Exact results for resonating-valence-bond states on two-dimensional (narrow) systems

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It is shown that the problem of calculating spin-spin correlation functions, in the dimer resonating-valence-bond states, on a possibly diluted two-dimensional square lattice, can be formulated in terms of a transfer matrix. The transfer matrix is used for exact numerical calculations of spin-spin correlation functions on ladders up to four units wide. [S0163-1829(96)07241-4]

In the last few years, the class of resonating valence bond (RVB) states has drawn much attention in connection to the long-lasting pursuit of the antiferromagnetic two-dimensional (2D) Heisenberg model ground state.[1,2] Especially important is the case of spin half, which is considered to be relevant to high-T_c superconductors. In this context, simulations had been performed to estimate the spin-spin correlation functions in these states,[3] and particularly the expectation values of the spin half Heisenberg Hamiltonian were calculated for variational considerations. In the two legged ladder lattice the short-range RVB states, which are in the focus of this article, were found to have low energies.[4] Despite this interest these simulations had not been backed by exact results. This article provides a way to extract such results, in the case of the 2D dimer RVB states on a (possibly) diluted lattice, by means of reducing the problem of calculating the spin-spin correlation functions, to the considerably simpler problem of treating a transfer matrix defined on a 1D lattice.

On a general lattice the class of RVB states is defined by[3]

$$|\Psi\rangle=\sum_{\{\Pi\}}\prod_{(\mathbf{i},\mathbf{j})\in\Pi}U(\mathbf{i},\mathbf{j})(\uparrow_{\mathbf{i}}\downarrow_{\mathbf{j}}-\uparrow_{\mathbf{j}}\downarrow_{\mathbf{i}}), \tag{1}$$

where $\{\Pi\}$ are all the possible divisions of the lattice into pairs of sites $(\mathbf{i},\mathbf{j})$, in which any site is a member of one and only one pair, and $U(\mathbf{i},\mathbf{j})$ is nonnegative. For the short-range RVB states $U(\mathbf{i},\mathbf{j})$ has a cutoff. We will restrict $|\Psi\rangle$ to be a dimer RVB state on a square lattice; hence the function $U(\mathbf{i},\mathbf{j})$ is given by

$$U(\mathbf{i},\mathbf{j})=\begin{cases} x & \text{if } \mathbf{i}-\mathbf{j}=\hat{\mathbf{x}},\\ y & \text{if } \mathbf{i}-\mathbf{j}=\hat{\mathbf{y}},\\ 0 & \text{otherwise,}\end{cases} \tag{2}$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors. In this case we can replace $\{\Pi\}$ by the dimer coverings of the lattice, denoted by $\{\Delta\}$.

The spin-spin correlation function in the dimer RVB states is defined by the expectation value[3,5]

$$\mathcal{S}_{\mathbf{ij}}=\frac{\langle\Psi|\mathbf{S_i}\cdot\mathbf{S_j}|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{3}$$

where $\mathbf{i}$ and $\mathbf{j}$ are two sites on the lattice. Two quantities are evaluated for the calculation of this expectation value. The norm

$$\mathcal{D}=\langle\Psi|\Psi\rangle=\sum_{\{\Delta_L,\Delta_R\}}2^{\mathcal{N}_\lambda}y^{n_y}x^{n_x}=y^{MK}\sum_{\{\Delta_L,\Delta_R\}}2^{\mathcal{N}_\lambda}\eta^{n_x}, \tag{4}$$

where Δ_L and Δ_R are any two dimer coverings of the lattice which are placed on each other, $\{\Delta_L,\Delta_R\}$ is the ensemble of all the loop configurations which are given by overlaps of dimer coverings, this ensemble on a 2×2 lattice is depicted in Fig. 1; n_x and n_y are the numbers of horizontally and vertically placed dimers, respectively (with $n_x+n_y=N$, where N is the number of sites in the lattice), $\mathcal{N}_\lambda$ is the number of loops in this overlap, and $\eta=x/y$. And

