Exact Solution of a Three-Dimensional Dimer System

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Abstract

We consider a three-dimensional lattice model consisting of layers of vertex models coupled with interlayer interactions. For a particular non-trivial interlayer interaction between charge-conserving vertex models and using a transfer matrix approach, we show that the eigenvalues and eigenvectors of the transfer matrix are related to those of the two-dimensional vertex model. The result is applied to analyze the phase transitions in a realistic three-dimensional dimer system.

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An outstanding unsolved problem in the statistical mechanics of critical phenomena is the pursuit of exact solutions for realistic three-dimensional (3D) systems. While a large number of 2D systems have yielded to analyses [1], only a limited number of 3D systems have been solved. They include the 3D Ising model solved by Suzuki [2], the Zamolodchikov model [3] solved by Baxter [4] and its more recent $N$-state extension by Bazhanov and Baxter [5]. However, these models invariably suffer defects in one way or another: The Suzuki model turns out to be a 2D system in disguise, while the Zamolodchikov model and its extension involve unphysical negative Boltzmann weights. Similarly, a continuous string model in general $d$ dimensions solved by two of us [6] also involves negative weights. The solution of realistic physical 3D models has remained very much an open problem.

One approach toward solving realistic 3D models is to build from 2D systems. Indeed, such an approach has been suggested [7] and applied with some success recently [8,9]. However, in these considerations much attention has been placed to the algebraic structure of the transfer matrix and the associated Yang-Baxter equation, to the extent of masking the elegance of the solution. Here, we present a more general formulation, and deduce its solution via an alternate and yet much simpler consideration. The result is applied to analyze a realistic layered 3D dimer system.

Consider a simple-cubic lattice $\mathcal{L}$ of size $K \times M \times N$ with periodic boundary conditions. Regard $\mathcal{L}$ as consisting of $K$ copies of square lattices, of $M$ rows and $N$ columns each and stacked together as shown in Fig. 1. For simplicity, we shall speak of the square lattices as “layers” of $\mathcal{L}$. Label sites of $\mathcal{L}$ by indices $\{m, j, k\}$, with $1 \leq m \leq M$, $1 \leq j \leq N$ and $1 \leq k \leq K$. Within each layer of $\mathcal{L}$ define a 2D $q$-state vertex model whose lattice edges can be in $q$ distinct states. Label the state of the horizontal (vertical) edge incident at the site $\{m, j, k\}$ in the direction of, say, decreasing $\{m, j\}$ by $\alpha_{mjk}$ ($\beta_{mjk}$). It is convenient at times to suppress the subscripts $m$ and/or $k$ by adopting the notation

$$ \beta_{m+1,j,k} \to \beta'_j, \quad \beta_{m,j,k+1} \to \tilde{\beta}_j; \quad (1) $$

and similarly for the $\alpha$’s. Associate vertex weight $W_{mjk}$ to site $\{m, j, k\}$ which is a function
of the configuration \( C_{m,j,k} \equiv \{ \alpha_{mjk}, \beta_{mjk}, \alpha_{m,j+1,k}, \beta_{m+1,j,k} \} \rightarrow \{ \alpha_j, \beta_j, \alpha_{j+1}, \beta_j' \} \) of the four edges incident at the site \( \{m,j,k\} \). Let the \( \{m,j\} \) sites of two adjacent layers \( k \) and \( k + 1 \) interact with a Boltzmann factor \( B_{mjk} \) which in the most general case is a function of the configurations \( C_{m,j,k} \) and \( C_{m,j,k+1} \) of the eight edges incident to the two sites. Then, the problem at hand is the evaluation of the partition function

\[
Z_{MNK} = \sum_{\alpha_{mjk}} \sum_{\beta_{mjk}} \prod_{k=1}^{K} \prod_{m=1}^{M} \prod_{j=1}^{N} (B_{mjk} W_{mjk})
\]  

where the summations are taken over all edge states \( \alpha_{mjk} \) and \( \beta_{mjk} \), and the per-site “free energy” for any \( K \)

\[
f_K = K^{-1} \lim_{M,N \to \infty} (MN)^{-1} \ln Z_{MNK}.
\]  

