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Critical Behavior of a Three-Dimensional Dimer Model

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The phase transition behavior of a dimer model on a three-dimensional lattice is studied. This model is of biological interest because of its relevance to the lipid bilayer main phase transition. The model has the same kind of inactive low-temperature behavior as the exactly solvable Kasteleyn dimer model on a two-dimensional honeycomb lattice. Because of low-temperature inactivity, determination of the lowest-lying excited states allows one to locate the critical temperature. In this paper the second-lowest-lying excited states are studied and exact asymptotic results are obtained in the limit of large lattices. These results together with a finite-size scaling ansatz suggest a logarithmic divergence of the specific heat above T_c for the three-dimensional model. Use of the same ansatz recovers the exact divergence ($\alpha = 1/2$) for the two-dimensional model.

KEY WORDS: Dimer model; phase transition; lipid bilayer; transfer matrix; random walk; generating function; critical exponent.

1. INTRODUCTION

Exact solutions show that dimer models on two-dimensional lattices exhibit a variety of phase transition behavior. There is one class of model which exhibits a logarithmic divergence of the specific heat, familiar from the two-dimensional Ising model. One example is the dimer model on the 4–8 lattice,[1] which has been used to model the transition in $SnCl_2 2H_2O$. Another class of dimer model exhibits "3/2-order" transitions[2]; in such transitions the specific heat diverges as $(T - T_c)^{-1/2}$ in the disordered phase but there is no divergence in the ordered phase. The first model in

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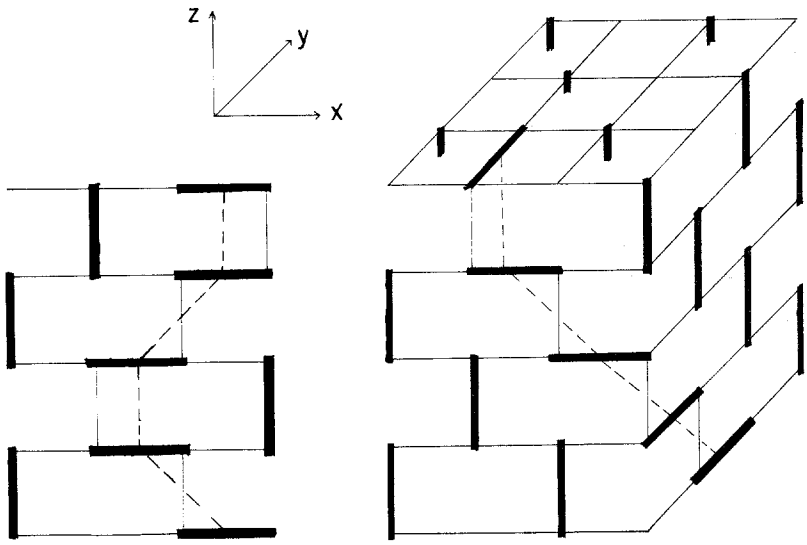

Fig. 1. The models considered in the paper. Each vertical dimer has zero energy and each horizontal dimer has energy ϵ. (a) Kasteleyn model (the K-model) on a "brick" lattice. Each lattice site is paired by one dimer to a nearest-neighbor site. The particular state shown has one horizontal dimer in each z-level. This forms a domain wall as indicated by the dashed lines, with no change of phase ($p = 1$) between domains. (b) The three-dimensional IA model. Here each lattice site can be paired by a dimer to one of the five nearest-neighbor sites. The particular state shown also has one horizontal dimer in each lattice plane corresponding to an $n = 1$ excitation of the transfer matrix (see text).

this class was discovered by Kasteleyn[3]; it is defined in Fig. 1a and has been called the K-model.[4] The K-model is inactive or "frozen" in the low-temperature phase in the sense that the equilibrium state is the ground state for all $T < T_c$. Although another model in this same class has a nonzero specific heat[5] below T_c, it too exhibits a stiffness or frozen behavior, though only partial, in the low-temperature phase[3]: in particular, the specific heat is completely nonsingular below T_c.