$$\mathcal{C}_{\mathbf{ij}}=\pm\tfrac{4}{3}\langle\Psi|\mathbf{S_i}\cdot\mathbf{S_j}|\Psi\rangle=y^{\mathrm{MK}}\sum_{\{\Delta_L,\Delta_R\}_{\mathbf{ij}}}2^{\mathcal{N}_\lambda}\eta^{n_x}, \tag{5}$$

where the sign is $+$ when the two sites are on the same sublattice and $-$ otherwise, and $\{\Delta_L,\Delta_R\}_{\mathbf{ij}}$ is the ensemble of all the loop configurations in which the sites $\mathbf{i}$ and $\mathbf{j}$ are on the same loop $\lambda_{\mathbf{ij}}$ (this loop is particular to each of the loop configurations). See Fig. 1 for further explanation.

As an introduction, let us recall the construction of the transfer matrix, formulated to solve the dimer problem,[6] that is, to calculate the partition function

$$Z=\sum_{\{\Delta\}}y^{n_y}x^{n_x}. \tag{6}$$

In an M row by K column square lattice the transfer matrix V is an operator defined in a 2^K-dimensional Hilbert space of the Ising states of K spins half placed in the sites of a K site row, each in a site. In a certain dimer configuration, each row in the lattice is represented by an Ising state. This Ising state denotes the *vertical* dimers which are placed on the bonds between this row and the row above it. An up spin in a site signifies the presence of a vertical dimer on the bond between this site and the site above it (an up dimer), while a down spin signifies the absence of an up dimer on this bond. We will use the Fock representation where the spins are represented by bosons (or fermions) of spin half and

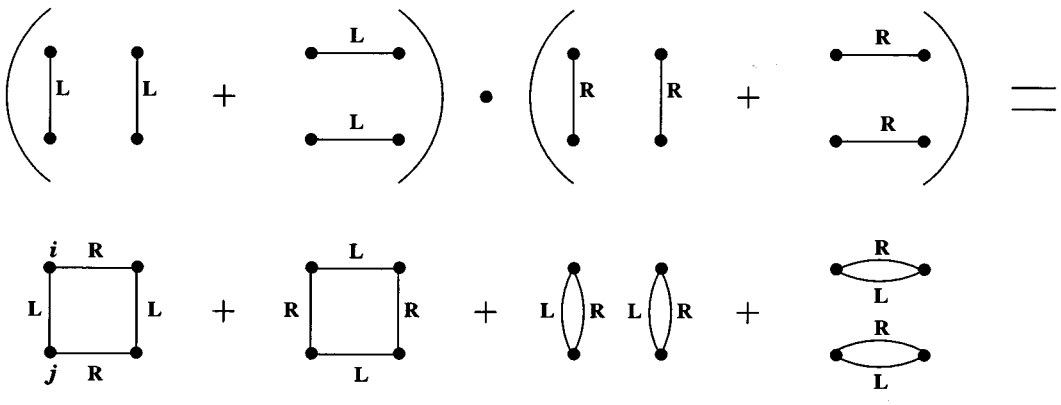

FIG. 1. The four possible loop configurations, made by overlaps of dimers coverings, on a 2×2 lattice. The dimer configurations from the **L** side are placed on the dimer configurations from the **R** side. In the sum of Eq. (5), for the two sites marked by **i** and **j**, the first (from left to right) three loop configurations have to be included.

$$|s_1,\ldots,s_K\rangle\equiv\prod_i^K (c^\dagger_{i,s_i}|0\rangle_i), \tag{7}$$

where $s_i=\uparrow$ or$\downarrow$.

