ref. 21, but the detailed relationship of the two approaches is

TABLE I. First loop correction for the square lattice for the density of dimers ($\pi \equiv \bar{N}_D/N$) as a function of $z$. Here $\pi_0$ is the value for the Bethe lattice for $q=4$, $\pi_1$ is the value when the first loop correction, Eq. (57), is included, and $\pi_E$ is the "exact" result obtained by extrapolation (Ref. 5) of the series of Gaunt (Ref. 22).

| $z$ | $\pi_0$ | $\pi_1$ | $\pi_E$ |
|---|---|---|---|
| 0.005 180 | 0.010 000 | 0.010 000 | 0.010 000 |
| 0.010 742 | 0.020 000 | 0.020 000 | 0.020 000 |
| 0.023 156 | 0.039 999 | 0.039 999 | 0.040 000 |
| 0.037 575 | 0.059 997 | 0.060 000 | 0.060 000 |
| 0.054 413 | 0.079 990 | 0.080 000 | 0.080 000 |
| 0.074 195 | 0.099 978 | 0.100 000 | 0.100 000 |
| 0.097 587 | 0.119 954 | 0.119 999 | 0.120 000 |
| 0.125 452 | 0.139 917 | 0.139 998 | 0.140 000 |
| 0.158 915 | 0.159 862 | 0.159 996 | 0.160 000 |
| 0.199 466 | 0.179 784 | 0.179 991 | 0.180 000 |
| 0.249 111 | 0.199 679 | 0.199 982 | 0.200 000 |
| 0.310 597 | 0.219 543 | 0.219 968 | 0.220 000 |
| 0.387 766 | 0.239 370 | 0.239 945 | 0.240 000 |
| 0.486 115 | 0.259 158 | 0.259 909 | 0.260 000 |
| 0.613 728 | 0.278 904 | 0.279 857 | 0.280 000 |
| 0.782 881 | 0.298 607 | 0.299 783 | 0.300 000 |
| 1.012 941 | 0.318 271 | 0.319 684 | 0.320 000 |
| 1.335 914 | 0.337 903 | 0.339 556 | 0.340 000 |
| 1.807 776 | 0.357 516 | 0.359 397 | 0.360 000 |
| 2.533 661 | 0.377 128 | 0.379 204 | 0.380 000 |
| 3.730 072 | 0.396 761 | 0.398 970 | 0.400 000 |
| 5.902 289 | 0.416 436 | 0.418 682 | 0.420 000 |
| 10.466 788 | 0.436 180 | 0.438 318 | 0.440 000 |
| 22.802 101 | 0.456 068 | 0.457 892 | 0.460 000 |
| 81.673 705 | 0.476 432 | 0.477 641 | 0.480 000 |

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

TABLE II. First loop correction for the triangular lattice. The notation is as in Table I, but where $\pi_1$ includes the loop correction of Eq. (60) and $\pi_G$ includes the loop correction derived geometrically in Appendix C.

| $z$ | $\pi_0$ | $\pi_1$ | $\pi_E$ | $\pi_G$ |
|---|---|---|---|---|
| 0.003 459 | 0.009 999 | 0.009 999 | 0.010 000 | 0.009 999 |
| 0.011 206 | 0.030 004 | 0.029 999 | 0.030 000 | 0.029 999 |
| 0.025 331 | 0.060 040 | 0.059 998 | 0.060 000 | 0.059 997 |
| 0.043 360 | 0.090 121 | 0.089 991 | 0.090 000 | 0.089 987 |
| 0.066 712 | 0.120 261 | 0.119 975 | 0.120 000 | 0.119 962 |
| 0.097 473 | 0.150 457 | 0.149 943 | 0.150 000 | 0.149 912 |
| 0.138 811 | 0.180 705 | 0.179 892 | 0.180 000 | 0.179 831 |
| 0.195 705 | 0.210 994 | 0.209 822 | 0.210 000 | 0.209 712 |
| 0.276 329 | 0.241 312 | 0.239 741 | 0.240 000 | 0.239 559 |
| 0.394 826 | 0.271 650 | 0.269 667 | 0.270 000 | 0.269 386 |
| 0.577 329 | 0.302 001 | 0.299 629 | 0.300 000 | 0.299 221 |
| 0.876 264 | 0.332 353 | 0.329 663 | 0.330 000 | 0.329 101 |
| 1.408 720 | 0.362 668 | 0.359 786 | 0.360 000 | 0.359 056 |
| 2.477 977 | 0.392 849 | 0.389 972 | 0.390 000 | 0.389 084 |
| 5.067 826 | 0.422 724 | 0.420 118 | 0.420 000 | 0.419 135 |
| 13.932 546 | 0.452 078 | 0.450 085 | 0.450 000 | 0.449 161 |
| 91.850 988 | 0.480 860 | 0.479 893 | 0.480 000 | 0.479 338 |

not clear to us. We note that the disconnected diagram of Fig. 3(d) of Nagle[21] (which "is required" for his dimer series) does not appear in our approach.

## D. ANISOTROPY

We may generalize the above model to allow for different activities along different coordinate axes. (The dimers all come from a common reservoir but have different interaction energies with the horizontal and vertical bonds.) For that purpose we relate the square lattice to a Bethe lattice in which each site is surrounded by four bonds, two of which we arbitrarily label as "horizontal" (or $x$) bonds and the others as "vertical" (or $y$) bonds. The unnormalized probability of a particular configuration with $N_x$ horizontal dimers and $N_y$ vertical dimers is $z_x^{N_x} z_y^{N_y}$. If the chemical potential of a dimer is $\mu$ and the interaction energy of a dimer with the underlying bond is $\epsilon_\alpha$ ($\alpha = x, y$), then $z_\alpha = e^{\beta(\mu-\epsilon_\alpha)}$. The fraction of $\alpha$ bonds covered by dimers will be denoted $\rho_\alpha$ and the fraction of $\alpha$ bonds which are dimer vacancies will be denoted $\rho_{V\alpha}$

### 1. Geometrical approach

The geometrical reasoning used before yields

$$z_\alpha^{-1} = \rho_{V\alpha}/\rho_\alpha. \tag{61}$$

The tree approximation, which is exact for the Bethe lattice, then yields

$$\rho_{V\alpha} = W/(1-\rho_\alpha), \tag{62}$$

where $W^{1/2}$ is the probability that a given site is vacant, where

$$W = (1 - 2\rho_x - 2\rho_y)^2, \tag{63}$$

so that

$$\frac{\rho_x(1-\rho_x)}{z_x} = \frac{\rho_y(1-\rho_y)}{z_y} = W. \tag{64}$$

Thus

$$\rho_\alpha = [1 - \sqrt{1 - 4z_\alpha W}]/2 \tag{65}$$

and

$$W = (\sqrt{1-4z_x W} + \sqrt{1-4z_y W} - 1)^2. \tag{66}$$

This equation allows one to calculate $W$ as a function of $z_x$ and $z_y$, from which all the other relevant quantities can be obtained.

### 2. Algebraic approach

We use the Hamiltonian

$$e^{-\beta\mathcal{H}} = \prod_{\langle ij\rangle \in H} [1 + z_x s_i s_j] \prod_{\langle ij\rangle \in V} [1 + z_y s_i s_j], \tag{67}$$

where the sum $\in H$ means we sum over horizontal ($x$) bonds and similarly for $\in V$. The operators $s_i$ obey the same trace rules as before. We write the partition function as

$$Z = \mathrm{Tr} \prod_i g_{ix}^2 g_{iy}^2 \prod_{\langle ij\rangle} [1 + V_{ij}], \tag{68}$$

where for horizontal bonds

$$V_{ij} = [1 + z_x s_i s_j]/g_{ix} g_{jx} - 1 \tag{69}$$

and for vertical bonds

$$V_{ij} = [1 + z_y s_i s_j]/g_{iy} g_{jy} - 1. \tag{70}$$

Now we expand in powers of $V_{ij}$ and require that diagrams with either a vertical or a horizontal free end vanish. For horizontal bonds we require that

$$\mathrm{Tr}_j\, g_{jx}^2 g_{jy}^2 V_{ij} = 0, \tag{71}$$

so that

$$g_{ix} = \frac{\mathrm{Tr}_j\, g_{jx} g_{jy}^2 [1 + z_x s_i s_j]}{\mathrm{Tr}_j\, g_{jx}^2 g_{jy}^2}. \tag{72}$$

For vertical bonds we require that

$$\mathrm{Tr}_j\, g_{jx}^2 g_{jy}^2 V_{ij} = 0, \tag{73}$$

so that

$$g_{ix} = \frac{\mathrm{Tr}_j\, g_{jx}^2 g_{jy} [1 + z_y s_i s_j]}{\mathrm{Tr}_j\, g_{jx}^2 g_{jy}^2}. \tag{74}$$

These equations have a solution of the form

$$g_{i\alpha} = A_\alpha + B_\alpha s_i. \tag{75}$$

Thus

$$A_x + B_x s_i = \frac{\mathrm{Tr}_j [1 + z_x s_i s_j][A_x + B_x s_j][A_y + B_y s_j]^2}{\mathrm{Tr}_j [A_x + B_x s_j]^2 [A_y + B_y s_j]^2} = \frac{A_x A_y^2 + B_x A_y^2 + 2A_x A_y B_y + s_i z_x A_x A_y^2}{A_x^2 A_y^2 + 2A_x B_x A_y^2 + 2A_x^2 A_y B_y} \tag{76}$$

and

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

$$A_y + B_y s_i = \frac{\mathrm{Tr}_j[1 + z_y s_i s_j][A_x + B_x s_j]^2[A_y + B_y s_j]}{\mathrm{Tr}_j[A_x + B_x s_j]^2[A_y + B_y s_j]^2} = \frac{A_x^2 A_y + 2A_x B_x A_y + A_x^2 B_y + s_i z_y A_x^2 A_y}{A_x^2 A_y^2 + 2A_x B_x A_y^2 + 2A_x^2 A_y B_y}. \tag{77}$$