The transfer matrix: The partition function (2) can be evaluated by applying a transfer matrix in the vertical direction. In a horizontal cross section of \( L \) there are \( NK \) vertical edges. Let \( \{ \beta_m \} \equiv \{ \beta_{mjk} | 1 \leq j \leq N, 1 \leq k \leq K \} \), \( 1 \leq m \leq M \) denote the states of these \( NK \) vertical edges, and define a \( 2^{NK} \times 2^{NK} \) matrix \( T \) with elements

\[
T(\{\beta_m\}, \{\beta_{m+1}\}) = \sum_{\alpha_{mjk}} \prod_{k=1}^{K} \prod_{j=1}^{N} (B_{mjk} W_{mjk}), \quad 1 \leq m \leq M.
\]  

Then one has

\[
Z_{MNK} = \sum_{\beta_{mjk}} \prod_{m=1}^{M} T(\{\beta_m\}, \{\beta_{m+1}\})
= \text{Tr} T^M
\sim \Lambda_{\text{max}}^M
\]  

where \( \Lambda_{\text{max}} \) is the largest eigenvalue of \( T \).

It is clear that we need to restrict considerations to models which are soluble when the interlayer interaction is absent, or \( B_{mjk} = 1 \). This leads us to build 3D systems from soluble 2D models. It is also clear that the interlayer interaction \( B_{mjk} \) should be such that the overall interlayer factor \( \prod_{m,j,k} B_{mjk} \) can be conveniently treated. For this purpose we restrict considerations to 2D charge-conserving models.
For definiteness let the labels $\alpha_{mjk}$ and $\beta_{mjk}$ take on a set $I$ of $q$ integral values. For example, one can take $I = \{+1, -1\}$ for $q = 2$ and $I = \{+1, 0, -1\}$ for $q = 3$. A 2D vertex model is charge-conserving if its vertex weights are non-vanishing only when

$$\alpha_j + \beta_j = \alpha_{j+1} + \beta'_{j} \quad \text{(charge conservation)}$$

holds at all sites. Examples of charge conserving models are the $q = 2$ ice-rule models, the $q$-state string model, the $q = 3$ Izergin-Korepin model, and others.

A direct consequence of the charge-conserving rule (6) is deduced by summing (6) from $j = 1$ to $j = N$. This yields

$$y_k = \frac{1}{N} \sum_{j=1}^{N} \beta_j = \frac{1}{N} \sum_{j=1}^{N} \beta'_{j}$$

showing that the quantity $-1 \leq y_k \leq 1$ is independent of $m$. (For ice-rule models this fact is well-known.)

Next one introduces the interlayer interaction

$$B_{mjk} = \exp\left(h(\alpha_{j}\bar{\beta}_j - \tilde{\alpha}_{j+1}\beta'_j)\right).$$

Since the negation of $h$ corresponds to a reversal of the layer numberings, without loss of generality we can take $h \geq 0$. We now show quite generally that the interlayer interaction (8) leads to a considerable simplification of the transfer matrix. Consider first the product

$$\prod_{j=1}^{N} B_{mjk} = \exp\left(h \sum_{j=1}^{N} (\alpha_{j}\bar{\beta}_j - \tilde{\alpha}_{j+1}\beta'_j)\right).$$

Summing over (8), or $\alpha_i + \beta_i = \alpha_{i+1} + \beta'_i$, for $i = \{1, j - 1\}$ and $i = \{j + 1, N\}$ for the layer $k + 1$, one obtains, respectively, the identities

$$\alpha_j = \alpha_1 + \sum_{i=1}^{j-1} (\beta_i - \beta'_i), \quad j = 2, 3, \ldots, N$$

$$\tilde{\alpha}_{j+1} = \tilde{\alpha}_1 - \sum_{i=j+1}^{N} (\bar{\beta}_i - \tilde{\beta}'_i), \quad j = 1, 2, \ldots, N - 1$$

