Exact Entropy of Dimer Coverings for a Class of Lattices in Three or More Dimensions

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We construct a class of lattices in three and higher dimensions for which the number of dimer coverings can be determined exactly using elementary arguments. These lattices are a generalization of the two-dimensional kagome lattice, and the method also works for graphs without translational symmetry. The partition function for dimer coverings on these lattices can be determined also for a class of assignments of different activities to different edges.

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The dimer model is a well-known problem in classical lattice statistics. The Ising model can be reformulated as a dimer model on a modified graph [1]. The dimer model is a simple, nontrivial but analytically tractable model that provides a starting point for the studies of systems of nonspherical molecules with hard-core interactions [2]. The latter can show a variety of geometrical phase transitions, e.g., in liquid crystals [3]. Recently there has been a lot of interest in quantum dimer models, to describe the ground states of frustrated quantum antiferromagnets, and some exotic phases expected in assemblies of hard-core bosons on pyrochlore lattices [4].

Kasteleyn's pioneering solution of the problem for general two-dimensional planar lattices [5] led to a lot of follow-up work on the two-dimensional problem [2], but the problem in higher dimensions is much less studied. For a nonzero fraction of sites not covered by dimers, it is known that there is no phase transition as a function of the density of dimers [6]. This result is similar to the Lee-Yang circle theorem and is valid for arbitrary graphs with different activities for different bonds. Huse *et al.* have given nonrigorous arguments that the dimer-dimer orientational correlations have a power-law decay in all dimensions on bipartite lattices [7]. For graphs made of corner-sharing triangles, where each vertex has a coordination number four, the entropy of dimer coverings per site can be determined exactly in any dimension [8]. Huang *et al.* studied the dimer problem in three dimensions, where the lattice is a stack of 2D planes, but the problem is not fully three-dimensional as the dimers were confined to lie in planes [9]. Priezzhev calculated exactly the number of a *subset* of all dimer configurations on the cubic lattice [10]. For some anisotropic dimer models in three dimensions, the phase transition point can be determined exactly [11], but not the total entropy.

Elser [12] provided a simple argument to show that entropy per site of dimer covering of the kagome lattice [Fig. 1(a)] has a very simple form and equals $\frac{1}{3}\log 2$. This argument was extended to arbitrary graphs made of corner-sharing triangles by Misguich *et al.* [8]. This problem was investigated again recently by Wang and Wu [13]. The arguments of Misguich *et al.* are valid only for graphs in which each vertex has coordination number 4, and belongs to exactly two triangles. In this Letter, we present an argument that is similar to Elser's, but is valid for graphs in which the coordination number of vertices is not restricted to 4. Our arguments are applicable to a large class of lattices with arbitrary dimension, and also to graphs

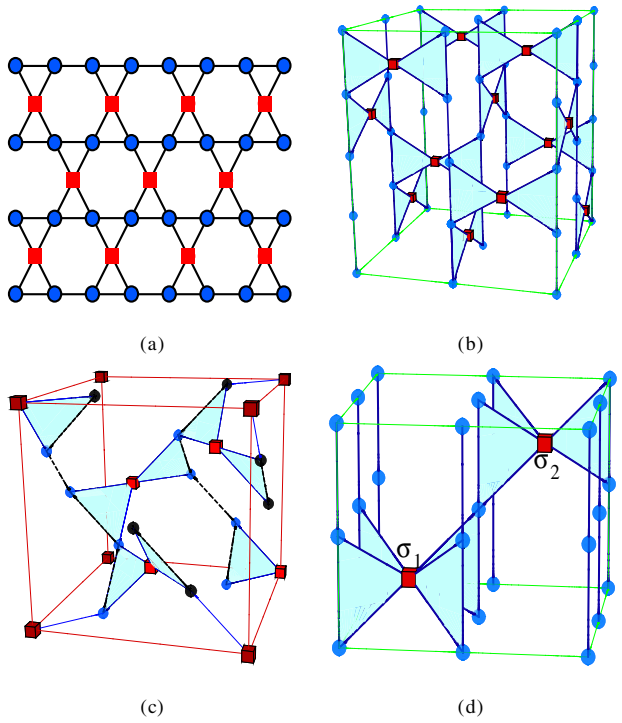

FIG. 1 (color online). Some examples of lattices for which the exact entropy is calculated in this Letter. (a) The kagome lattice. (b) A three-dimensional lattice with corner-sharing triangles. (c) The unit cell of the $Na_4Ir_3O_8$ lattice. There are 12 iridium atoms per unit cell (shown as red cubes or blue spheres). Sodium and oxygen atoms are not shown. The (red) cubes mark the articulation points of the lattice and the spheres mark the rest. The lattices in (b) and (c) can be shown to be equivalent. (d) Unit cell of a lattice obtained by the decoration procedure discussed in text.

without translational invariance. Some examples of lattices where our method can be used are shown in Fig. 1.