Given an up-dimers configuration of a certain row, starting with the first row, V will generate all the permitted dimers configurations of the next row, each marked by its up dimers. V is composed of two operators:

$$V=V_2V_1.$$

The first is

$$V_1=\prod_{i=1}^K \sigma_i^x, \tag{8}$$

where

$$\sigma_i^x=\sigma_i^+ +\sigma_i^-, \quad \sigma_i^+\equiv \mathbf{c}^\dagger_{\mathbf{i}\uparrow}\mathbf{c}_{\mathbf{i}\downarrow}, \quad \sigma_i^-\equiv \mathbf{c}^\dagger_{\mathbf{i}\downarrow}\mathbf{c}_{\mathbf{i}\uparrow}.$$

This operator reverses all the spins for the next row. After this operation a vertical or horizontal dimer can be placed on any up-spin site. A vertical dimer is placed by leaving the spin up in the site, and a horizontal dimer, between any two adjacent up-spin sites i and $(i+1)$, is placed by the operator $\sigma_i^-\sigma_{i+1}^-$. The operator which places m horizontal dimers in arbitrary locations along the row is

$$\frac{1}{m!}\left(\sum_{i=1}^K \sigma_i^-\sigma_{i+1}^-\right)^m.$$

An arbitrary number of horizontal dimers, each accompanied by the weight η, is placed by the operator

$$V_2=\exp\left(\eta\sum_{i=1}^K \sigma_i^-\sigma_{i+1}^-\right), \tag{9}$$

where in the case of periodic boundary conditions (which are henceforth assumed) $\sigma_{K+1}^-\equiv\sigma_1^-$. Hence we get [note that in Eq. (6) $n_x+n_y=MK/2$]

$$Z=y^{MK/2}\mathrm{Tr}V^M. \tag{10}$$

Let us now consider the square of Eq. (6):

$$Z^2=\sum_{\{\Delta_L,\Delta_R\}} y^{n_y}x^{n_x}. \tag{11}$$

This is just summing over loop configurations in which each site is connected by dimers of two flavors, L and R, which are independent of each other. To formulate a transfer matrix, we denote each of the flavored dimers in any site, by a flavored spin. These spins are propagating along the columns by the operator

$$\overline{V}=V_LV_R,$$

where V_L and V_R are defined in a Hilbert space which is the tensor product of a L and R Ising spaces, and V_L (V_R) effects only the L (R) spins in each of the product states.

After the prepatatory examples above we are ready to tackle the transfer matrix represantation of Eq. (4), with the additional term of $2^{\mathcal{N}_\lambda}$ for each loop configuration. Imagine that there are two colors of dimers, red (r) and green (g). A dimer from each of the colors is distinguished by an additional flavor index $\alpha\in\{L,R\}$. We will define the ensemble $\{\Theta\}$ to include all the possible colored-dimer configurations in which each site in the lattice is connected with two dimers, of identical colors, marked by a distinct flavor index. In $\{\Theta\}$ there are exactly $2^{\mathcal{N}_\lambda}$ different configurations for any loop configuration in Eq. (11), since each of the loops in this overlap can appear in two forms, all red or all green, and we can write

$$\mathcal{D}=y^{MK}\sum_{\{\Theta\}} \eta^{n_x}. \tag{12}$$

We denote the colored dimers in each site by colored spins. Accordingly we expand further our Hilbert space to be the 8^K-dimensional space of a row of K sites; on each site i two spin-half bosons, of the flavors L and R, both labeled by the *same* color index $c_i\in\{r,g\}$. Each of the states in this space is specified by

$$|s_{(1,L)},s_{(1,R)},c_1;\ldots;s_{(K,L)},s_{(K,R)},c_K\rangle \equiv \prod_i^K (\mathbf{c}^\dagger_{\mathbf{i},\mathbf{c_i},\mathbf{L},\mathbf{s}_{(i,L)}}\mathbf{c}^\dagger_{\mathbf{i},\mathbf{c_i},\mathbf{R},\mathbf{s}_{(i,R)}}|0\rangle_i). \quad (13)$$