Thus if we set $B_x = b_x A_x$ and $B_y = A_y b_y$, then

$$A_x^2 = \frac{1 + b_x + 2b_y}{1 + 2b_x + 2b_y},$$
$$A_y^2 = \frac{1 + 2b_x + b_y}{1 + 2b_x + 2b_y},$$
$$A_x^2 b_x = \frac{z_x}{1 + 2b_x + 2b_y},$$
$$A_y^2 b_y = \frac{z_y}{1 + 2b_x + 2b_y}. \tag{78}$$

Thus

$$b_x = \frac{z_x}{1 + b_x + 2b_y},$$
$$b_y = \frac{z_y}{1 + 2b_x + b_y}. \tag{79}$$

These equations reproduce those from the geometrical approach if one makes the identification

$$\rho_\alpha = b_\alpha / [1 + 2b_x + 2b_y] \tag{80}$$

and

$$W = (1 + 2b_x + 2b_y)^{-2}. \tag{81}$$

The density of dimer bonds along $\alpha$ is given by

$$\rho_\alpha = \frac{1}{N}\frac{\partial Z}{\partial z_\alpha} z_\alpha = z_\alpha \frac{\partial}{\partial z_\alpha} \ln(A_x^2 A_y^2 [1 + 2b_x + 2b_y]). \tag{82}$$

This can be shown to be equivalent to Eq. (64). Thus we conclude that the algebraic approach agrees with the much simpler geometrical approach. But, in principle, the algebraic approach can be used to generate corrections to the tree approximation for $d$-dimensional lattices.

## III. INTERACTING DIMERS

### A. Geometrical derivation of the exact result

Here we consider the case when two dimers separated by a single bond (an interacting bond as shown in Fig. 1) have an interaction energy $-\alpha$. Thus the energy of a configuration of dimers on the lattice is $-N_I\alpha$, where $N_I$ is the number of interacting bonds. We start by expressing $N_I$ in terms of $N_V$. For that purpose we record the following sum rules for periodic lattices. The first sum rule expresses the fact that each bond is uniquely a member of one of the four sets shown in Fig. 1, so that the total number of bonds of the lattice $N_B$ is given by

$$N_V + N_I + N_D + N_H = N_B = Nq/2, \tag{83}$$

where $N_H$ is the number of half bonds (see Fig. 1). The second sum rule is obtained by imagining putting a stick on each of the $q$ bonds emanating from each occupied site. The total number of sticks is obviously $q(2N_D)$. Each half bond has one stick, whereas each interacting bond and each dimer bond is covered by two sticks, so that

$$2qN_D = N_H + 2N_I + 2N_D. \tag{84}$$

Combining these two relations we get

$$N_I = -Nq/2 + (2q-1)N_D + N_V. \tag{85}$$

Thus the probability $P(N_D)$ that there are $N_D$ dimers on the lattice is

$$P(N_D) = Q^{-1}\sum_{\mathcal{G}} e^{\beta\alpha N_I} z^{N_D} = \mathrm{const}[z e^{\beta\alpha(2q-1)}]^{N_D} \sum_{\mathcal{G}} e^{\beta\alpha N_V(\mathcal{G})}, \tag{86}$$

where $Q$ is the partition function, the sum over $\mathcal{G}$ runs over all configurations with $N_D$ dimers on the lattice, and $N_V(\mathcal{G})$ is the number of dimer vacancies in the graph $\mathcal{G}$. Similarly

$$P(N_D + 1) = \mathrm{const} \times [z e^{\beta\alpha(2q-1)}]^{N_D+1} \sum_{\mathcal{G}'} e^{\beta\alpha N_V(\mathcal{G}')}, \tag{87}$$

where the sum over $\mathcal{G}'$ runs over all the graphs with $N_D+1$ dimers on the lattice. Let $\mathcal{G}''(\mathcal{G})$ be a graph formed by adding an additional dimer to a graph $\mathcal{G}$. The additional dimer is, of course, placed on one of the dimer vacancies $AB$ in the graph $\mathcal{G}$. The number of vertices adjacent to $A$ (excluding $B$) is $\sigma$, and the number of vertices adjacent to $B$ (excluding $A$) is also $\sigma$. If $m$ of these $2\sigma$ vertices are vacant, then the number of dimer vacancies in the graph $\mathcal{G}''(\mathcal{G})$ is $N_V(\mathcal{G}) - m - 1$. If we look at all the different graphs $\mathcal{G}''(\mathcal{G})$ which can be generated by adding a dimer to a particular graph $\mathcal{G}$, $m$ assumes the values $(1, \ldots, 2\sigma)$ with the respective probabilities $p(m)$ which we shall calculate. Furthermore, since it is quite clear that the configurations of two small subsections of a large graph $\mathcal{G}$ which are distant from each other are statistically independent, we assert that the probability distribution $p(m)$ is the same for almost all graphs $\mathcal{G}$ [but $p(m)$ does depend on $N_D/N$ which has the same value for all the graphs $\mathcal{G}$]. Thus for almost all graphs $\mathcal{G}$ we have

$$\sum_{\mathcal{G}''(\mathcal{G})} e^{\beta\alpha N_V[\mathcal{G}''(\mathcal{G})]} = N_V(\mathcal{G}) e^{\beta\alpha N_V(\mathcal{G})} \sum_{m=0}^{2\sigma} p(m) e^{-\beta\alpha(m+1)}. \tag{88}$$

If $\{\mathcal{G}''(\mathcal{G})\}$ is the set of all graphs which can be generated by adding a dimer to a particular graph $\mathcal{G}$, and $\Sigma_{\mathcal{G}}\{\mathcal{G}''(\mathcal{G})\}$ is the set which is the union of all the sets $\{\mathcal{G}''(\mathcal{G})\}$, then $\Sigma_{\mathcal{G}}\{\mathcal{G}''(\mathcal{G})\}$ is identical to the set of graphs $\{\mathcal{G}'\}$, except that each graph $\mathcal{G}'$ occurs $N_D+1$ times in the union (since each graph $\mathcal{G}'$ has $N_D+1$ "ancestors" $\mathcal{G}$ which can be obtained by removing a single dimer). Thus we obtain

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

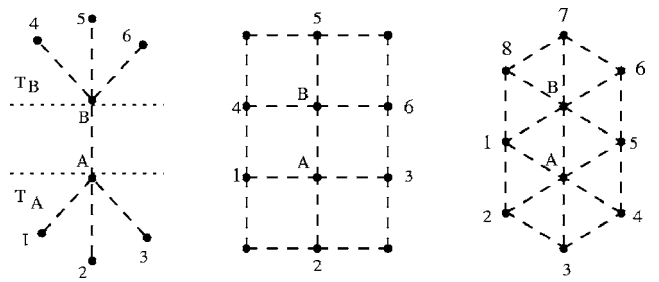


FIG. 4. Left: the bond $AB$ and its environment in a Bethe lattice with $q=4$. The subsystems $T_A$ and $T_B$ are the regions outside the dotted lines. We show the sites neighboring to $A$ and $B$, which are numbered 1–6 $(1-2\sigma)$. There are no indirect paths connecting any pairs of numbered sites which do not pass through $A$ and/or $B$. Middle: environment of a bond $AB$ on a square lattice where we show indirect paths which connect adjacent numbered sites, in which case the strong form of tree decoupling is not exact. Right: environment of a bond $AB$ on a triangular lattice. Here the decoupling is worse than for a square lattice because (a) there are nearest neighbor bonds connecting numbered sites and (b) some neighbors of $A$ are simultaneously neighbors of $B$.

$$
\begin{aligned}
(N_D+1)\sum_{\mathcal{G}'} e^{\beta\alpha N_V(\mathcal{G}')} &= \sum_{\mathcal{G}}\sum_{\mathcal{G}''(\mathcal{G})} e^{\beta\alpha N_V[\mathcal{G}''(\mathcal{G})]} \\
&= \left(\sum_{m=0}^{2\sigma} p(m)e^{-\beta\alpha(m+1)}\right) \\
&\quad\times\sum_{\mathcal{G}} N_V(\mathcal{G})e^{\beta\alpha N_V(\mathcal{G})} \\
&= \left(\sum_{m=0}^{2\sigma} p(m)e^{-\beta\alpha(m+1)}\right)\bar{N}_V(N_D) \\
&\quad\times\sum_{\mathcal{G}} e^{\beta\alpha N_V(\mathcal{G})},
\end{aligned}
\tag{89}
$$

where

$$
\bar{N}_V(N_D) = \sum_{\mathcal{G}} N_V(\mathcal{G})e^{\beta\alpha N_V(\mathcal{G})} \Big/ \sum_{\mathcal{G}} e^{\beta\alpha N_V(\mathcal{G})}. \tag{90}
$$

For a given value of $z$, the value of $N_D$ which maximizes $P(N_D)$ satisfies the condition $P(N_D+1)/P(N_D)=1$,

$$
1 = ze^{\beta\alpha(2q-1)}\frac{\bar{N}_V(\bar{N}_D)}{\bar{N}_D+1}\sum_{m=0}^{2\sigma} p(m)e^{-\beta\alpha(m+1)}. \tag{91}
$$

[Note that when $\alpha=0$ this reduces to Eq. (6) for noninteracting dimers.] The preceding statements are true on all lattices with $q$ nearest neighbors.

