Exact results for resonating valence bonds states on 2D (narrow) systems

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Abstract

It is shown that the problem of calculating spin-spin correlation functions, in the dimers RVB states, on a possibly diluted 2D 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.
In the last few years, the class of Resonating Valence Bonds (RVB) states have drawn much attention in connection to the long lasting pursuit of the anti-ferromagnetic 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 dimers 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 \[3\]

\[
|\Psi\rangle = \sum_{\{\Pi\}} \prod_{(i, j) \in \Pi} U(i, j) \left( \langle \uparrow_i \downarrow_j \rangle - \langle \uparrow_j \downarrow_i \rangle \right)
\]

(1)

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

\[
U(i, j) = \begin{cases} 
  x & \text{if } i - j = \hat{x} \\
  y & \text{if } i - j = \hat{y} \\
  0 & \text{otherwise}
\end{cases}
\]

(2)

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

The spin-spin correlation function in the dimers RVB states is defined by the expectation value \[3,4\]

\[
S_{ij} = \frac{\langle \Psi | S_i \cdot S_j | \Psi \rangle}{\langle \Psi | \Psi \rangle}
\]

(3)
where \( i \) and \( j \) are two sites on the lattice. Two quantities are evaluated for the calculation of this expectation value. The norm:

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

where \( \Delta_L \) and \( \Delta_R \) are any two dimers coverings of the lattice which are placed on each other to create \( \{\Delta_L, \Delta_R\} \) which is the ensemble of all the loops configurations given by overlaps of dimers coverings, this ensemble on a \( 2 \times 2 \) 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); \( N_\lambda \) is the number of loops in this overlap; and \( \eta = \frac{x}{y}. \) And

\[
\mathcal{C}_{ij} = \pm \frac{4}{3} \langle \Psi | \mathbf{S}_i \cdot \mathbf{S}_j | \Psi \rangle = y^{MK} \sum_{\{\Delta_L, \Delta_R\} \Delta_{ij}} 2^{N_\lambda} \eta^{n_x} \tag{5}
\]

where the sign is ‘+’ when the two sites are on the same sub-lattice and ‘−’ otherwise, and \( \{\Delta_L, \Delta_R\} \Delta_{ij} \) is the ensemble of all the loops configurations in which the sites \( i \) and \( j \) are on the same loop - \( \lambda_{i,j} \) (this loop is particular to each of the loops configurations). See Fig. [1] for further explanation.

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

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

In an \( M \) rows by \( K \) columns 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 \( K \) sites row, each in a site. In a certain dimers 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

\[ |s_1, \ldots, s_K\rangle \equiv \prod_i^K (c_{i,s_i}^\dagger |0\rangle_i) \]  

(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:

\[ V = V_2 V_1. \]

The first is

\[ V_1 = \prod_{i=1}^K \sigma_i^x \]  

(8)

where

\[ \sigma_i^x = \sigma_i^+ + \sigma_i^-, \quad \sigma_i^+ \equiv c_{i\uparrow}^\dagger c_{i\downarrow}, \quad \sigma_i^- \equiv c_{i\downarrow}^\dagger c_{i\uparrow}. \]

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 \( \eta \), are placed by the operator

\[ V_2 = \exp \left( \eta \sum_{i=1}^K \sigma_i^- \sigma_{i+1}^- \right) \]  

(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. \( B \) \( n_x + n_y = MK/2 \))
Let us now consider the square of Eq. (6)

\[ Z^2 = \sum_{\{\Delta_L, \Delta_R\}} \eta^{n_y} x^{n_x}. \]  

(11)

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

\[ \bar{V} = V_L V_R \]

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 preparatory examples above we are ready to tackle the transfer matrix representation of Eq. (4), with the additional term of $2^{N_{\lambda}}$ for each loops configuration. Imagine that there are two colours of dimers - red ($r$) and green ($g$). A dimer from each of the colours is distinguished by an additional flavour index - $\alpha \in \{L, R\}$. We will define the ensemble $\{\Theta\}$ to include all the possible coloured-dimers configurations in which each site in the lattice is connected with two dimers, of identical colours, marked by distinct flavour index. In $\{\Theta\}$ there are exactly $2^{N_{\lambda}}$ different configurations for any loops 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

\[ D = y^{MK} \sum_{\{\Theta\}} \eta^{n_x}. \]  

(12)

We denote the coloured dimers in each site by coloured 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 flavours $L$ and $R$, both labeled by the same colour index - $c_i \in \{r, g\}$. Each of the states in this space is specified by
\[ | s_{(1,L)}, s_{(1,R)}, c_1; \ldots; s_{(K,L)}, s_{(K,R)}, c_K \rangle \equiv \prod_{i}^{K} \left( c_{i,i,L}^{\dagger}, c_{i,i,R}^{\dagger}, c_{i,i,L}, c_{i,i,R}, |0\rangle_i \right) \] (13)