Flipping spins must now include the two color options, and so

$$\widetilde{V}_1=\prod_{i=1}^K (\sigma^x_{i,r,L}\sigma^x_{i,r,R}+\sigma^x_{i,g,L}\sigma^x_{i,g,R}), \quad (14)$$

where, for example,

$$\sigma^x_{i,r,R}\equiv\sigma^+_{i,r,R}+\sigma^-_{i,r,R}\equiv\mathbf{c}^\dagger_{\mathbf{i,r,R},\uparrow}\,\mathbf{c}_{\mathbf{i,r,R},\downarrow}+\mathbf{c}^\dagger_{\mathbf{i,r,R},\downarrow}\mathbf{c}_{\mathbf{i,r,R},\uparrow}.$$

Horizontal dimers are placed by lowering spins of the same flavor and color by four operators of the form

$$\widetilde{V}_2^{c,\alpha}=\exp\left(\eta\sum_{i=1}^K \sigma^-_{i,c,\alpha}\sigma^-_{i+1,c,\alpha}\right), \quad (15)$$

where $\alpha=L,R$ and $c=r,g$, and now

$$\widetilde{V}_2=\prod_{\substack{\alpha=L,R,\\ c=r,g.}}\widetilde{V}_2^{c,\alpha}, \quad (16)$$

But this is not all. The operator defined in Eq. (14) preserves the color of a column, hence imposing the monocolor propagation of a loop with a vertical dimer. But if a site is not connected by a vertical dimer from ''below,'' its pair of dimers should be of either colors, as there are two color opetions for the loop passing through this site. Since the absence of vertical dimers is denoted by two down spins, the additional color-flipping options are provided by the operator

$$\widetilde{V}_0=\prod_{i=1}^K (1+\mathbf{c}^\dagger_{\mathbf{i,r,L},\downarrow}\mathbf{c}^\dagger_{\mathbf{i,r,R},\downarrow}\mathbf{c}_{\mathbf{i,g,L},\downarrow}\mathbf{c}_{\mathbf{i,g,R},\downarrow} + \mathbf{c}^\dagger_{\mathbf{i,g,L},\downarrow}\mathbf{c}^\dagger_{\mathbf{i,g,R},\downarrow}\mathbf{c}_{\mathbf{i,r,L},\downarrow}\mathbf{c}_{\mathbf{i,r,R},\downarrow}). \quad (17)$$

Combining Eq. (14), (16), and (17), the transfer operator is

$$\widetilde{V}=\widetilde{V}_2\widetilde{V}_1\widetilde{V}_0 \quad (18)$$

and

$$\mathcal{D}=y^{MK}Tr\widetilde{V}^M. \quad (19)$$

On narrow lattices, such as the two-legged ladder, it is possible to extend this treatment to longer range, like the first- and second-, or the first- and third-nearest neighbors, RVB states.[7] These extensions, although straightforward, require a more complicated transfer matrix, which is usually larger in its dimension (for a given lattice width).

The transfer matrix formulation will be concluded in adding that a disconnected site (a static hole) ***i*** can be placed by positioning the operator

$$\widetilde{V}^d_{\mathbf{i}}=\frac{1}{y}\sigma^-_{\mathbf{i},r,L}\sigma^-_{\mathbf{i},r,R} \quad (20)$$

TABLE I. Results of the one-lattice-unit spin-spin correlation functions, energies, and correlation lengths, for the isotropic dimer RVB state on nondiluted ladders of the width two, three, and four lattice units. The results in the second row are for the absolute values of the one-lattice-unit correlations: (1) in the vertical case along one of the side legs of the ladders, (2) in the vertical case along the middle leg of a 3×40 ladder, and (3) in the horizontal case. The results in the third row are for the expactation values of the isotropic Heisenberg Hamiltonian for each of the lattices. The expactation values are in units of J/site. The results in the fourth row are for the correlation lengths along the (4) side legs of the ladders, and (5) middle leg of a 3×40 ladder. The results for the correlation lengths are according to the values of the correlation function in distances of five and six lattice units along the lattice.