Isomorphic transformations of dimer models from the second class have been used to study phase transitions in hydrocarbon chain systems of lipids[7] and polymers.[8] One clear shortcoming of these models is the loss of a relevant dimension.[9] Unfortunately, presently available methods do not permit exact solution of three-dimensional dimer models. Nevertheless,

[3] Incidentally, the transition in the K-model may also be described as an example of a $p = 1$ commensurate–incommensurate transition. The square root divergence in the specific heat supports the general phenomenological argument of Fisher and Fisher[6] concerning critical exponents.

exploratory research on three-dimensional models is in order, and recently Izuyama and Akutsu[10] (to be referred to as IA) have initiated this line of investigation. They have introduced a model, to be called the IA model, that is a possible three-dimensional extension of the two-dimensional K-model. This model is shown in Fig. 1b. Actually, the three-dimensional dimer model which is the best analog of the lipid hydrocarbon model is somewhat different from the IA model. Compared to Fig. 1b it would have no bonds parallel to the x axis in even-numbered lattice planes and no bonds parallel to the y axis in odd-numbered ones. The lipid hydrocarbon analog would then have a ratio of two gauche rotamers/one trans rotamer compared to the four gauche/one trans rotamers in the three-dimensional IA model. The analysis carried out here for the IA model has also been done for this model and the main result is the same as for the IA model. This strongly suggests that the two models have the same transition behavior. We shall therefore discuss the IA model because it is simpler. Basically the IA model involves a simple cubic lattice with regularly spaced forbidden bonds in the vertical direction. Each vertical dimer has zero energy, each horizontal dimer has energy ϵ, and each site must be occupied by a dimer.[4]

The thermodynamic behavior of the IA model has many similarities to the behavior of the two-dimensional K-model. In particular, it is completely inactive in the low-temperature phase. This feature is easily seen by starting with the ground state and trying to shift one vertical dimer into a horizontal position. This requires shifting one vertical dimer in each of the M layers of the system, thereby costing an energy $M\epsilon$. Even though this energy is very large for large M, there are four ways to shift each dimer. Therefore, the free energy of this set of lowest-lying excited states is $M(\epsilon - kT\ln 4)$. Such states will be thermodynamically preferred to the ground state only when $kT > \epsilon/\ln 4 = kT_c$. This simple argument[5] locates the critical temperature T_c exactly. In addition to locating T_c, IA also claimed to show rigorously that, unlike the K-model, the specific heat, $\mathbf{C}(T)$, remains finite as $T \to T_c$ from the disordered phase. Their derivation involves a kind of random

[4] Incidentally Priezzhev[11] has recently proposed a three-dimensional lattice model for which the dimer problem can be solved exactly. The lattice is also a simple cubic lattice with the restriction that dimers cannot form a closed path (for definition see Ref. 11). The model, however, has regular thermodynamic behavior and shows no phase transition. In contrast the IA model exhibits a phase transition at finite temperature.

[5] Such a simple argument was also instrumental in locating the exact transition temperature of the Slater KDP six-vertex model in any dimension. A rigorous proof was given for the KDP model using series expansions.[12] For the lipid analog model such an argument gives $T_c = \epsilon/(k\ln 2)$.

phase approximation utilizing the free fermion basis states. This derivation does not appear to us to be rigorous. However, their derivation does obtain the correct specific heat divergence for the two-dimensional K-model, so it cannot be dismissed out of hand.

The first purpose of this paper is to provide evidence that contradicts the claim of IA to have proved rigorously the finiteness of the specific heat at T_c. The second purpose is to provide evidence that $\mathbf{C}(T)$ diverges as $-\ln(T - T_c)$ as $T \to T_c +$ for the IA model, although we emphasize that this is not a rigorous result. Our method involves an exact calculation in Section 4 of the asymptotic behavior of the largest eigenvalue of the transfer matrix for statistical states which are twice perturbed from the ground state and so have *two* horizontal dimers in each horizontal lattice plane. Although such low-lying states play little role in most phase transitions, we have already seen that consideration of just the singly perturbed states in these dimer models yields the exact transition temperature, so one can expect there to be more information in low-lying excitations in this kind of model than in other models, such as spin models, which have nontrivial low-temperature phases. In Section 3 an *ansatz* is developed which relates the behavior of the twice-perturbed states to the critical behavior of the specific heat. This is preceded by a discussion of the transfer matrix in Section 2.