We now obtain $N_V$ and $p(m)$ explicitly as functions of $N_D$, so that Eq. (91) becomes an explicit equation of state for dimers. We do this using an approximation, which for reasons explained below we call the "strong form of tree decoupling," in which we replace the $d$-dimensional lattice by a Bethe lattice. To obtain $p(m)$ we first relate $p(m)$ to the quantity $p_{\text{con}}$ which we define to be the conditional probability that site $i$ is vacant when site $j$ is known to be vacant, where sites $i$ and $j$ are nearest neighboring sites. Recall that $A$ and $B$ are vacant neighboring sites. We label the vertices adjacent to $A$ (excluding $B$) by the index $i$ $(i=1,\ldots,\sigma)$ and the vertices adjacent to $B$ (excluding $A$) by the values $i=\sigma+1,\ldots,2\sigma$, as shown in Fig. 4. We define a random variable $X_i$ which has the value 1 if the vertex $i$ is vacant and the value 0 if a dimer is touching vertex $i$. On the Bethe lattice the $X_i$ $(i=1,2,\ldots,2\sigma)$ are independent random variables. Note that $P(X_i=1)$ is the conditional probability that a neighbor of $B$ is vacant given that not only $B$ but also $A$ is vacant. On a Bethe lattice the condition that $A$ is also vacant is irrelevant in this context, in which case $P(X_i=1)$ is just $p_{\text{con}}$, so that

$$
\begin{aligned}
p(m) &= P(X_1+X_2+\cdots+X_{2\sigma}=m) \\
&= \frac{(2\sigma)!}{m!(2\sigma-m)!}p_{\text{con}}^m(1-p_{\text{con}})^{2\sigma-m}
\end{aligned}
\tag{92}
$$

and

$$
\sum_{m=0}^{2\sigma} p(m)e^{-\beta\alpha(m+1)} = e^{-\beta\alpha}[p_{\text{con}}e^{-\beta\alpha}+1-p_{\text{con}}]^{2\sigma}. \tag{93}
$$

Thus, Eq. (91) becomes

$$
1 = z\frac{\bar{N}_V}{\bar{N}_D}[\epsilon+1-p_{\text{con}}\epsilon]^{2\sigma}, \tag{94}
$$

where $\epsilon=e^{\beta\alpha}-1$ and we replaced $\bar{N}_D+1$ by $\bar{N}_D$ in the thermodynamic limit. Now we use Eq. (9) which we write in the form

$$
\rho_V = (1-q\rho)p_{\text{con}}. \tag{95}
$$

Then Eq. (94) becomes

$$
1 = zp_{\text{con}}\frac{1-q\rho}{\rho}[\epsilon+1-p_{\text{con}}\epsilon]^{2\sigma}. \tag{96}
$$

It remains to determine $p_{\text{con}}$ in terms of $\rho$.

In order to calculate $p_{\text{con}}$ (as a function of $\rho$), we first calculate a simpler quantity $p'$, the conditional probability that $B$ is vacant, given that bond $AB$ is unoccupied (i.e., not covered by a dimer). Note that an unoccupied bond is not necessarily a dimer vacancy, since a dimer may be touching one or both ends of the bond. We write

$$
\begin{aligned}
p' &= P(B \text{ vacant}|\text{bond } AB \text{ unoccupied}) \\
&= \frac{P(B \text{ vacant and bond } AB \text{ unoccupied})}{P(\text{bond } AB \text{ unoccupied})} \\
&= P(B \text{ vacant})/P(\text{bond } AB \text{ unoccupied}) \\
&= (1-q\rho)/(1-\rho).
\end{aligned}
\tag{97}
$$

On the other hand, we will calculate $p'$ in terms of the weights (unnormalized probabilities) of certain graphs, yielding the information which is needed to calculate $p_{\text{con}}$.

We focus our attention on a bond $AB$ and we continue to consider the Bethe lattice. For this discussion we divide the lattice into two parts by cutting the bond $AB$, so that one part, $T_A$, contains site $A$ and all sites accessible to site $A$ without going through site $B$ and the other part, $T_B$, is defined similarly, as shown in Fig. 4. On the Bethe lattice, when the bond $AB$ is unoccupied, these two parts $T_A$ and $T_B$ are independent

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

subsystems. In that case we see, from Eq. (86), that the "weight" of a configuration of either $T_A$ or $T_B$ is obtained as the product of (a) a factor $\zeta = z\exp[\beta\alpha(2q-1)]$ for every bond covered by a dimer[33] (the actual value of $\zeta$ will not appear in the final results) and (b) a factor $e^{\beta\alpha}$ for every bond which is a dimer vacancy. We define

$$\begin{aligned} w_{A,0} &= \text{sum of weights of all graphs on } T_A \text{ which contain no dimers touching } A, \\ w_{A,1} &= \text{sum of weights of all graphs on } T_A \text{ which contain one dimer touching } A, \\ w_{B,0} &= \text{sum of weights of all graphs on } T_B \text{ which contain no dimers touching } B, \\ w_{B,1} &= \text{sum of weights of all graphs on } T_B \text{ which contain one dimer touching } B. \end{aligned} \tag{98}$$

Note that we are only concerned with graphs in which the bond $AB$ is fixed (to be unoccupied), so that weights of graphs on the subtrees $T_A$ and $T_B$ are well defined. Then

$$p' = \frac{P(B \text{ vacant})}{P(AB \text{ unoccupied})} = \frac{w_{A,0}w_{B,0}e^{\beta\alpha} + w_{A,1}w_{B,0}}{w_{A,0}w_{B,0}e^{\beta\alpha} + w_{A,0}w_{B,1} + w_{A,1}w_{B,1} + w_{A,1}w_{B,0}}. \tag{99}$$

The first term in the numerator is the total weight of graphs in which $A$ and $B$ are vacant (so that bond $AB$ is a dimer vacancy), and the second term is the total weight of graphs in which $B$ is vacant and $A$ is occupied (so that bond $AB$ is not a dimer vacancy). The terms in the denominator are similarly interpreted. Since $P(B \text{ vacant}) = P(A \text{ vacant})$ far from the boundary, we have $w_{B,0}w_{A,1} = w_{B,1}w_{A,0}$. Thus $w_{A,1}/w_{A,0} = w_{B,1}/w_{B,0}$.

Dividing the numerator and denominator of Eq. (99) by $w_{A,0}w_{B,0}$ we obtain the following relation between $p'$ and $u \equiv w_{A,1}/w_{A,0}$:

$$p' = \frac{e^{\beta\alpha} + u}{e^{\beta\alpha} + u^2 + 2u}, \tag{100}$$

so that

$$\frac{e^{\beta\alpha} + u}{e^{\beta\alpha} + u^2 + 2u} = \frac{1 - q\rho}{1 - \rho}. \tag{101}$$

Now we relate $p_{\text{con}}$ to $u$,

$$p_{\text{con}} = \frac{P(A \text{ and } B \text{ vacant})}{P(A \text{ vacant})} = \frac{w_{A,0}w_{B,0}e^{\beta\alpha}}{w_{A,0}w_{B,0}e^{\beta\alpha} + w_{A,0}w_{B,1}} = \frac{\epsilon + 1}{\epsilon + 1 + u}. \tag{102}$$

We now solve Eq. (102) for $u$ and substitute the result into Eq. (101) to get

$$\epsilon p_{\text{con}} - (2\epsilon + \lambda + 1) + (\epsilon + 1)/p_{\text{con}} = 0, \tag{103}$$

where $\lambda = \rho\sigma/(1 - q\rho)$. (Note that as $\alpha \to 0$, $p_{\text{con}}$ becomes equal to $p'$, as expected.) Thus we get

$$\frac{1 - q\rho}{\rho} = \frac{p_{\text{con}}\sigma}{[\epsilon p_{\text{con}} - \epsilon - 1][p_{\text{con}} - 1]}, \tag{104}$$

so that Eq. (96) can be written as

$$1 = \frac{\sigma z p_{\text{con}}^2}{1 - p_{\text{con}}}[\epsilon + 1 - p_{\text{con}}\epsilon]^{2\sigma - 1}, \tag{105}$$

or

$$-\ln(\sigma z) = G(\rho), \tag{106}$$

where

$$G(\rho) = 2\ln p_{\text{con}}(\rho) - \ln[1 - p_{\text{con}}(\rho)] + (2\sigma - 1)\ln[\epsilon + 1 - \epsilon p_{\text{con}}(\rho)], \tag{107}$$

where $p_{\text{con}}(\rho)$ is determined by Eq. (103).[34]

The physical range of $\rho$ is $[0, 1/q]$. As $\rho \to 0$, $p_{\text{con}} \to 1$ and $G(\rho) \to +\infty$. As $\rho \to 1/q$, $p_{\text{con}} \to 0$ and $G(\rho) - \infty$. One can show, either analytically or by making computer plots, that if $\epsilon$ is less than a certain critical value $\epsilon_c$ (which we shall calculate) then $G(\rho)$ is a monotone decreasing function of $\rho$ in the interval $[0, 1/q]$. In this case there is a unique solution of Eq. (106) for $\rho$ for each positive value of the activity $z$. If $\epsilon > \epsilon_c$, then $dG/d\rho$ is negative for small $\rho$ and for $\rho$ near $1/q$, but there is an intermediate region in which $dG/d\rho > 0$, as is illustrated in Fig. 5. In this case there is a certain range of $z$ in which there are three values of $\rho$ which satisfy Eq. (106). As explained in Appendix A, for $z$ less than a certain value $z_0(\epsilon)$, which is determined by an equal-area construction, the physical solution (i.e., the most probable state) is a homogeneous state whose density of dimers is given by the smallest solution of Eq. (106). For $z > z_0(\epsilon)$ the physical solution is a homogeneous state whose density of dimers is given by the largest solution of Eq. (106). For $z = z_0(\epsilon)$ the physical solution is the coexistence of two homogeneous phases whose densities are the smallest and largest solutions of Eq. (106).