where we have used $\tilde{\alpha}_{N+1} = \tilde{\alpha}_1$. Substituting (10) into (9) and making use of the identity $\sum_{j=2}^{N} \sum_{i=1}^{j-1} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N}$ in the first summation in (9), one arrives after a little algebra at
\[ \prod_{j=1}^{N} B_{mjk} = \exp \left( N h (\alpha_1 \tilde{y} - \tilde{\alpha}_1 y) + N h [f(\beta, \tilde{\beta}) - f(\beta', \tilde{\beta}')] \right), \quad (11) \]

where \( f(\beta, \tilde{\beta}) \equiv \sum_{j=2}^{N} \sum_{i=1}^{j-1} \beta_i \tilde{\beta}_j \). The numerical factor \( f(\beta, \tilde{\beta}) \), which is defined for each fixed \( m \), is cancelled in the further product

\[ \prod_{m=1}^{M} \prod_{j=1}^{N} B_{mjk} = \prod_{m=1}^{M} \exp \left( N h (\alpha_{m,1,k} y_{k+1} - \alpha_{m,1,k+1} y_k) \right). \quad (12) \]

As a result, only the conserved quantities \( y_k \) and the state \( \alpha_{m,1,k} \) of the extremities of a row of horizontal edges appear in the product (12). This leads us to rewrite the partition function (4) as

\[ Z_{MNK} = \text{Tr} (T^{\text{eff}})^M \quad (13) \]

where \( T^{\text{eff}} \) is a matrix with elements

\[ T^{\text{eff}}(\{\beta_m\}, \{\beta_{m+1}\}) = \sum_{\alpha_{mjk}} K \prod_{k=1}^{K} \left( e^{Nh \alpha_{m,1,k} (y_{k+1} - y_k - 1)} \prod_{j=1}^{N} W_{mjk} \right). \quad (14) \]

The problem is now reduced to one of finding the largest eigenvalue of \( T^{\text{eff}} \). In fact, expression (11) shows that \( T^{\text{eff}} \) is related to \( T \) by a similarity transformation \( T^{\text{eff}} = S T S^{-1} \) where \( S \) is diagonal. It follows that \( T \) and \( T^{\text{eff}} \) have the same eigenvalues, and their eigenvectors are related. The task is now considerably simpler since one needs only to keep track of the 2D system. The problem is solved if the eigenvalues of the transfer matrix for the 2D vertex model can be evaluated for fixed \( y_k \) and \( \alpha_{m,1,k} \).

The ice-rule model: To illustrate the usefulness of this formulation, we now apply it to layers of ice-rule model with vertex weights \( \{\omega_1, \omega_2, ..., \omega_6\} \) (for standard notations relevant to present discussions see, for example, [10]). Let \( \alpha = +1 \) (−1) denote arrows pointing toward right (left), and \( \beta = +1 \) (−1) arrows pointing up (down). Then one verifies that the charge-conserving condition (3) is satisfied with \( y_k = 1 - 2n_k/N \), where \( n_k \) is the number of down arrows in a row of vertical edges in the \( k \)th layer. Introducing next the interlayer interaction (8), the eigenvalues of the matrix (14) are obtained by applying a global Bethe
ansatz consisting of the usual Bethe ansatz for each layer. The algebra is straightforward
and one obtains

$$Z_{MNK} \sim \max_{1 \leq n_k \leq N} \prod_{k=1}^{K} \left[ \Lambda_R(n_k) + \Lambda_L(n_k) \right]^M, \quad (15)$$

with

$$\Lambda_R(n_k) = e^{-2h(n_{k+1} - n_{k-1})\omega_1^n - n_k} \prod_{j=1}^{n_k} \left( \frac{\omega_3 \omega_4 - \omega_5 \omega_6 - \omega_1 \omega_3 z_j^{(k)}}{\omega_4 - \omega_1 z_j^{(k)}} \right),$$