For simplicity of presentation, we first describe our arguments as applied to the kagome lattice [shown in Fig. 1(a)] and discuss the generalizations later. We select a *suitable* subset of the sites of the lattice. The condition for the choice of sites in this subset will become clear with the example below. We will call these the red sites, and denote the set by $\mathcal{R}$. In the figures they are marked with (red) squares or cubes while the remaining sites are shown with (blue) circles or spheres. For the kagome lattice, we choose the red sites to be the sites of one of its three sublattices [Fig. 1(a)]. For any dimer covering $\mathcal{C}$ of the lattice, to each red site s of the lattice, we assign a discrete variable σ_s. This variable takes only two possible values: σ_s is $+1$ if the other vertex of the dimer covering s is above s, and -1 if it is below.

We now arbitrarily choose a value of σ_s for each site s in $\mathcal{R}$. Let us denote this set by $\{\sigma_s\}$, and ask how many dimer configurations are consistent with $\{\sigma_s\}$. We note that if $\sigma_s = +1$, then the two bonds connecting the site s to sites below it would not be used in dimer coverings. Then we can safely delete these bonds, and consider dimer covering of the remaining graph. Similarly, if $\sigma_s = -1$, we remove two bonds connecting s to sites above. If we do this for all sites of the red sublattice, the full lattice breaks up into a set of mutually disconnected chains of the type shown in Fig. 2.

It is easy to see that each chain can be covered by dimers in at most one way. For example, in Fig. 2, for the top chain, starting from left, we see that site 1 has to be matched with site 3, and then site 2 has to be matched with site 4. And so on.

It is convenient to adopt the boundary conditions that a site on the *right boundary* can be either covered by a dimer or left uncovered [14]. Then there is exactly one dimer covering consistent with any given set $\{\sigma_s\}$. The number of red sites is $N/3$, and so the number of different possible choices of $\{\sigma_s\}$ is $2^{N/3}$. This is also the total number of dimer coverings.

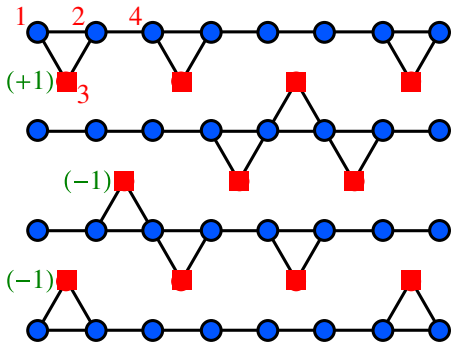

FIG. 2 (color online). On deleting two edges from each (red) square, the kagome lattice breaks into disconnected chains. The values of the σ variables at some of the (red) squares are indicated by the numbers in parentheses.

We define entropy per site C by the relation that number of dimer coverings increases as $\exp(CN)$, for a lattice with N sites, for large N. Then for the kagome lattice,

$$C = \tfrac{1}{3}\log 2. \tag{1}$$

The above argument can be generalized to more general connected graphs made of corner-sharing triangles. Consider, for example, the lattices shown in Figs. 1(b) and 1(c). To construct the lattice of Fig. 1(b), we start with a simple cubic lattice with only the vertical edges present. For each pair of neighboring vertical chains, we add a red site in between every fourth pair of opposing edges and join it to the ends of the edges. The opposing edges in between which we add these additional sites are displaced with respect to each other so that no two triangles share an edge, as shown in Fig. 1(b).

The unit cell of a hyperkagome lattice is shown in Fig. 1(c). There are experimental materials like the sodium iridate ($Na_4Ir_3O_8$) where this structure, known as the GGG structure, is realized in nature [15]. To obtain this lattice, we start from the pyrochlore lattice, which consists of corner-sharing tetragons, their centers forming a diamond lattice. The hyperkagome lattice in Fig. 1(c) is obtained by removing one site from each tetragon to leave a lattice of corner-sharing triangles. In fact, the graph of Fig. 1(c) can be shown to be isomorphic to 1(b).

For these cases, we choose the red sites as shown in Figs. 1(b) and 1(c), and as in the kagome case, to each red site assign a binary variable σ, specifying whether the dimer covering that site belongs to one or the other of the two triangles meeting at that point. Then, as before, we ask how many different dimer coverings are consistent with an arbitrary choice of $\{\sigma_s\}$.

If now, from each red site, we delete two edges that are not consistent with the given choice, the lattice breaks up into mutually disconnected chains of single edges and triangles similar to Fig. 2. These chains have a ''backbone'' of bonds in the z direction in Fig. 1(b), and a zigzag array of roughly vertical lines in Fig. 1(c) (shown by black dashed lines). If we assume free boundary conditions on one (say, the top) face, there is a unique dimer covering of the lattice consistent with any arbitrary choice of $\{\sigma_s\}$. For large N, the number of red sites is $N/3$ (up to surface correction terms), and the number of dimer coverings is $2^{N/3}$. Hence, for both the three-dimensional lattices shown in Figs. 1(b) and 1(c), we get

$$C = \tfrac{1}{3}\log 2. \tag{2}$$

For graphs in which each vertex is shared by two triangles, this result was obtained earlier by Misguich *et al.* [8]. But our argument is extended easily to graphs where more than two triangles meet at a single vertex. Consider a graph formed by the vertices and edges of a collection of

nonintersecting (possibly nonstraight) lines, which may be imagined as embedded in a d-dimensional lattice ($d \geq 2$). We add a number of additional vertices not lying on any line and call these additional vertices red vertices. The red vertices can be labeled by integers $1, 2, \ldots, N_r$. For the jth red vertex, we choose a positive integer $r_j \geq 1$, choose r_j different edges from the original lines, and join both ends of each edge to the red vertex j by additional edges. Then the jth red vertex is the shared corner vertex of r_j triangles, and its coordination number is $2r_j$. We ensure that the edges selected do not already have some vertex in common, and that no edge of the original lines is selected more than once, so that no edge belongs to more than one triangle. This defines the graph $\mathcal{L}$ for which we want to calculate the number of possible dimer covers.