We now will calculate $\epsilon_c$ by determining the range of $\epsilon$ for which the equation $G'(\rho) = 0$ has two solutions for $\rho$ in $[0, 1/q]$. We have

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

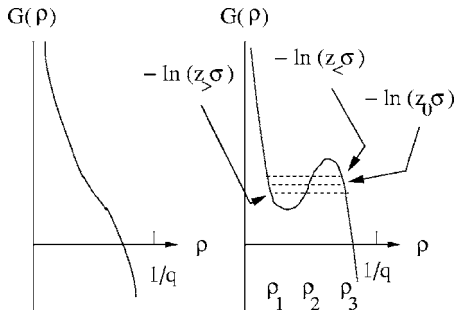


FIG. 5. Schematic graphs of $G(\rho)$ for $\epsilon<\epsilon_c$ (left) and for $\epsilon>\epsilon_c$ (right). In the right panel we show the line at $-\ln[\sigma z_0(\epsilon)]$ at which the net area between the line and the curve of $G(\rho)$ is zero. This is the "equal area" construction which gives $z_0(\epsilon)$. We also show lines for a value of $z$ ($z_<$) which is less than $z_0(\epsilon)$ and a value of $z$ ($z_>$) which is larger than $z_0(\epsilon)$. The values of $\rho_j$ are the values of $\rho$ at which the line for $z_0(\epsilon)$ intersects $G(\rho)$.

$$G'(\rho)=\left[\frac{2}{p_{\rm con}}+\frac{1}{1-p_{\rm con}}-\frac{\epsilon(2\sigma-1)}{\epsilon+1-p_{\rm con}\epsilon}\right]\frac{dp_{\rm con}}{d\rho}. \tag{108}$$

By differentiating Eq. (103) with respect to $\rho$ one can show that $dp_{\rm con}/d\rho<0$ for $p_{\rm con}$ in [0, 1] and $\rho$ in $[0,1/q]$. Accordingly, setting $G'(\rho)=0$ leads to the quadratic equation

$$2\sigma\epsilon p_{\rm con}^2-p_{\rm con}(1+2\epsilon+2\sigma\epsilon)+2\epsilon+2=0. \tag{109}$$

This equation has two real roots for either $\epsilon>\epsilon_+$ or $\epsilon<\epsilon_-$ and no real roots otherwise, where $\epsilon_\pm$ satisfies

$$(1+2\epsilon+2\sigma\epsilon)^2=16\sigma\epsilon(\epsilon+1), \tag{110}$$

which gives

$$\epsilon_\pm=\frac{3\sigma-1\pm2\sqrt{\sigma(2\sigma-1)}}{2(\sigma-1)^2}. \tag{111}$$

Since the two values of $p_{\rm con}$ corresponding to $\epsilon_-$ are both greater than 1, we see that two relevant solutions for $G'(\rho)=0$ occur only for $\epsilon>\epsilon_c\equiv\epsilon_+$. From the value of $\epsilon_c$ we obtain the transition temperature $T_c$ for the liquid-gas transition for interacting dimers from

$$\epsilon_c=e^{\alpha/(kT_c)}-1. \tag{112}$$

We close this section by discussing the accuracy of the "strong form of tree decoupling" in which we approximate a $d$-dimensional lattice by a Bethe lattice of the same coordination number. Recall that in the tree decoupling introduced above in Eq. (11) it was only assumed that we could neglect indirect paths which connect nearest neighboring sites $A$ and $B$. A comparable approximation here is to assume that the conditional probability that a neighbor of site $A$ is vacant given that both sites $A$ and $B$ are vacant is the same as the conditional probability when only site $A$ is vacant. If this were the only approximation, then the present treatment of the interacting dimer system would be expected to be quite accurate—as is the tree decoupling for noninteracting dimers.[5] However, here we also started from the much stronger assumption that the random variables $X_i$ introduced above in Eq. (92) are independent of one another. On the Bethe lattice this is obviously true, as can be seen from Fig. 4. However, on a real lattice, this assumption neglects the many next-nearest neighbor connections between the $X_i$ sites. This same neglect reappears if one tries to apply the subsequent calculation of $p'$ to a $d$-dimensional lattice. Accordingly it would not be surprising if the Bethe approximation for interacting dimers had an accuracy similar to that of mean field theory for the Ising model in the same spatial dimensionality. In two dimensions, this would imply that the Bethe lattice value of $\epsilon_c$ may differ from the exact value for a $d$-dimensional lattice by about 30%.

### B. Solution by construction of an effective Hamiltonian

In this section we generalize the effective Hamiltonian for noninteracting dimers to include dimer-dimer interactions. We continue to mark sites with operators $s_i$ which obey the trace rules of Eq. (15). But in addition we need to have operators which keep track of interactions. So at each site $i$ we introduce operators $t_i$ which have zero trace unless accompanied by an $s_i$ operator. These operators commute with one another and obey

$$\mathrm{Tr}_j\, s_j^p t_j^r=\delta_{p,0}\delta_{r,0}+\delta_{p,1} \tag{113}$$

for $p$ and $r$ each assuming the values $0,1,\ldots,q$. Now we set

$$e^{-\beta\mathcal{H}}=\prod_{\langle ij\rangle}[(1+xs_is_j)(1+\delta t_it_j)]. \tag{114}$$

For a configuration of $N_D$ dimer bonds and $N_I$ interacting bonds this Hamiltonian gives a contribution to the partition function of

$$[x(1+\delta)]^{N_D}[1+\delta]^{N_I}. \tag{115}$$

To get the desired partition function we thus set $\delta=e^{\alpha\beta}-1=\epsilon$ and $x=ze^{-\beta\alpha}$.

We now obtain the exact solution for the Bethe lattice. We could introduce replicas to obtain an expansion for the free energy rather than for the partition function. However, in the interest of simplicity we work with the partition function to obtain an exact solution for the Bethe lattice. Accordingly Eq. (21) in this case assumes the form

$$g_i=\frac{\mathrm{Tr}_j[(1+ze^{-\beta\alpha}s_is_j)(1+\epsilon t_it_j)g_j^\sigma]}{\mathrm{Tr}_j\, g_j^q}. \tag{116}$$

The solution to this equation is of the form

$$g_i=A+Bs_i+Ct_i+Ds_it_i. \tag{117}$$

To satisfy Eq. (116) the constants must obey

$$\begin{aligned}A&=\mathrm{Tr}_j\, g_j^\sigma/\mathrm{Tr}_j\, g_j^q,\\ B&=ze^{-\beta\alpha}\,\mathrm{Tr}_j\, s_jg_j^\sigma/\mathrm{Tr}_j\, g_j^q,\\ C&=\epsilon\,\mathrm{Tr}_j\, t_jg_j^\sigma/\mathrm{Tr}_j\, g_j^q,\\ D&=z\epsilon e^{-\beta\alpha}\,\mathrm{Tr}_j\, s_jt_jg_j^\sigma/\mathrm{Tr}_j\, g_j^q.\end{aligned} \tag{118}$$

These equations may be written in terms of $A$, $r_B\equiv B/A$, $r_C\equiv C/A$, and $r_D=D/A$, as

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

$$A^2 = \frac{1+\sigma(r_B+r_D)(1+r_C)^{\sigma-1}}{1+q(r_B+r_D)(1+r_C)^{\sigma}},$$
$$r_B = \frac{ze^{-\beta\alpha}(1+r_C)^{\sigma}}{1+\sigma(r_B+r_D)(1+r_C)^{\sigma-1}},$$
$$r_C = \frac{\epsilon\sigma(r_B+r_D)(1+r_C)^{\sigma-1}}{1+\sigma(r_B+r_D)(1+r_C)^{\sigma-1}}, \tag{119}$$
$$r_D = \frac{z\epsilon e^{-\beta\alpha}(1+r_C)^{\sigma}}{1+\sigma(r_B+r_D)(1+r_C)^{\sigma-1}} = \epsilon r_B.$$

From the equation for $r_C$ we obtain

$$r_B + r_D = \frac{r_C}{\sigma(1+r_C)^{\sigma-1}(\epsilon - r_C)}. \tag{120}$$

Using this in conjunction with the equation for $r_B$ we obtain an equation which determines $r_C$,

$$\frac{r_C/(1+\epsilon)}{\sigma(\epsilon-r_C)(1+r_C)^{\sigma-1}} = \frac{z(1+r_C)^{\sigma}}{(1+\epsilon)[1+r_C/(\epsilon-r_C)]}, \tag{121}$$

which can be put into the form

$$-\ln(\sigma z) = 2\ln(\epsilon - r_C) - \ln(\epsilon r_C) + (2\sigma-1)\ln(1+r_C). \tag{122}$$

This is identical to (106) when we make the identification $r_C/\epsilon = p_{\text{con}}$. (It has to be admitted that this physical interpretation of $r_C$ is not obvious if one only has the effective Hamiltonian.)

In Appendix B we develop mean field theory by a suitable decoupling of the effective Hamiltonian and, as expected, we obtain results qualitatively similar to those for the Bethe lattice.