2. QUALITATIVE CHARACTERISTICS OF THE TRANSFER MATRIX

We consider the generalization of the two-dimensional K-model to arbitrary dimensionality, including the three-dimensional IA model. "Finite" versions of these models consist of finite cross sections with linear dimension N along $(d-1)$-dimensional lattice planes perpendicular to the z axis in Figs. 1a and 1b and with periodic boundary conditions in these lattice planes; the system remains infinite along the z axis, i.e., $M \to \infty$, where M is the number of such lattice planes. A plane midway between two such adjacent lattice planes will be called a *layer* and is pierced by $\frac{1}{2}N^{d-1}$ vertical bonds. (Even N will be assumed.) A vertical bond not occupied by a dimer will be said to produce a *hole* in the layer. The transfer matrix, $\mathbb{Q}$, transfers from layer to layer in the z direction. The basis set, $\{\psi\}$, for $\mathbb{Q}$ designates the positions of the holes in a layer. The ground state therefore consists of the "vacuum" state with no holes, ψ_0 and $\mathbb{Q}\psi_0 = \lambda_0\psi_0$, where $\lambda_0 = 1$. The lowest-lying excited states, $\{\psi\}_1$, consist of one hole in a layer, and from the Introduction it is clear that $\mathbb{Q}$ operating upon any state in this set gives a sum of states from this set. Similarly, if there are n holes in one layer, then all other layers have n holes. Therefore, the transfer matrix is already block diagonal in the $\{\psi\}$ basis and every nonzero element of the

nth block has the Boltzmann factor $e^{-n\beta\epsilon}$ as the statistical weight. For finite models of size MN^{d-1} the largest eigenvalue, $\lambda_1 e^{-\beta\epsilon}$, from the $n=1$ block (which is $\frac{1}{2}N^{d-1} \times \frac{1}{2}N^{d-1}$ in size) becomes degenerate with λ_0 at T_c, and for $T > T_c$, $\lambda_1 e^{-\beta\epsilon} > \lambda_0$. For $T < T_c$, λ_0 is the largest eigenvalue of $\mathbb{Q}$. Therefore, there is a first-order transition with latent heat $M\epsilon$ at T_c. For finite systems there is also a temperature $T_2 > T_c$ at which the largest eigenvalue $\lambda_2 e^{-2\beta\epsilon}$ from the $n=2$ block becomes degenerate with $\lambda_1 e^{-\beta\epsilon}$, and so on. Therefore, the finite system exhibits a sequence of first-order transitions each with $\Delta E = M\epsilon$. This is equivalent to a sequence of delta functions in the specific heat at a sequence of temperatures, $T_c < T_2 < T_3 < \cdots$, until the system becomes maximally disordered. (This behavior is also seen in the Slater KDP ferroelectric six-vertex model.) As the width, N, of the system becomes larger, there are more transitions, $T_n(N)$, and the limit of $T_n(N)$ approaches T_c as $N \to \infty$ for fixed n. Also, the first-order jump becomes smaller at each $T_n(N)$ when measured per lattice site, $\Delta E/MN^{d-1} = \epsilon/N^{d-1}$. As the limit of an infinite system is approached, the infinite sequence of delta functions approaches a specific heat function which should be analytic except at T_c (assuming only one true phase transition in the infinite limit). The way in which an infinite specific heat could develop at T_c as $N \to \infty$ is for the local density of first-order jumps to approach infinity more rapidly than N^{d-1}. Stated more mathematically, let us approximate the specific heat for $T_{n-1}(N) < T < T_n(N)$ by

$$\mathbf{C}(T) \approx (\Delta E/MN^{d-1})/\left[T_n(N) - T_{n-1}(N)\right] \tag{1}$$

and, quite generally, introduce the scaled density of jumps, $g(N;\rho)$, as

$$g(N; n/N^{d-1}) = N^{-(d-1)}/\left[T_n(N) - T_{n-1}(N)\right] \tag{2}$$

where $\rho = n/N^{d-1}$ represents the density of holes. Then for large N we have

$$\mathbf{C}(T) \approx \epsilon g(N;\rho) \tag{3}$$

and it is reasonable to hope that $g(N;\rho)$ approaches, as $N \to \infty$, a smooth function of ρ and N. Thus if $g_n(N) \equiv g(N; n/N^{d-1})$ diverges to ∞ in the limit $N \to \infty$ at *fixed* n (i.e., as $\rho \to 0$), one may conclude that the specific heat diverges to ∞ at the transition. We shall, in fact, show that $g_2(N)$ remains bounded for $d > 3$, diverges logarithmically with N when $d = 3$, and diverges as N for $d = 2$.