Flipping spins must now include the two colour options so

\[ \tilde{V}_1 = \prod_{i=1}^{K} \left( \sigma_{i,r,L}^{x} \sigma_{i,r,R}^{x} + \sigma_{i,g,L}^{x} \sigma_{i,g,R}^{x} \right) \] (14)

where for example

\[ \sigma_{i,r,R}^{x} \equiv \sigma_{i,r,R}^{+} + \sigma_{i,r,R}^{-} \equiv c_{i,r,R,\uparrow}^{\dagger} c_{i,r,R,\downarrow} + c_{i,r,R,\uparrow} c_{i,r,R,\downarrow}^{\dagger} \]

Horizontal dimers are placed by lowering spins of the same flavour and colour by four operators of the form

\[ \tilde{V}_2^{c,\alpha} = \exp \left( \eta \sum_{i=1}^{K} \sigma_{i,c,\alpha}^{-} \sigma_{i+1,c,\alpha}^{-} \right) \] (15)

where \( \alpha = L, R \) and \( c = r, g \), so now

\[ \tilde{V}_2 = \prod_{\alpha = L, R} \prod_{c = r, g} \tilde{V}_2^{c,\alpha} \] (16)

But this is not all. The operator defined in Eq.(14) preserves the colour of a column, hence imposing the mono-colour 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 colours, as there are two colour options for the loop passing through this site. Since the absence of vertical dimers is denoted by two down spins, the additional colour flipping options are provided by the operator

\[ \tilde{V}_0 = \prod_{i=1}^{K} \left( 1 + c_{i,r,L,\downarrow}^{\dagger} c_{i,r,R,\downarrow}^{\dagger} c_{i,g,L,\downarrow} c_{i,g,R,\downarrow} + c_{i,g,L,\uparrow}^{\dagger} c_{i,g,R,\uparrow}^{\dagger} c_{i,r,L,\uparrow} c_{i,r,R,\uparrow} \right) \] (17)

Combining equations (14), (16), and (17), the transfer operator is
\[ V = \tilde{V}_2 \tilde{V}_1 \tilde{V}_0 \]  

(18)

and

\[ \mathcal{D} = y^{MK} \text{Tr} \tilde{V}^M. \]  

(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 neighbours, RVB states. This extension, although straightforward, requires 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

\[ \tilde{V}_i^d = \frac{1}{y} \sigma_{i,r,L}^\sigma \sigma_{i,r,R}^\sigma \]  

(20)

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

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

\[ \mathcal{Y}_{ij} = y^{MK} \sum_{\{\Upsilon\}_{ij}} 2^{N_{\lambda}} \eta^{n_x} \]  

(21)

where \( \{\Upsilon\}_{ij} \) is the ensemble of all the loops 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 colours, or by calculating the colour-colour correlation function

\[ \mathcal{Y}^{r,q}_{ij} = y^{MK} \text{Tr} \left( \tilde{V}^{(M-p)} n_{j,\alpha}^{r} \tilde{V}_{i,\alpha}^{p} n_{i,\alpha}^{q} \right) \]  

(22)

where the two sites are \( p \) rows apart, and

\[ n_{i,\alpha}^{c} = n_{i,\alpha,\uparrow}^{c} + n_{i,\alpha,\downarrow}^{c} \]
(the flavour index - $\alpha$ is arbitrary). In Eq. (22) we calculate the contributions to $Y_{ij}$ from configurations in which $\lambda_i$ is a green loop and $\lambda_j$ is a red loop. Each of the other configurations in which $\lambda_i \neq \lambda_j$ (that is, loops configurations which do not contribute to $Y_{ij}^{r,g}$, but must be counted in $Y_{ij}$) has its duplicate in one and only one of the configurations which do contribute to $Y_{ij}^{r,g}$, since each of the two loops may appear in either of the two colours. Because there are four colours possibilities for the two loops, we conclude that

$$Y_{ij} = 4 \cdot Y_{ij}^{r,g}. \quad (23)$$

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

$$C_{ij} = D - Y_{ij}. \quad (24)$$

The spin-spin correlation functions were numerically calculated, in the isotropic dimers RVB state ($y = \eta = 1$), on non-diluted ladders of the sizes $2, 3, 4 \times 40$, with vertical (along the ladders legs) periodic boundary conditions, and horizontal periodic boundary conditions in the case of $4 \times 40$ 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 dimers 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 kind of calculations are possible when longer range RVB states are considered.

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[9] In the case of 3 units width lattice, the correlation function is slightly wavy, hence a slightly different result may appear, if the correlation length is to be calculated by the values of the correlation function in different distances.
TABLE I. Results of the one lattice unit spin-spin correlation functions, energies, and correlation lengths, for the isotropic dimers RVB state on non-diluted ladders of the width 2, 3, and 4 lattice units. The results in the second row are for the absolute values of the one lattice unit correlations: (a) in the vertical case along one of the side legs of the ladders; (b) in the vertical case along the middle leg of a $3 \times 40$ ladder; and (c) in the horizontal case. The results in the third row are for the expectation values of the isotropic Heisenberg Hamiltonian for each of the lattices. The expectation values are in units of $J/site$. The results in the fourth row are for the correlation lengths along the (a) side legs of the ladders, and (b) middle leg of a $3 \times 40$ 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.
FIG. 1. The four possible loops configurations, made by overlaps of dimers coverings, on a $2 \times 2$ lattice. The dimers configurations from the L side are placed on the dimers 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 loops configurations have to be included.