## IV. QUENCHED RANDOMNESS

### A. Dimers on percolation clusters at infinite fugacity

Here we consider the statistics of dimers on a quenched random lattice in which sites can be either $X$ sites with probability $p$ or $Y$ sites with probability $1-p$. For a given configuration $\mathcal{C}$ (i.e., for a given distribution of $X$ and $Y$ sites), the grand canonical partition function, $Z(\mathcal{C};\{z\})$, for dimer coverings is calculated as

$$Z(\mathcal{C};\{z\}) = \sum_{\mathcal{A}} z_{XX}^{n_{XX}(\mathcal{A})} z_{XY}^{n_{XY}(\mathcal{A})} z_{YY}^{n_{YY}(\mathcal{A})}, \tag{123}$$

where the sum is over all arrangements $\mathcal{A}$ of 0, 1, 2, etc., hard-core dimers, $n_{AB}(\mathcal{A})$ is the number of dimers covering an $A$ site and a $B$ site in the arrangement $\mathcal{A}$ (where $A$ and $B$ each assume the values $X$ and $Y$), and $z_{AB}$ is the activity of an $AB$ dimer. Then the quenched average free energy $F$ is calculated as

$$F(p;\{z\}) = \sum_{\mathcal{C}} P(\mathcal{C};p)\ln Z(\mathcal{C};\{z\}), \tag{124}$$

with $P(\mathcal{C};p)=p^{n_x(\mathcal{C})}(1-p)^{n_y(\mathcal{C})}$, where $n_x(\mathcal{C})$ ($n_y(\mathcal{C})$) is the number of $X$ ($Y$) sites in the configuration $\mathcal{C}$. From this quenched free energy one then obtains the average number of $AB$ dimers as

$$N_{AB}(p;\{z\}) = z_{AB}\frac{\partial F(p;\{z\})}{\partial z_{AB}}. \tag{125}$$

An exact result for the dimer density on a Bethe lattice does not seem easy to obtain. However, we now give an exact solution for the dimer density on a Bethe lattice in the limit $z_{XX}\to\infty$ and $z_{XY}=z_{YY}\to 0$. Thus we consider $M_D(p)$, the average of the maximal number of dimers which can be placed on percolation clusters of $X$ sites. Even in this limit the result is not trivial because the constraint that dimers do not overlap plays a variable role depending on the compactness of the cluster.

To obtain the exact solution we will explicitly evaluate the expansion of $M_D(p)$ in powers of $p$. For this purpose we temporarily consider $M_D$ as a function of the set of $p_i$'s, where $p_i$ is the probability that site $i$ is present (i.e., is an $X$ site). Then we write

$$\begin{aligned} M_D(\{p_i\}) &= \sum_i M_D(0,\ldots,0,p_i,0,\ldots,0) \\ &\quad + \sum_{i<j}[M_D(0,\ldots,0,p_i,0,\ldots,0,p_j,0,\ldots,0) \\ &\quad - M_D(0,\ldots,0,p_i,0,\ldots,0) \\ &\quad - M_D(0,\ldots,0,p_j,0,\ldots,0)] + \cdots. \end{aligned} \tag{126}$$

We write this as

$$\begin{aligned} M_D(\{p_i\}) &= \sum_i M_D(p_i)_c + \sum_{i<j} M_D(p_i,p_j)_c \\ &\quad + \sum_{i<j<k} M_D(p_i,p_j,p_k)_c \cdots, \end{aligned} \tag{127}$$

where we only indicate as arguments those $p_i$'s which are nonzero and we introduce the cumulants via

$$\begin{aligned} M_D(p_i)_c &= M_D(p_i), \\ M_D(p_i,p_j)_c &= M_D(p_i,p_j) - M_D(p_i) - M_D(p_j), \end{aligned} \tag{128}$$

etc., as in Eq. (47). Note that $M_D(p_i)=0$ because a dimer requires two sites being present. Similarly $M_D(p_i,p_j)\neq 0$ only if sites $i$ and $j$ are nearest neighbors. One can show that the cumulant vanishes for a disconnected diagram. The general term (evaluated for $p_i=p$) is

$$\begin{aligned} M_D(\Gamma)_c &= \sum_{\gamma\in\Gamma} M_D(\gamma)(-1)^{N_\Gamma - N_\gamma} \\ &= \text{The terms of order } p^{N_\Gamma} \text{ in } M_D(\Gamma) \\ &= p^{N_\Gamma}\sum_{x_i=\pm 1} M_D(x_1,x_2,\ldots,x_{N_\Gamma})\prod_{j=1}^{N_\Gamma} x_j. \end{aligned} \tag{129}$$

In the first line $\Gamma$ denotes a set of $p_i$'s, $\gamma$ is a subset of $\Gamma$ (with $\gamma=\Gamma$ allowed), and $N_\Gamma$ is the number of $p_i$'s in the set $\Gamma$. In the last line $x_i=1$ means that the site $i$ is included in the set and $x_i=-1$ means that the site $i$ is not included. (These definitions follow from the fact that to get a term of order $p^{N_\Gamma}$, we take a factor of $p$ if the site is included and $(1-p)$

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

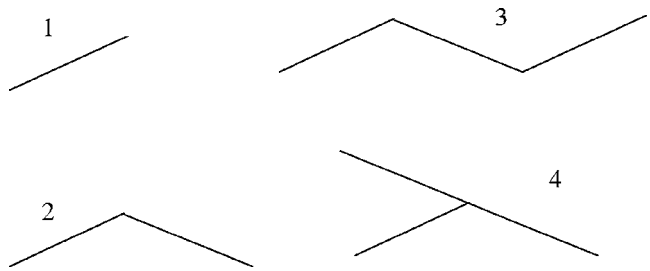


FIG. 6. Small clusters for which we give the cumulant value of $M$.

$\rightarrow(-p)$ if the site is not included.) For example, for the sets of sites shown in Fig. 6 we find that

$$\begin{aligned} M_D(\Gamma_1)_c &= p^2, \\ M_D(\Gamma_2)_c &= p^3[1-2(1)] = -p^3, \\ M_D(\Gamma_3)_c &= p^4[2-4(1)+3(1)] = p^4, \\ M_D(\Gamma_4)_c &= p^4[1-3(1)+3(1)] = p^4. \end{aligned} \tag{130}$$

For $\Gamma_2$ there is one term with all the $x$'s equal to +1 and two nonzero terms with one $x_i$ equal −1. For $\Gamma_3$ there is one term with all the $x$'s equal to +1, four nonzero terms with one $x_i$ equal −1, and three nonzero terms with two $x_i$'s equal to −1. For $\Gamma_4$ there is one term with all the $x$'s equal to +1, three nonzero terms with one $x_i=-1$, and three nonzero terms with two $x_i$'s equal to −1. These results suggest that for any connected cluster of sites $\Gamma$ on the Bethe lattice one has

$$M_D(\Gamma)_c = (-p)^{N_\Gamma}. \tag{131}$$

Note that in contrast to the cumulant, the bare value $M_D(\Gamma)$ is not simply a function of $N_\Gamma$.

The proof of Eq. (131) is by induction on $N_\Gamma$. We have explicitly shown this result to be true for $N_\Gamma$ equal to 2, 3, and 4. We now show that if Eq. (131) is assumed to hold for $N_\Gamma \leqslant N-1$, then it holds for $N_\Gamma = N$ (assuming $N>2$). When this is proved, the general result is established.

Consider a diagram with $N$ sites and label the sites so that the $N$th site is an "end," that is, it is connected to only one other site in the diagram and this other site is labeled $N-1$, as shown in Fig. 7. For a Bethe lattice (in contrast to the case of hypercubic lattices) this construction is possible because all diagrams have at least one free end.

We will use Eq. (129) for the cumulant, so that

$$M_D(\Gamma_N)_c = p^N \sum_{x_1,x_2\cdots x_N=\pm 1} x_1 x_2 \cdots x_N F(x_1,x_2,\ldots,x_N), \tag{132}$$

which we write as

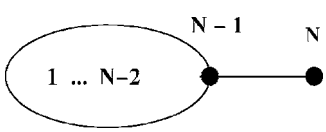


FIG. 7. Cluster of $N$ sites in which site $N$ is a free end.

$$M_D(\Gamma_N)_c = p^N \sum_{x_1,x_2\ldots x_{N-2}} x_1 x_2 \cdots x_{N-2}[A-B+C-D], \tag{133}$$

where the algebraic signs reflect the values of the quantity $(x_{N-1}x_N)$ with

$$\begin{aligned} A &= M_D(x_1,x_2\cdots x_{N-2},1,1), \\ B &= M_D(x_1,x_2\cdots x_{N-2},1,-1), \\ C &= M_D(x_1,x_2\cdots x_{N-2},-1,-1), \\ D &= M_D(x_1,x_2\cdots x_{N-2},-1,1). \end{aligned} \tag{134}$$

In terms $B$, $C$, and $D$, the maximal covering by dimers does *not* include the bond $N-1$ to $N$, because for this bond to be included obviously both sites $N-1$ and $N$ must be occupied (so that $x_{N-1}=x_N=1$). Consider

$$Y(\Gamma_N) = p^N \sum_{x_1,x_2\cdots x_{N-2}} x_1 x_2 \cdots x_{N-2}[-B+C]. \tag{135}$$

This is almost the contribution to the cumulant when the site $N$ is not included either in the summations or in the covering. We say "almost" because the sum includes the factor $-px_N$ which ought to be taken out if we want to identify this with the $N-1$ site problem. We have

$$\begin{aligned} p^N &\sum_{x_1,x_2\cdots x_{N-2}} x_1 x_2 \cdots x_{N-2}[-B+C] \\ &= (-p)p^{N-1} \sum_{x_1,x_2\cdots x_{N-2}} x_1 x_2 \cdots x_{N-2}[B-C] \\ &= (-p)M_D(\Gamma'_{N-1})_c, \end{aligned} \tag{136}$$

where $\Gamma'_{N-1}$ is the diagram obtained from $\Gamma_N$ by omitting the $N$th site.