3. PROCEDURE FOR TESTING THE IA APPROXIMATION AND FOR OBTAINING ESTIMATES OF THE SPECIFIC HEAT EXPONENT

In their treatment IA introduced an approximation for computing the largest eigenvalue in any block of the transfer matrix corresponding to n

holes.[10] They express their result in terms of the free energy per lattice site, $f(\rho)$, where, as above, $\rho = n/N^{d-1}$ is the density (we will extend IA's discussion for $d = 2$ and $d = 3$ to arbitrary dimensionality d) and

$$f(\rho) = -(kT/N^{d-1})\ln\lambda_n + \rho\epsilon = (\epsilon - kT\ln q)\rho - (kT/N^{d-1})\ln(\lambda_n/q^n) \tag{4}$$

In this expression q represents the number of nearest neighbors in a horizontal lattice plane. For our problem $q = 2(d-1)$. IA then claim that for $N \to \infty$

$$\ln(\lambda_n/q^n) \approx -B_d n^{(d+1)/(d-1)}/N^2 \tag{5}$$

where B_d is independent of N, so that

$$f(\rho) = (\epsilon - kT\ln q)\rho + bkT\rho^{(d+1)/(d-1)} + \text{higher-order terms} \tag{6}$$

From this it is easy to obtain the specific heat behavior in the following way. For $kT < kT_c = \epsilon/\ln q$, the minimum of $f(\rho)$ occurs at $\rho = 0$. Just above T_c the mean value of ρ is obtained by minimizing the first two terms in (6). Since $(\epsilon - kT\ln q)$ is proportional to $(T_c - T)$ this yields

$$\rho \sim (T - T_c)^{(d-1)/2} \tag{7}$$

and since the internal energy is just $\rho\epsilon$, one has

$$\mathbf{C}(T) = \epsilon d\rho/dT \sim \epsilon(T - T_c)^{(d-3)/2} \tag{8}$$

This yields the correct square root divergence for $d = 2$ but predicts a finite value for $\mathbf{C}$ at T_c when $d = 3$.

The focus of this paper is on Eq. (5). Although it seems very hard to do calculations for all values of n and N, the special case, $n = 2$, allows a critical evaluation of the central result in IA's approximation.[10] It may be emphasized that, although IA are interested in the limit $n \to \infty$ along with $N \to \infty$ at fixed ρ, their approximation does not specifically utilize the limit $n \to \infty$ and should apply equally for fixed n. Our studies confirm the known result[6]

$$\ln(\lambda_2/4) \approx -\pi^2/N^2 \tag{9}$$

for the two-dimensional K-model, in agreement with IA. However, in three dimensions, we prove that

$$\ln(\lambda_2/16) \approx -\pi/(N^2\ln N) \tag{10}$$

This proves that Eq. (5) is not correct for $d = 3$. It fails also for $d > 3$ where the correct variation is $1/N^{d-1}$.

Unfortunately, from these special results for $n = 2$ we cannot claim to have found a general formula to replace Eq. (5), as is really required.

However, let us make an *ansatz* that generalizes (9) and (10) to all values of n. For a given dimensionality, this ansatz requires λ_n for all n such that n/N^{d-1} is small to have the same N dependence as λ_2 when $N \to \infty$. In addition, for thermodynamic consistency, we need $N^{-(d-1)}\ln(\lambda_n/q^n)$ in (4) to be a function of ρ only, thereby requiring

$$\ln(\lambda_n/q^n) \approx -N^{(d-1)}\Lambda(n/N^{d-1}) \tag{11}$$

for $N \to \infty$ with n/N^{d-1} small but not necessarily vanishing. For $d = 2$ this ansatz predicts

$$\ln(\lambda_n/2^n) \sim -n^3/N^2 = -N\rho^3 \tag{12}$$

in agreement with (5) which gives the exact square root divergence in (8). For $d = 3$ the ansatz predicts

$$\ln(\lambda_n/4^n) \sim -n^2/\left[N^2\ln(N^2/n)\right] = N^2\rho^2/\ln\rho \tag{13}$$

Inserting this into (4) yields

$$f(\rho) = (\epsilon - kT\ln q)\rho - b'kT\rho^2/\ln\rho + \text{higher-order terms} \tag{14}$$

so that $\mathbf{C}(T) \sim \ln(T - T_c)$. This result is in disagreement with the prediction of IA that $\mathbf{C}(T)$ remains finite at T_c. However, the divergence is much weaker than in two dimensions.