Width	2	3	4
(1)	0.286139	0.328752	0.246393
(2)		0.277263	
(3)	0.539779	0.344843	0.395096
$\lvert E\rvert$	0.556029	0.656432	0.641489
(4)	0.696652 [a]	0.735272 [b]	0.723966
(5)		0.780763	

[a]This result, for the correlation length on the two-legged ladder, disagrees with the result in Ref. 4.

[b]In the case of a three-unit-width lattice, the correlation function is slightly wavy; hence a slightly different result may apear, if the correlation length is to be calculeted by the values of the correlation function in different distances.

to the left of $\widetilde{V}_1$, when propagating into **i**'s row. This operator colors the disconnected site red. A class of variational states, which include annealed holes, that obey Fermi statistics, will be treated elsewhere, using a similar technique.

In order to calculate $\mathcal{C}_{\mathbf{ij}}$ defined in Eq. (5), we will calculate the quantity $\mathcal{Y}_{\mathbf{ij}}$, defined by

$$\mathcal{Y}_{\mathbf{ij}}=y^{MK}\sum_{\{Y\}_{\mathbf{ij}}} 2^{\mathcal{N}_\lambda}\eta^{n_x}, \quad (21)$$

where $\{Y\}_{\mathbf{ij}}$ is the ensemble of all the loop configurations in which the sites **i** and **j** are *not* on the same loop. Some of these configurations are easily counted by fixing the two pairs of dimers, placed on the two sites, to be of distinct colors, or by calculating the color-color correlation function

$$\mathcal{Y}^{r,g}_{\mathbf{ij}}=y^{MK}\mathrm{Tr}(\widetilde{V}^{(M-p)}\mathbf{n}^r_{\mathbf{j},\alpha}\widetilde{V}^p\mathbf{n}^g_{\mathbf{i},\alpha}), \quad (22)$$

where the two sites are p rows apart, and

$$\mathbf{n}^c_{\mathbf{i},\alpha}=\mathbf{n}^c_{\mathbf{i},\alpha,\uparrow}+\mathbf{n}^c_{\mathbf{i},\alpha,\downarrow}$$

(the flavor index α is arbitrary). In Eq. (22) we calculate the contributions to $\mathcal{Y}_{\mathbf{ij}}$ from configurations in which $\lambda_{\mathbf{i}}$ is a green loop and $\lambda_{\mathbf{j}}$ is a red loop. Each of the other configurations in which $\lambda_{\mathbf{i}}\neq\lambda_{\mathbf{j}}$ (that is, loop configurations which *do not* contribute to $\mathcal{Y}^{r,g}_{\mathbf{ij}}$ but must be counted in $\mathcal{Y}_{\mathbf{ij}}$) has its

duplicate in one and only one of the configurations which do contribute to $\mathcal{Y}_{\mathbf{ij}}^{r,g}$ since the two loops may appear in either colors. Because there are four colors possibilities for the two loops, we conclude that

$$\mathcal{Y}_{\mathbf{ij}}=4\mathcal{Y}_{\mathbf{ij}}^{r,g}. \tag{23}$$

Finally, since the sum for the norm in Eq. (4) contains all the loop configurations, those in which the two sites are on the same loop and those in which they are not, we get

$$\mathcal{C}_{\mathbf{ij}}=\mathcal{D}-\mathcal{Y}_{\mathbf{ij}}. \tag{24}$$

The spin-spin correlation functions were numericaly calculated, in the isotropic dimer RVB state ($y=\eta=1$), on nondiluted ladders of the sizes 2,3, and 4×40, with vertical (along the ladder legs) periodic boundary conditions, and horizontal periodic boundary conditions in the case of a 4×40 lattice. The results are summarized in Table I.

In conclusion, using the transfer matrix method it was shown that it is possible to reduce the complexity of calculating spin-spin correlation functions in dimer RVB states on possibly diluted 2D lattices to the complexity of a 1D quantum many-body problem. This simplification permitted exact calculation of correlation functions on narrow lattices. We suggest that these kinds of calculations are possible when longer-range RVB states are considered.

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