Now consider $A$. Suppose the maximal covering does not actually include the bond $N-1$ to $N$. Then clearly, if this covering is to be maximal it must include a bond from some site to $N-1$. But now we may keep the number of dimers maximal by moving this bond which includes the site $N-1$ to cover the bond $N-1$ to $N$. So, without loss of generality, in the term $A$ the maximal covering can be chosen so as to include the bond $N-1$ to $N$. Thus for $N>1$,

$$\begin{aligned} p^N \sum_{x_1,x_2\cdots x_{N-2}} x_1 x_2 \cdots x_{N-2} A = p^N &\sum_{x_1,x_2\cdots x_{N-2}} x_1 x_2 \cdots x_{N-2} \\ &\times [M_D(x_1,x_2,\ldots,x_{N-2})+1]. \end{aligned} \tag{137}$$

Now if $N>2$ the term with the 1 will vanish when summed over $x_1$. (For $N=2$ there are no summations left and this is a special case.) Then we see that for $N>2$

$$p^N \sum_{x_1,x_2\cdots x_{N-2}} x_1 x_2 \cdots x_{N-2} A = p^2 M_D(\Gamma''_{N-2})_c, \tag{138}$$

where $\Gamma''_{N-2}$ is obtained from $\Gamma_N$ by deleting sites $N$ and $N-1$. The same reasoning can be applied to term $D$, but in this case there is no term with 1. So

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

$$p^N \sum_{\{x_i\}} x_1 x_2 \cdots x_{N-2}(-D) = -p^2 M_D(\Gamma''_{N-2})_c. \tag{139}$$

Combining all our results we have (for $N>2$)

$$M_D(\Gamma_N)_c = p^N \sum_{x_1,x_2\cdots x_{N-2}} x_1 x_2 \cdots x_n[A-B+C-D]$$
$$= (-p)M_D(\Gamma'_{N-1})_c. \tag{140}$$

This completes the proof by induction.

For a general lattice we may make the tree approximation in which the sum is carried over all diagrams with no loops. In that case the result is that the average dimer density is given by

$$M(p) \equiv M_D(p)/N_0 = N_0^{-1} \sum_{\mathcal{C}} (-p)^{N_{\mathcal{C}}}, \tag{141}$$

where $N_0$ is the total number of sites, the sum is over all loopless clusters $\mathcal{C}$ of two or more sites, and $N_{\mathcal{C}}$ is the number of sites in that cluster. Thus for the Bethe lattice Eq. (127) yields

$$M(p) = \sum_{n>1} (-p)^n W(n), \tag{142}$$

where $W(n)$ is the number (per site) of clusters of $n$ sites on a Bethe lattice. (To avoid edge effects it may be more precise to say that $nW(n)$ is the number of clusters of $n$ sites, one site of which is the central site in an arbitrarily large Cayley tree. This definition ensures that this result applies to hypercubic lattices in the asymptotic limit of large dimensionality.) We use the result of Fisher and Essam,[35]

$$W(n+1) = \frac{(\sigma+1)(\sigma n+\sigma)!}{(n+1)!(\sigma n+\sigma-n+1)!}. \tag{143}$$

Therefore the exact result can be written as

$$M(p) \equiv \sum_{n>1}^{\infty} (-p)^n \frac{(\sigma+1)(\sigma n)!}{n!(\sigma n-n+2)!}. \tag{144}$$

This result indicates that the singularity in $M(p)$ is at $p=-p^*$, where $p^*=(\sigma-1)^{\sigma-1}/\sigma^\sigma$ is the critical concentration for branched polymers on the Bethe lattice.[31] Curiously then, dimer statistics on percolation clusters is related to a somewhat artificial model of localization (which is also related to branched polymer statistics in the same way[31]).

For $\sigma=1$ (a linear chain) this gives

$$M(p) = \frac{p^2}{1+p}. \tag{145}$$

This result could be obtained far more simply by noting that the expected number of clusters per site of length $n$ sites is $p^n(1-p)^2$ and for a cluster of length $2n$ or $2n+1$ the maximal number of dimers is $n$, so that

$$M(p) = \sum_{n=1}^{\infty} (p^{2n}+p^{2n+1})(1-p)^2 n, \tag{146}$$

which reproduces the result of Eq. (145).

### B. Alternate expression

We now give a closed form expression for $M(p)$. To do this we construct an expression for $d^2M/dp^2$. In this quantity the binomial coefficient can be expressed as a contour integral,

$$\frac{d^2M}{dp^2} = (\sigma+1)\sum_{n=2}^{\infty}(-p)^{n-2}\int \frac{dz}{2\pi i}\frac{(1+z)^{\sigma n}}{z^{n-1}}, \tag{147}$$

where the contour surrounds the origin. The sum over $n$ is a geometric series which can be summed. After some manipulations we found that

$$M(p) = p + z_0 - \frac{\sigma-1}{2}z_0^2, \tag{148}$$

where $z_0$ is the root of the algebraic equation

$$(1+z_0)^\sigma = -z_0/p, \tag{149}$$

which is proportional to $p$ for small $p$. One can check that this gives the correct result for $\sigma=1$. For $\sigma=2$ it gives

$$M(p) = \frac{1}{4p^2}[-1-6p-6p^2+4p^3+(1+4p)^{3/2}]. \tag{150}$$

It is necessary to discuss the status of this result. The step of summing the geometric series and deforming the contour to surround the singularity at $z=z_0$ requires that the ratio of the geometric series, $r=-p(1+z)^\sigma/z$, have magnitude less than unity somewhere on the positive real axis. The minimum value of $|r|$ on the positive real axis is $p\sigma^\sigma/(\sigma-1)^{\sigma-1}$ and this leads to the condition $p<p^*$ whose value is given just below Eq. (144). So the result of Eq. (150) is thereby established for $p<p^*$. Now we argue that the range of validity of Eq. (150) actually extends beyond $p^*$. To see this, suppose we express $M(p)$ as a sum over clusters. Since a cluster of $n$ sites has probability $p^n(1-p)^{\sigma+1+(n-1)(\sigma-1)}$, $M(p)$ must be of the form

$$M(p) = (1/p)^2\Phi[p(1-p)^{\sigma-1}], \tag{151}$$

where $\Phi(x)$ has a power series expansion which should converge as long as $p<p_c$, where $p_c=(1/\sigma)$ is the critical concentration for the percolation problem on the Bethe lattice. Since the argument of $\Phi$ has its maximum value when $p=p_c$, the form of Eq. (151) provides an exact mapping of the regime $p>p_c$ onto the regime $p<p_c$. Therefore Eq. (151) can be extended to $p_c<p\leqslant 1$ provided that we understand that this equation only gives the contribution to $M(p)$ from finite clusters. For $\sigma=2$ this mapping is very simple: it implies that we replace $p$ by $(1-p)$ inside the square bracket of Eq. (150). We have not been able to calculate the contribution to $M(p)$ from the infinite cluster which appears when $p$ is greater than $p_c$. Clearly the complete formula for $M(p)$, including the contribution from the infinite cluster, should yield $M(1)=1/2$. Since Eq. (150) does not give $M(1)=1/2$, it cannot possibly represent the complete formula for $M(p)$.

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

## V. RANDOM DEPOSITION

### A. Introduction

Here we consider a special case of a model of catalysis[4] in which hard-core dimers are randomly deposited on bonds and the hard-core constraint does not allow two dimers to intersect the same site. Deposition on all allowable bonds is equiprobable. A quantity of interest is the final concentration when no further dimers can be deposited. We have not been able to construct such a solution on a Bethe lattice. However, here we give an exact solution of this model in one dimension.

To characterize this process it is essential to consider deposition on a line of bonds of finite length in one dimension. In order to consider deposition recursively, we therefore introduce the function $F(i,j)$, (with $i<j$), which is defined to be the average number of dimers which will ultimately be deposited in the interval between two preexisting dimers, one on bond $i$ and the other on bond $j$. Obviously $F(i,j)=F(i-n,j-n)$ and as shorthand we set $F(1,j)\equiv F(j)$.

Let us see what this function is for small argument. It is clear that $F(1,3)=F(1,4)=0$ because a new dimer cannot be deposited on a bond neighboring an occupied bond, since neighboring bonds share a site which cannot be occupied by two hard-core dimers. Next consider $F(1,5)\equiv F(5)$. If we start with dimers on bonds 1 and 5, then an additional dimer can only be deposited on bond 3, so

$$F(1,5)=F(5)=1 \tag{152}$$

is the average number of dimers which will be deposited between dimers at sites 1 and 5. Similar considerations indicate that $F(6)=1$ and $F(7)=5/3$.

Next consider $F(1,8)$. In the first step an additional dimer will be placed on bonds 3, 4, 5, or 6, each with probability $1/4$. If it is placed on bond 3 (or equivalently on bond 6), then we have added one dimer and will be able to add (on average) $F(1,3)+F(3,8)=0+1=1$ further dimer in later step(s). Therefore in each case these two processes lead to the deposition of two dimers. So the combined contribution to $F(1,8)$ from these two cases, each occurring with probability $(1/4)$, is $\delta F(1,8)=1$. Similarly, if the first new dimer is placed on bond 4 (or equivalently on bond 5), then we have added one dimer and will be able to add (on average) $F(1,4)+F(4,8)=0+1=1$ further dimer. As before, the contribution to $F(1,8)$ from these two cases, each occurring with probability $(1/4)$, is $\delta F(1,8)=1$. Therefore we see that $F(8)=2$.