4. ASYMPTOTIC BEHAVIOR OF THE LARGEST EIGENVALUE OF THE $n = 2$ BLOCK

For finite N, the $n = 2$ block of the transfer matrix can be constructed easily by counting the number of ways the state of a layer goes into the states of the next layer. Many of these states are symmetrically related because of the translational symmetry of the system, and this allows one to consider a reduced matrix for which the basis set consists of each class of symmetrically related states.[12]

For the two-dimensional K-model there are $N' = N/2$ sites in each layer and so there will be $N'/2$ reduced basis states (we shall consider only even values of N'). The reduced transfer matrix has the form

$$\mathbb{Q}_{i,j} = 2\delta_{i,j} + \delta_{i,j+1} + \delta_{i+1,j} + \delta_{i,(N/4)-1}\delta_{j,(N/4)} \tag{15}$$

The eigenvalues of this matrix (which is almost a Toeplitz matrix) are simply $4\cos^2(\theta_p/2)$ where $\theta_p = (2p-1)\pi/N'$ with p going from 1 to $N'/2$. The largest eigenvalue λ_2 is therefore $4\cos^2(\pi/N)$ which behaves as $\lambda_2 \approx 4(1 - \pi^2/N^2)$ when $N \to \infty$, so yielding the result quoted in (9). This agreement lends confidence to the ansatz introduced in the previous section.

For the three-dimensional IA model construction of the transfer matrix is quite straightforward but we have not succeeded in completely diagonalizing the $n = 2$ block. However, it is possible to obtain the asymptotic behavior of the largest eigenvalue of the $n = 2$ block by using random walk techniques[13–15] as we show in the remainder of this section. Think of each of the two holes in a given layer as corresponding to a random walker on a square lattice, the sites of which correspond to the projection of the vertical bonds of the three-dimensional IA lattice onto the (x, y) plane. Each hole on an adjacent layer to the original layer in the IA lattice then corresponds to one of the random walkers moving by one lattice spacing on the square lattice. Each $n = 2$ state of the IA three-dimensional model with M layers has a 1–1 correspondence with a random walk of *two* random walkers on the square lattice with M steps/walker, but with the restriction that after both walkers have taken the same number of steps, they are not both at the same site. Since the starting points of the random walkers are on the same sublattice of the square lattice, one has another obvious restriction, namely, that they will both be on the same sublattice after the same number of steps. We note that this random walk isomorphism extends directly to other dimensionalities (and lattice structures) and to other values of n. For the two-dimensional K-model the random walk lattice is one dimensional. This leads to an important distinction between the IA model and the K-model, namely, that in the K-model the walkers cannot exchange positions (except by using the periodic boundary conditions): this allows the free-fermion method to be exact.

Because of the periodic boundary conditions in the (x, y) plane and the resulting translational symmetry, it is much simpler to consider a *relative* random walk of a single new walker defined as follows: Let the position of the single new walker be the vector position of the first original walker minus the position of the second original walker so that this relative walker is always on a sublattice of the original square lattice. One way to think of this relative walker is as a *giant* who takes large steps on one sublattice only. We can also think of the relative walker as a *midget* who takes smaller steps on the original lattice such that the odd-numbered steps of the midget [e.g., the $(2m + 1)$st step] correspond to the steps of the first original walker [in fact the $(m + 1)$st step] and the even-numbered steps of the midget [e.g., the $(2m + 2)$nd step] correspond to the steps of the second walker [the $(m + 1)$st step] in the opposite direction. Each pair of successive odd-numbered and even-numbered steps of the midget corresponds to one step of the giant on the sublattice. The restriction that the original walkers can never be at the same site at the same time corresponds to the relative random walker (in either giant or midget representation) not being allowed to visit the origin.

For the giant, let C'_M be the total number of random walks with M steps that start on the sublattice containing the origin **o**, but never visit the origin. (The primed quantities will henceforth refer to the giant's walk and the unprimed quantities to the midget's walk.) The finite square lattice contains N^2 lattice sites. Then, the largest eigenvalue of the $n = 2$ block of the transfer matrix is related to C'_M by

$$\lambda_2 = \lim_{M\to\infty} (C'_M)^{1/M} \tag{16}$$

It is most convenient to consider the generating function defined by

$$C'(z) = \sum_{M=0}^{\infty} z^M C'_M \tag{17}$$

because from (16) and the root test, the radius of convergence of $C'(z)$ gives the reciprocal of λ_2. In computing C'_M we shall use an open boundary condition along the z direction on the original three-dimensional IA lattice; this corresponds to allowing the walker to be anywhere on the sublattice at the end of the M-step walk and not necessarily at the starting point as would be required by complete periodic boundary conditions. Although the periodic boundary condition gives a more complicated expression for C'_M, we have shown that the limiting behavior as $M \to \infty$ is the same, as is to be expected. Therefore we have