$$\Lambda_L(n_k) = e^{2h(n_{k+1} - n_{k-1})\omega_4^n - n_k} \prod_{j=1}^{n_k} \left( \frac{\omega_1 \omega_2 - \omega_5 \omega_6 - \omega_2 \omega_4 / z_j^{(k)}}{\omega_1 - \omega_4 / z_j^{(k)}} \right), \quad (16)$$

where $\Lambda_R$ ($\Lambda_L$) refers to the eigenvalue for $\alpha_{m,1,k} = +1$ ($-1$) and, for each $1 \leq k \leq K$, the $n_k$ complex numbers $z_j^{(k)}$, $j = 1, 2, \ldots, n_k$ are the solutions of the Bethe ansatz equations

$$e^{4h(n_{k+1} - n_{k-1})}(z_j^{(k)})^N = (-1)^{n_k+1} \prod_{i=1}^{n_k} \left( \frac{B(z_i, z_j)}{B(z_j, z_i)} \right), \quad j = 1, 2, \ldots, n_k \quad (17)$$

where $B(z, z') = \omega_2 \omega_4 + \omega_1 \omega_3 zz' - (\omega_1 \omega_2 + \omega_3 \omega_4 - \omega_5 \omega_6)z'$. Note that the Bethe ansatz equation (17), which is obtained by imposing the cancellation of unwanted terms in the Bethe ansatz solution, differs from its usual form (see, for example, [14]) in the inclusion of the exponential factor involving $h$. Various special forms of this solution has been given previously [7–9].

A dimer system with interlayer interactions: We now consider a 3D lattice model consisting of layers of honeycomb dimer lattices. The dimers, which carry weights $u, v, w$ along the three honeycomb edge directions, are close packed within each layer and, in addition, interact between layers. For two dimers incident at the same $\{m, j\}$ site in adjacent layers, the interaction energy is given in Table I.

The 2D honeycomb dimer system can be formulated as a five-vertex model, namely, an ice-rule model with the weights [14,15]

$$\{\omega_1, \omega_2, \omega_3, \omega_4, \omega_5, \omega_6\} = \{0, w, v, u, \sqrt{uv}, \sqrt{uv}\}. \quad (18)$$

The 5-vertex model is defined on a square lattice of size $M \times N$ mapping to an honeycomb lattice of $2MN$ sites [14,15]. The mapping is such that the edge state $\alpha = +1$ ($\beta = +1$)
corresponds to the presence of a $v$ ($u$) dimer. It can then be verified that the interlayer interaction given in Table I can be written precisely in the form of \cite{16}, and therefore we can use the ice-rule model results.

Substituting (18) into (15), one obtains

$$Z_{MNK} \sim u^{MNK} \max_{1 \leq n_k \leq N} \prod_{k=1}^{K} \prod_{j=1}^{n_k} \left( \frac{w}{u} + \frac{v}{u} z_j^{(k)} \right)^{M}$$

(19)

with the Bethe ansatz solution

$$z_j^{(k)} = e^{i \theta_j} e^{2h(y_{k+1} - y_k - 1)}, \quad j = 1, 2, \ldots, n_k$$

(20)

where $e^{i \theta_j}$ are $n_k$ distinct $N$th roots of $(-1)^{n_k+1}$. For a given $n_k$, the factor inside the parentheses in (19) attends its maximum if the $\theta_j$’s lie on an arc crossing the positive real axis and extending from $-\pi(1 - y_k)/2$ to $\pi(1 - y_k)/2$. Using (3) this leads to the per-site free energy

$$f_K = \ln u + \max_{-1 \leq y_k \leq 1} \frac{1}{K} \sum_{k=1}^{K} \frac{1}{2\pi} \int_{-\pi(1 - y_k)/2}^{\pi(1 - y_k)/2} \ln \left( \frac{w}{u} + \frac{v}{u} e^{2h(y_{k+1} - y_k - 1)} e^{i \theta} \right) d\theta.$$ 

(21)

This is our main result.