### B. Recursion relation

Now imagine starting with dimers on bonds 1 and $N$, with $N>4$. The first added dimer can go on bond $3,4,\ldots,N-3,N-2$, each with probability $1/(N-4)$. So, if we include this added dimer we have

$$\begin{aligned} F(1,N) &= 1+\frac{1}{N-4}\sum_{j=3}^{j=N-2}[F(1,j)+F(j,N)] \\ &= 1+\frac{2}{N-4}\sum_{j=3}^{j=N-2}F(1,j) \\ &= 1+\frac{2}{N-4}\sum_{j=3}^{j=N-2}F(j). \end{aligned} \tag{153}$$

Also

$$F(N-1)=1+\frac{2}{N-5}\sum_{j=3}^{j=N-3}F(j). \tag{154}$$

Using these we see that

$$(N-4)F(N)=(N-5)F(N-1)+1+2F(N-2). \tag{155}$$

Now we form the generating function

$$\bar{F}(x)=\sum_{N=5}^{\infty}F(N)x^N. \tag{156}$$

Now multiply Eq. (155) by $x^N$ and sum from $N=5$ to $N=\infty$. Keeping in mind that $F(N)$ vanishes for $N<5$ we get

$$x\bar{F}_x-4\bar{F}=x^2\bar{F}_x-4x\bar{F}+\frac{x^5}{1-x}+2x^2\bar{F}, \tag{157}$$

where $\bar{F}_x\equiv d\bar{F}(x)/dx$. From this we find that

$$\bar{F}(x)=\frac{x^4}{(1-x)^2}\left(\frac{1-e^{-2x}}{2}\right). \tag{158}$$

To see what this implies about $F(N)$ for large $N$ we write

$$\bar{F}(x)=\frac{H(x)}{(1-x)^2}=\frac{H(1)}{(1-x)^2}-\frac{H_1(1)}{1-x}+\sum_{n=2}^{\infty}\frac{H_n(1)}{n!}(x-1)^{n-2}, \tag{159}$$

where $H_n(1)\equiv d^nH(x)/dx^n|_{x=1}$. From this we see that

$$F(N)\sim H(1)N=(1-\delta)(N/2), \tag{160}$$

where

$$\delta=e^{-2}\approx 0.1354 \tag{161}$$

is the fraction of sites which remain vacant in the jamming limit (after deposition is completed).

## VI. SUMMARY

In this paper we have presented two approaches, which we call geometric and algebraic, for the analysis of dimer statistics. Both approaches yield exact results when the lattice does not have loops, as for a Bethe lattice. The charm of the geometrical method is that it starts from the most basic statement, namely, that in a grand canonical ensemble, the activity $z$ is precisely the ratio of the statistical weights of the $N$-particle system to that of the $N+1$-particle system. The virtue of the algebraic approach is that once the Hamiltonian is constructed using operators whose trace rules incorporate kinematic restrictions, the standard procedures of statistical

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

mechanics can be applied, for instance, to obtain series expansions for finite dimensional lattices. (This approach was used[27] to give a field theoretic analysis of the monomer-dimer problem.) Here we also show that the use of replicas (which normally are invoked to implement quenched averages of a random Hamiltonian) can be useful in converting a series for the partition function into one for its logarithm, the free energy. Exact solutions for generalizations in which (a) the lattice is anisotropic or (b) dimer-dimer interactions are included were also developed using both approaches. We give an exact solution for dimer statistics on a Bethe lattice in a simple quenched random potential in which dimers are placed on percolation clusters. Finally, we developed an exact solution for the fraction of sites which remain vacant after random disposition is completed in a one-dimensional system.

## ACKNOWLEDGMENT

We thank J. F. Nagle and M. E. Fisher for helpful correspondence.

## APPENDIX A: ANALYSIS OF THE PHASE TRANSITION

The phase transition in the presence of dimer-dimer interactions is entirely similar to that in the van der Waals gas.

The right-hand side of Eq. (105) gives an explicit formula for $zP(N_D+1)/P(N_D)$ when Eq. (103) is used.[33] Thus we have

$$\ln[P(N_D+1)/P(N_D)] = G(\rho) + \ln(\sigma z). \tag{A1}$$

Figure 5 shows schematic graphs of $G(\rho)$ vs $\rho$ for $\epsilon$ slightly less than and slightly greater than $\epsilon_c$. For $\sigma=2$ we find $\epsilon_c \approx 4.95$ and the value of $\rho$ at the critical point is $\rho_c \approx 0.159$, $G(\rho_c)=3.226$, and $z_c \approx 0.0199$.

If $\epsilon > \epsilon_c$ and $z$ is close to $z_0$, a horizontal line (dashed in Fig. 5) at height $\ln(1/\sigma z)$ will intersect the graph of $G(\rho)$ three times, each of the intersections corresponding to a value of $N_D$ for which $P(N_D+1)/P(N_D)=1$. If the densities of dimers at the intersections are $\rho_1 < \rho_2 < \rho_3$, then we have

$$\ln[P(\rho_3)/P(\rho_1)] = \frac{Nq}{2}\int_{\rho_1}^{\rho_3} [G(\rho) - \ln(1/\sigma z)]d\rho. \tag{A2}$$

If $z_0(\epsilon)$ is the value of $z$ such that the area of the loop below the dashed line at height $\ln(1/\sigma z)$ is equal to the area of the loop above that line, then $P(\rho_3)/P(\rho_1)=1$. If $z$ is slightly less than $z_0$, then the negative area exceeds the positive area and $P(\rho_3)/P(\rho_1)<1$, in which case the stable phase has $\rho=\rho_1$. Note that $\rho_2$ is always less probable than $\rho_1$. Similarly, if $z$ is slightly greater than $z_0 z=z_<$, then the stable (most probable) phase corresponds to $\rho=\rho_3$. Note that because of the prefactor $Nq/2$ before the integral, "most probably" means "overwhelmingly most probable."

If we place a density of dimers on the lattice which is intermediate between $\rho_1(z_0)$ and $\rho_3(z_0)$, the lattice will separate into regions with coverage at densities $\rho_1(z_0)$ and $\rho_3(z_0)$, the size of the two regions being determined by the requirement that the total number of dimers is that specified.

If $\epsilon$ is slightly greater than $\epsilon_c$, then the temperature $T$ is slightly less than $T_c$ and the definition of $\epsilon$ implies that $(T_c-T)\propto(\epsilon-\epsilon_c)$. In this case the distance between the two roots of Eq. (109) is proportional to $(\epsilon-\epsilon_c)^{1/2}$, and thus the distance between the corresponding values of $\rho$ is also proportional to $(\epsilon-\epsilon_c)^{1/2}$, which is proportional to $(T_c-T)^{1/2}$. Examination of Fig. 5, without additional analysis, makes it clear that the difference in density between the two coexisting phases, $\rho_3(z_0)-\rho_1(z_0)$, is also proportional to $(T_c-T)^{1/2}$.

## APPENDIX B: MEAN FIELD THEORY

In this appendix we obtain mean field theory for interacting dimers from the Hamiltonian using the standard decoupling even though this Hamiltonian involves operators which obey unusual trace rules.

In view of the trace rules (extended to infinite $q$) we may write

$$e^{-\beta\mathcal{H}} = \prod_{\langle ij\rangle} e^{\hat{z}s_i s_j + \alpha\beta t_i t_j}, \tag{B1}$$

where $\hat{z}=ze^{-\beta\alpha}$. Mean field theory is obtained by ignoring correlated fluctuations and writing

$$-\beta\mathcal{H} = \sum_{\langle ij\rangle} [\hat{z}(s_i\langle s\rangle + s_j\langle s\rangle - \langle s\rangle^2) + \alpha\beta(t_i\langle t\rangle + t_j\langle t\rangle - \langle t\rangle^2)]. \tag{B2}$$

Then

$$\langle s\rangle = \frac{\mathrm{Tr}_i\, s_i e^{s_i q\hat{z}\langle s\rangle + q\alpha\beta\langle t\rangle t_i}}{\mathrm{Tr}_i\, e^{s_i q\hat{z}\langle s\rangle + q\alpha\beta\langle t\rangle t_i}} = \frac{e^{q\alpha\beta\langle t\rangle}}{1+q\hat{z}\langle s\rangle e^{q\alpha\beta\langle t\rangle}}, \tag{B3}$$

$$\langle t\rangle = \frac{\mathrm{Tr}_i\, t_i e^{s_i q\hat{z}\langle s\rangle + q\alpha\beta\langle t\rangle t_i}}{\mathrm{Tr}_i\, e^{s_i q\hat{z}\langle s\rangle + q\alpha\beta\langle t\rangle t_i}} = \frac{q\hat{z}\langle s\rangle e^{q\alpha\beta\langle t\rangle}}{1+q\hat{z}\langle s\rangle e^{q\alpha\beta\langle t\rangle}}. \tag{B4}$$

We solve Eq. (B4) for $\langle s\rangle$ to get

$$\langle s\rangle = \frac{\langle t\rangle}{q\hat{z}e^{q\alpha\beta\langle t\rangle}[1-\langle t\rangle]}, \tag{B5}$$

so that Eq. (B3) gives

$$\ln\langle t\rangle = \ln(q\hat{z}) + 2q\alpha\beta\langle t\rangle + 2\ln[1-\langle t\rangle]. \tag{B6}$$

To shorten the discussion we assume a second order transition in which case the above equations *and* its two derivatives with respect to $\langle t\rangle$ are zero. Differentiating twice we get

$$\frac{1}{\langle t\rangle} = 2q\alpha\beta - \frac{2}{1-\langle t\rangle} \tag{B7}$$

and

$$-\frac{1}{\langle t\rangle^2} = -\frac{2}{(1-\langle t\rangle)^2}. \tag{B8}$$

The last equation gives $t_c$, the value of $\langle t\rangle$ at the critical point, to be $t_c=\sqrt{2}-1$. Putting this into the preceding equation gives $q\alpha\beta_c=\sqrt{2}+(3/2)$.

We may compare this with the solution for the Bethe lattice. For simple models (such as the Ising model) it is known that the Bethe lattice solution only coincides with

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

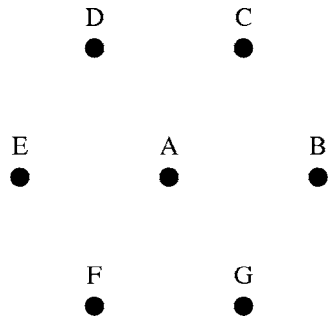


FIG. 8. A portion of the triangular lattice.

mean field theory for large $q$. For large $q$ the Bethe lattice solution for $T_c$ given by Eq. (112) agrees with the present result.