$$C'_M = \sum_{\mathbf{p}}{}' \sum_{\mathbf{q}}{}' C'_M(\mathbf{p}\to\mathbf{q}) \tag{18}$$

where $C'_M(\mathbf{p}\to\mathbf{q})$ is the number of walks which begin at **p** and end at **q** after M steps avoiding the origin and the primed sums run over all **p** and **q** on the sublattice containing the origin.

The expression of $C'(z)$ in terms of simpler functions follows a procedure used by Montroll for walks which become trapped at the origin.[15] Let $W'_M(\mathbf{p}\to\mathbf{q})$ be the number of ways of going from **p** to **q** in exactly M steps, and $F'_M(\mathbf{p}\to\mathbf{q})$ be the number of ways of going from **p** to **q** for the first time in M steps. The fundamental relation among these quantities is

$$W'_M(\mathbf{p}\to\mathbf{q}) = C'_M(\mathbf{p}\to\mathbf{q}) + \sum_{j=0}^{M} F'_j(\mathbf{p}\to\mathbf{o})\, W'_{M-j}(\mathbf{o}\to\mathbf{q}) \tag{19}$$

because the first term on the right side gives the number of ways of going to **q** avoiding the origin, **o**, whereas the second term gives the number of ways of visiting the origin at least once in M steps. Defining the generating functions

$$G'(z;\mathbf{p}\to\mathbf{q}) = \sum_{M=0}^{\infty} z^M G'_M(\mathbf{p}\to\mathbf{q}) \tag{20}$$

where G' may be W', C', or F', allows the fundamental relation (19) to be written more simply as

$$W'(z;\mathbf{p}\to\mathbf{q}) = C'(z;\mathbf{p}\to\mathbf{q}) + F'(z;\mathbf{p}\to\mathbf{o})W'(z;\mathbf{o}\to\mathbf{q}) \tag{21}$$

Next, define the overall generating functions

$$G'(z) = \sum_{\mathbf{p}}{}' \sum_{\mathbf{q}}{}' G'(z;\mathbf{p}\to\mathbf{q}) \tag{22}$$

where, again, $G' = W'$, C', and F' in turn. Summing (21) over $\mathbf{p}$ and $\mathbf{q}$ on the sublattice and using the translational invariance of W' and F' (but not of C') on $\mathbf{p}-\mathbf{q}$, one obtains

$$N_s^2 W'(z) = N_s^2 C'(z) + F'(z)W'(z) \tag{23}$$

because the sublattice has $N_s \equiv \frac{1}{2}N^2$ lattice sites; therefore, one has

$$C'(z) = W'(z)\left[1 - F'(z)/N_s^2\right] \tag{24}$$

Expressions for $W'(z)$ and $F'(z)$ are well known[13–15] and will not be rederived[6]: we have

$$F'(z) = W'(z)/W'(z;\mathbf{o}\to\mathbf{o}) \tag{25}$$

$$W'(z) = N_s\left[1 - zw_1'(\mathbf{0})\right]^{-1} \tag{26}$$

$$W'(z;\mathbf{o}\to\mathbf{o}) = N_s^{-1}\sum_{\mathbf{k}'}\left[1 - zw_1'(\mathbf{k}')\right]^{-1} \tag{27}$$

where the $\mathbf{k}'$ are the reciprocal vectors for the finite sublattice with components k_i', $i = 1, 2, \ldots, d-1$, and $w_1'(\mathbf{k}')$ is the Fourier transform of the giant's single-step walk, i.e.,

$$w_1'(\mathbf{k}') = \sum_{\mathbf{p}}\left[\exp(i\mathbf{k}'\cdot\mathbf{p})\right]w_{\mathbf{p}}' \tag{28}$$

in which the sum runs only over lattice sites $\mathbf{p}$ to which the giant can go in a single step from the origin, in $w_{\mathbf{p}}'$ distinct ways. As the total number of allowed single steps of the giant is q^2 we have the relation $\sum_{\mathbf{p}} w_{\mathbf{p}}' = q^2$.