We have carried out analytic as well as numerical analyses of the free energy (21) for $K = 3 \times$ integer. Here we summarize the findings. For $h = 0$, the layers are decoupled and the property of the system is the same as that of the 2D system \cite{14,15}. For large $h$, it is readily seen from Table I that the energetically preferred state is one in which each layer is occupied by one kind of dimers, $u$, $v$, or $w$, and the layers are ordered in the sequence of \{w, v, u, w, v, u, \ldots\}. It is also clear that for large $u$, $v$, or $w$, the system is also frozen with complete ordering of $u$, $v$, or $w$ dimers. These orderings are referred to as the $H$, $U$, $V$, and $W$ phases, respectively. The system can also be in two other phases. A $Y$ phase in which all layers have the same value of $y_k = y$ determined straightforwardly by maximizing (21), or

$$w^2 + v^2 + 2wv \cos \left( \frac{\pi}{2} (1 - y) \right) = u^2,$$

(22)
and an I phase which is the $H$ phase with any of the $w$, $v$, or $u$ layers replaced by layers with $y_k = y$. If the $v$ layer is replaced by a $y$ layer so that the ordering is \{w, y, u, w, y, u, \ldots\}, for example, then $y$ is given by \((22)\) with $v$ replaced by $ve^{\text{th}}$.

The phase diagram is found to be symmetric in $w$, $v$, and $u$. It is then convenient to plot the phase diagram using the coordinates

\[
X = \ln(v/w) \quad Y = (\sqrt{3})^{-1} \ln(vw/u^2)
\]

so that any interchange of the three variables $w$, $v$, and $u$ corresponds to a 120° rotation in the \{X, Y\} plane. The phase diagram for $h < h_0 = 0.2422995...$ is the same as in Fig. 2a but without the $H$ regime. Increasing the value of $h$ one finds the $H$ phase appear in $h_0 < h < h_1 = 0.2552479...$ as shown in Fig. 2a. At $h = h_1$ the I phase appears (Fig. 2b), with its region extending to infinity when $h$ reaches $h_2 = (\ln 3)/4 = 0.2746531...$ (Fig. 2c). When $h$ reaches $h_3 = 0.3816955...$ and higher, the $Y$ phase disappears completely as shown in Fig. 2d. All transitions are found to be of first-order except the transitions between the \{U, V, W\} and $Y$ phases, and between the I and $H$ phases, which are found to be of second-order with a square-root divergence in the specific heat.

In summary, we have presented the formulation of a general 3D lattice model, and applied it to solve a realistic dimer system. The analysis can be extended to include dimer-dimer interactions within each layer \[14\], and further-neighbor interlayer interactions. Details of the present and further analyses will be presented elsewhere. Work has been supported in part by NSF Grant DMR-9313648 and by INTAS Grants 93-1324 and 93-0633. One of us (VP) thanks Prof. D. Kim for discussions.
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[16] To be more precise, (8) leads to Table I with $uu$ and $vv$ interactions $-\epsilon h$ instead of 0. But the two energies are equivalent, since the interacting $uu$ or $vv$ dimers are parallel covering the same A and B sites.
FIGURES

FIG. 1. A three-dimensional lattice model consisting of layered vertex models.

FIG. 2. Phase diagrams of the dimer system. (a) $h_0 < h < h_1$, (b) $h_1 < h < h_2$, (c) $h_2 < h < h_3$, (d) $h > h_3$. 
TABLES

TABLE I. Interaction energy between two dimers incident at the same \(\{m,j\}\) site of adjacent layers. For example, a \(v\) dimer in the \(k\)th layer interacts with a \(u\) dimer in the \((k+1)\)th layer with an energy \(\epsilon h\). Here \(\epsilon = +1 \ (-1)\) if the site is in sublattice A (B).

| layer \(k \rightarrow k+1\) | \(w\) | \(v\) | \(u\) |
|--------------------------|------|------|------|
| \(w\)                    | 0    | \(-h\) | \(h\) |
| \(v\)                    | \(h\) | 0    | \(\epsilon h\) |
| \(u\)                    | \(-h\) | \(\epsilon h\) | 0    |