## APPENDIX C: GEOMETRICAL CALCULATION OF FIRST LOOP CORRECTION FOR THE TRIANGULAR LATTICE

For the triangular lattice, a simple geometrical argument permits us to calculate most of the difference between the "exact" value of $\bar{N}_D/N$ (notation as in Table I) and the value given by the Bethe approximation. The argument depends on the "tight" structure of the triangular lattice, and we have not been able to extend the argument to the square lattice. Furthermore, unlike the "loop corrections" calculated in Sec. II C, our geometrical calculation is not the first term in a systematic series of corrections. Nevertheless, the calculation is simple and remarkably accurate. From Eq. (7) we have

$$1/z = \rho_V/\rho, \tag{C1}$$

where $\rho_V$ is the probability that adjacent sites $A$ and $B$ are both vacant and $\rho$ is the probability that a bond is occupied. Clearly

$$P(B \text{ vacant}) = P(B \text{ vacant and } A \text{ vacant}) + P(B \text{ vacant and } A \text{ occupied}). \tag{C2}$$

Consider the section of the triangular lattice shown in Fig. 8. We see that

$$P(B \text{ vacant}) = P(A \text{ vacant}) = 1 - 6\rho \tag{C3}$$

and we set

$$P(B \text{ vacant and } A \text{ vacant}) = (1 - 6\rho)(p'), \tag{C4}$$

where

$$p' = P(B \text{ vacant}|A \text{ vacant}). \tag{C5}$$

Furthermore

$$\begin{aligned} P(B \text{ vacant and } A \text{ occupied}) &= P(B \text{ vac and } AE \text{ occ}) + P(B \text{ vac and } AD \text{ occ}) \\ &+ P(B \text{ vac and } AF \text{ occ}) + P(B \text{ vac and } AC \text{ occ}) \\ &+ P(B \text{ vac and } AG \text{ occ}). \end{aligned} \tag{C6}$$

We now estimate each of the terms on the right-hand side of this equation. It seems evident that there is very little difference between $P(B \text{ vacant}|AE \text{ occ})$ and $P(B \text{ vac}|A \text{ vacant})$, since the influence of the extra dimer would have to propagate over a long tortuous path. Thus we write $P(B \text{ vac and } AE \text{ occ}) = (\rho)(p')$. Similarly, and on slightly weaker ground, we write

$$\begin{aligned} &P(B \text{ vacant and } AD \text{ occupied}) \\ &\quad = P(B \text{ vacant and } AF \text{ occupied}) = (\rho)(p'). \end{aligned} \tag{C7}$$

To estimate $P(B \text{ vac and } AC \text{ occ})$ we note that if $AC$ is occupied then $AB$ and $CB$ must be unoccupied. As far as state of site $B$ is concerned, it makes little difference whether we specify that bond $AC$ is occupied or that bonds $AB$ and $CB$ are unoccupied, because the effect of the presence of the dimer $AC$ on the state of site $B$ is very indirect. Thus we make the approximation that

$$\begin{aligned} &P(B \text{ vacant}|AC \text{ occupied}) \\ &\quad = P(B \text{ vacant}|AB \text{ and } BC \text{ unoccupied}). \end{aligned} \tag{C8}$$

However, the conditional probability that $B$ is vacant, given that $AB$ and $CB$ are unoccupied, is $(1-6\rho)/(1-2\rho)$, so that approximately

$$P(B \text{ vac}|AC \text{ occ}) = (1 - 6\rho)/(1 - 2\rho), \tag{C9}$$

and thereby that

$$P(B \text{ vac and } AC \text{ occ}) = \rho(1 - 6\rho)/(1 - 2\rho). \tag{C10}$$

Now we use our evaluation of each term on the right-hand side of Eq. (C6) to write Eq. (C2) as

$$\begin{aligned} (1 - 6\rho) &= (1 - 6\rho)(p') + (3\rho)(p') \\ &+ (2\rho)(1 - 6\rho)/1 - 2\rho. \end{aligned} \tag{C11}$$

Solving for $p'$ we find that

$$p' = (1 - 6\rho)(1 - 4\rho)/(1 - 2\rho)(1 - 3\rho) \tag{C12}$$

and Eq. (C1) yields

$$\begin{aligned} 1/z = (1 - 6\rho)(p')/(\rho) &= (1 - 6\rho)^2(1 - 4\rho)/ \\ &(\rho)(1 - 2\rho)(1 - 3\rho). \end{aligned} \tag{C13}$$

The computer readily calculates $\rho$ for each value of $z$ in Table II. The corresponding value of $\bar{N}_D/N$, which we call $\pi_G$, is $3\rho$ and is exhibited in Table II.

Thus, a simple geometrical argument yields a good estimate of the "first loop correction" for the triangular lattice. However, we have been unable to make a corresponding argument for the square lattice, nor can we extend this argument in an orderly way to make higher order corrections.

[1] P. Fendley, R. Moessner, and S. L. Sondhi, Phys. Rev. B **66**, 214513 (2002); R. Moessner and S. L. Sondhi, *ibid.* **68**, 054405 (2003).
[2] C. J. Olson, C. Reichhardt, M. McCloskey, and R. J. Zieve, Europhys. Lett. **57**, 904 (2002).
[3] R. van Roij, Phys. Rev. Lett. **76**, 3348 (1996).
[4] J. Kohler and D. ben-Avraham, J. Phys. A **24**, L621 (1991).
[5] J. Cohen and M. Cohen, Biophys. J. **36**, 623 (1981).
[6] T. S. Chang, Proc. R. Soc. London, Ser. A **169**, 512 (1939).
[7] A. R. Miller, Proc. Cambridge Philos. Soc. **38**, 109 (1942).
[8] W. J. C. Orr, Trans. Faraday Soc. **40**, 306 (1944).
[9] H. A. Bethe, Proc. R. Soc. London, Ser. A **150**, 552 (1935).
[10] R. E. Peierls, Proc. R. Soc. London, Ser. A **154**, 207 (1936).
[11] P. R. Weiss, Phys. Rev. **74**, 1493 (1948).
[12] M. F. Sykes, Ph. D. thesis, Oxford University, 1956. We thank Professor

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04

M. E. Fisher for providing this reference.
[13] T. P. Eggarter, Phys. Rev. B **9**, 2989 (1974).
[14] H. Matsuda, Prog. Theor. Phys. **51**, 1053 (1974).
[15] E. Müller-Hartmann and J. Zittartz, Phys. Rev. Lett. **33**, 893 (1974).
[16] H. Falk, Phys. Rev. B **9**, 05184 (1974).
[17] M. E. Fisher and D. S. Gaunt, Phys. Rev. **133**, A224 (1964).
[18] See, for example, P. Pfeuty and G. Toulouse, *Introduction to the Renormalization Group and Critical Phenomena* (Wiley, New York, 1977).
[19] C. Domb, Adv. Phys. **9**, 149 (1960).
[20] For a recent Bethe lattice calculation, see J. M. Schwarz, A. J. Liu, and L. Chayes, Europhys. Lett. **73**, 560 (2006); A. B. Harris and J. M. Schwarz, Phys. Rev. E **72**, 046123 (2005).
[21] J. F. Nagle, Phys. Rev. **152**, 190 (1966).
[22] D. S. Gaunt, Phys. Rev. **179**, 174 (1969).
[23] J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (Wiley, New York, 1940).
[24] G. S. Rushbrooke and H. I. Scoins, Proc. R. Soc. London, Ser. A **230**, 74 (1955).
[25] L. Degrève, Physica (Amsterdam) **66**, 395 (1973).
[26] O. D. Brazhnik and K. F. Freed, J. Chem. Phys. **105**, 837 (1996). The extension of our geometrical approach to the case of noninteracting $n$-mers on a Bethe lattice is simple.
[27] Y. Shapir, J. Phys. A **15**, L433 (1982).
[28] J. Cohen and M. Cohen (unpublished).
[29] This relation actually holds for any finite lattice.
[30] Either or both subsystems of bonds $S_1$ and $S_2$ may include bonds which intersect the boundary of the tree.
[31] A. B. Harris, Phys. Rev. B **26**, 337 (1982).
[32] We have developed a formalism to obtain $Z^n$ for integer values of $n$. Mathematically, the limit $n \to 0$ involves an analytic continuation which, in principle, is not unique. However, in cases of Hamiltonians involving $n$ component *vectors*, no problems seem to arise from assuming the simplest possible analytic continuation. Compare G. Grinstein, AIP Conf. Proc. **24**, 313 (1975) and T. C. Lubensky and A. B. Harris, AIP Conf. Proc. **24**, 311 (1975).
[33] Implicitly we treat the independent subsystems $T_A$ and $T_B$ via a grand canonical formulation in which each dimer carries an activity $\zeta$, which has to be adjusted to give the equilibrium value of the total number of dimers in the combined system. In equilibrium, the correct value of $\zeta$ is indeed $z \exp[\beta\alpha(2q-1)]$. However, the final result for $p_{\text{con}}$ in Eq. (103), below, does not involve $\zeta$. Therefore we can use Eqs. (96) and (103) for values of $N_D$ which are not equal to $\bar{N}_D$, as we do in Appendix A.
[34] An equation equivalent to Eq. (107) was obtained in Ref. 6, but was not related to the Bethe lattice.
[35] M. E. Fisher and J. W. Essam, J. Math. Phys. **2**, 609 (1961).

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 165.123.108.243 On: Thu, 09 Jul 2015 17:56:04