Now, the relation (24) becomes

$$C'(z) = N_s\left[1 - zw_1'(\mathbf{0})\right]^{-1}\left(1 - \left\{\left[1 - zw_1'(\mathbf{0})\right]\sum_{\mathbf{k}'}\left[1 - zw_1'(\mathbf{k}')\right]^{-1}\right\}^{-1}\right) \tag{29}$$

At first glance it would appear that this expression has a singularity at

[6] Montroll uses P in place of W' and there is the inconsequential difference that P is a probability rather than a number of walks. The sum over M for $F'(z)$ in our definition goes from 0 to ∞ and not from 1 as in these references. This is the reason why we do not have a δ-function term in Eq. (25).

$z = 1/w_1'(\mathbf{0}) = 1/q^2$. However, this is not so, as can be seen by expanding the sum in the denominator about $z = 1/w_1'(\mathbf{0})$. Writing $X = [1 - zw_1'(\mathbf{0})]$, one has

$$C'(z) = N_s X^{-1}\left(1 - X^{-1}\{X^{-1} + a_0 + O[X]\}^{-1}\right) \tag{30}$$

where a_0 is a constant. Thus $C'(z)$ has a finite limit, namely, a_0, when $z \to 1/w_1'(\mathbf{0})$. Hence the radius of convergence of $C'(z)$ is determined by the smallest zero of the denominator which, by (24) and (25), is the zero of $W'(z; \mathbf{o} \to \mathbf{o})$, that lies closest to $z = 0$. We therefore need the solution of

$$W'(z; \mathbf{o} \to \mathbf{o}) = 0 \tag{31}$$

It is possible to analyze the above equation completely to obtain our results. However, it is also possible to utilize some asymptotic results obtained by Montroll,[15] by considering the midget's walk on the original lattice, and this is the procedure we follow in this paper. For the midget, using (20), we define

$$W(z; \mathbf{o} \to \mathbf{o}) = \sum_{M=0}^{\infty} z^M W_M(\mathbf{o} \to \mathbf{o}) \tag{32}$$

But as it is not possible for the midget to come back to the starting point in an odd number of steps, $W_{2M+1}(\mathbf{o} \to \mathbf{o})$ vanishes for all values of M. Also the relation between the midget's walk and the giant's walk shows that $W_M'(\mathbf{o} \to \mathbf{o}) = W_{2M}(\mathbf{o} \to \mathbf{o})$. Using these in (32), we find

$$\begin{aligned} W(z; \mathbf{o} \to \mathbf{o}) &= \sum_{M=0}^{\infty} z^{2M} W_{2M}(\mathbf{o} \to \mathbf{o}) \\ &= \sum_{M} z^{2M} W_M'(\mathbf{o} \to \mathbf{o}) \\ &= W_M'(z^2; \mathbf{o} \to \mathbf{o}) \end{aligned}$$

from (20). Hence the square z_0^2 of the solution of $W(z_0; \mathbf{o} \to \mathbf{o}) = 0$ will give the relevant zero of $W'(z; \mathbf{o} \to \mathbf{o})$.

For the midget walking on the original lattice, one has a relation similar to (27), namely,

$$W(z; \mathbf{o} \to \mathbf{o}) = N^{-2} \sum_{\mathbf{k}} \left[1 - zw_1(\mathbf{k})\right]^{-1} \tag{33}$$

where, for general dimensionality, the $\mathbf{k}$ are the reciprocal vectors for the finite $(d-1)$-dimensional hypercubic lattice with components $k_i = 2\pi r_i / N$ with $r_i = 1, 2, \ldots, N$ while

$$w_1(\mathbf{k}) = \sum_{\mathbf{p}} \left[\exp(i\mathbf{k} \cdot \mathbf{p})\right] = 2 \sum_{i=1}^{d-1} \cos \mathbf{k}_i \tag{34}$$

in which the sum runs only over the lattice sites $\mathbf{p}$ which are nearest neighbors of the origin. We therefore need the solution of

$$W(z;\mathbf{o}\to\mathbf{o}) = N^{-(d-1)}\sum_{\mathbf{r}}\left[1 - 2z\sum_{i=1}^{d-1}\cos(2\pi r_i/N)\right]^{-1} = 0 \qquad (35)$$

where $\mathbf{r} = (\mathbf{r}_1, \ldots, \mathbf{r}_{d-1})$ runs over the reciprocal lattice sites.