An example of such a graph is shown in Fig. 1(d). The lattice consists of vertices of a simple cubic lattice, labeled by coordinates (m_1, m_2, m_3), where m_1, m_2, and m_3 are integers. We start with edges only along the z direction. The lattice graph consists of disconnected vertical one-dimensional chains. We add extra connections to this graph to make it three-dimensional as follows: we pick an elementary cube of the lattice, add an extra vertex at the center of the cube, and connect it to two or more of the vertical edges of the cube by triangles [an example is shown in Fig. 1(d)]. We choose a unit cell of period p_1, p_2, p_3, where p_1, p_2, p_3 are integers >1. [In the case shown in Fig. 1(d), $p_1 = p_2 = p_3 = 2$.] We choose some extra cubes within the unit cell to connect this way, and then repeat this pattern to get a translationally invariant lattice. We ensure that these ''decorations'' are selected such that the resulting graph is connected, and that no edge belongs to more than one triangle.

In the example shown in Fig. 1(d), we chose two diagonally opposite cubes within the unit cell, and add a site each at the center of each cube. The site with coordinates $(1/2, 1/2, 1/2)$ is connected to all its four neighboring vertical edges, but we connect the site at $(3/2, 3/2, 3/2)$ to only three of its neighboring vertical edges.

Then, as before, at each red vertex j, we define a variable σ_j that takes r_j possible values. There is a unique dimer cover of $\mathcal{L}$ consistent with a particular arbitrarily chosen set of values $\{\sigma_s\}$. It follows that the total number of dimer covers of this graph Ω is given by

$$\Omega = \prod_{j=1}^{N_r} r_j. \tag{3}$$

In Fig. 1(d), we have two red vertices per unit cell, and $r_1 = 4$ and $r_2 = 3$. There are 10 sites per cell. Hence the entropy per site for the lattice shown in Fig. 1(d) is $\frac{1}{10}\log 12$.

It is easy to see that the arguments can be trivially extended to other choices of decorations, and also to higher dimensional lattices.

Our treatment can also be extended to the case where different edges are associated with different activities. This is illustrated most easily for the kagome lattice. Let us associate activity z_1 with a horizontal edge of the lattice [Fig. 1(a)]. Let us assume that the activity for a nonhorizontal edge is z_2 if it belongs to an up-pointing triangle, and z_3 if it belongs to a down-pointing triangle. Then, for a particular $\{\sigma_s\}$ having n values $+1$, the weight of the unique dimer cover is easily seen to be $z_2^n z_3^{N/3-n} z_1^{N/6}$. Summing over all choices of $\{\sigma\}$, we get total partition function $\Omega(z_1, z_2, z_3) = (z_2 + z_3)^{N/3} z_1^{N/6}$. This answer differs from that obtained by Wang and Wu [13], as our choice of edge weights differs from theirs.

It is easy to see that this same method works for the higher dimensional graphs [e.g., for the lattice shown in Fig. 1(d)], so long as (a) the two edges at a red vertex belonging to the same triangle always have the same weight, and (b) all edges not having a red end vertex have the same weight.

For example, consider the lattice shown in Fig. 1(d). In the unit cell shown in Fig. 1(d) there are seven triangles. Let the nonvertical edges of the respective triangles have the activities $z_1, z_2, \ldots, z_4$ for the bonds in the 4 triangles meeting at $(1/2, 1/2, 1/2)$, z_5, z_6, z_7 for the bonds meeting at the site $(3/2, 3/2, 3/2)$ and z_0 be the activity for the vertical edges. Then the free energy per site is $(1/10)\log[(z_1 + z_2 + z_3 + z_4)(z_5 + z_6 + z_7)z_0^3]$.

Note that the fact that σ variables are completely uncorrelated suggests that orientational correlations between dimers on these lattices may be short ranged. In fact, for the kagome lattice, the dimer-dimer orientational correlation function has been shown to be zero for all separations ≥ 2 unit cell spacings [13]. It is easy to see that this is true also of the lattice in Fig. 1(c) or 1(d).

We should emphasize that though the $\{\sigma_s\}$ variables are local, independent variables that uniquely specify the allowed dimer configurations, the procedure of finding the dimer configuration corresponding to a given $\{\sigma_s\}$ is nontrivial and nonlocal. If we change σ_s at only one red site, it changes the orientations of dimers very far along the two affected vertical chains.

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