The sum in (35) can be evaluated very easily[15] for $d = 2$ giving

$$W(z;\mathbf{o}\to\mathbf{o}) = (1 - 4z^2)^{-1/2}(1 + x^N)/(1 - x^N) \qquad (36)$$

where $x = [1 - (1 - 4z^2)^{1/2}]/2z$. Hence a zero occurs when $1 + x^N = 0$, whose solution is $z^2 = \frac{1}{4}\sec^2[(2p - 1)\pi/N]$ with $p = 1, \ldots, N$. The zero closest to the origin is at $z^2 = \frac{1}{4}\sec^2(\pi/N)$. The radius of convergence of $C'(z)$ for $d = 2$ is therefore $\frac{1}{4}\sec^2(\pi/N)$. The reciprocal of this radius then gives $\lambda_2 = 4\cos^2(\pi/N)$, which is precisely the expression we obtained by diagonalizing the transfer matrix at the beginning of this section.

For the three-dimensional IA model the sum in (35) cannot be evaluated in closed form but the asymptotic behavior of $W(z;\ \mathbf{o}\to\mathbf{o})$ has been determined by Montroll[15] to be[7]

$$W(z;\mathbf{o}\to\mathbf{o}) = 1/\left[N^2(1 - 4z)\right] + \pi^{-1}\ln N^2 + c_2 + c_3/N^2 + \cdots \qquad (37)$$

as $N\to\infty$ with $|1 - 4z|N^2$ sufficiently small. The relevant zero of $W(z;\mathbf{o}\to\mathbf{o})$ may be determined from the first two terms to be

$$z_0 \approx 1/4 + \pi/(8N^2\ln N) \qquad (38)$$

Therefore, for the IA model with $d = 3$ we have $\lambda_2 = 1/z_0^2 \approx 16[1 - \pi/(N^2\ln N)]$ and $\ln(\lambda_2/16) \approx -\pi/(N^2\ln N)$ as stated previously.

Following Ref. 14, the relevant asymptotic behavior of $W(z;\mathbf{o}\to\mathbf{o})$ for higher dimensions can be obtained as

$$W(z;\mathbf{o}\to\mathbf{o}) = \left[N^{d-1}(1 - qz)\right]^{-1} + N^{-(d-3)}\sum_{\mathbf{r}}\left(\sum_i r_i^2\right)^{-1} + \text{higher-order terms} \qquad (39)$$

where the first term represents the contribution from $\mathbf{r} = \mathbf{0}$ while in the second term $\mathbf{r} = \mathbf{0}$ is excluded from the summation. Replacing the summation by an integral, in polar coordinates, from $r = 1$ to $r = a(N - 1)$ where a is a constant, the zero of $W(z;\mathbf{o}\to\mathbf{o})$ is found to vary as $(1 - qz) \sim N^{-(d-1)}$ which gives $\lambda_2 \sim q^2(1 - c/N^{d-1})$. Therefore for $d > 3$ our ansatz suggests that $g_n(N)$, as defined after (3), remains bounded as $N\to\infty$

[7] This is Montroll's Eq. (B37) with two notational differences, namely, our z is 1/4 of his z and our N^2 is his N.

which yields a quadratic, ρ^2, term in the expansion of the free energy. This in turn gives a finite discontinuity in the specific heat. Thus, $d = 3$ is the critical dimensionality for the K-model generalized to arbitrary dimensions. For continuous dimensionalities in the range $1 < d < 3$ we believe (based on our ansatz and on our analysis of the random walk formula analytically continued to nonintegral dimensions) that (6) is correct. This gives $\alpha = (3 - d)/2$ for $1 < d < 3$.

A parallel analysis has also been carried out for the three-dimensional lipid analog model, mentioned in the Introduction: a logarithmic term of the same form as obtained for the three-dimensional IA model is again found.

5. CONCLUSION

We have obtained the exact asymptotic behavior of the largest eigenvalue of the $n = 2$ block of the transfer matrix for the IA dimer model in all dimensions. Together with the ansatz explained in Sections 2 and 3 these results suggest the following behavior of the specific heat, $\mathbf{C}(T)$, and its exponents α and α':

for $T < T_c$, $\alpha' = 0$ (finite) in all dimensions [with $\mathbf{C}(T) \equiv 0$];
for $T > T_c$;
$\alpha = 1/2$ for $d = 2$ in agreement with the exact solution[3] and $\alpha = (3 - d)/2$ more generally for $1 < d < 3$;
$\alpha = 0$ (log divergence) for $d = 3$;
$\alpha = 0$ (finite) for $d > 3$.

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