

Exact matrix representation of the RVB wavefunction

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It is shown that the RVB wave function can be expressed as the Pfaffian of an antisymmetric matrix whose size is equal to the number of lattice points. The matrix representation helps in proper counting of all the paired states.

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The resonating valence bond (RVB) approach for the two dimensional Heisenberg antiferromagnet shows that the energy one gets from such wavefunctions is very close to the estimate of the ground state energy known from other sources [1–4]. There are proposals that the RVB state can be stabilized by introducing disorder and/or hole in the system [see, e.g., 4]. Attempts have also been made to construct Hamiltonians that would have the RVB state as the ground state [5]. Our purpose in this paper is to show that many of the RVB wavefunctions considered in the literature can, in fact, be given an exact matrix representation. The RVB wavefunction is given by the Pfaffian (defined below) of an antisymmetric matrix of order equal to the number of lattice points. This is reminiscent of, but not analogous to, the Slater determinant for fermions. In the Slater determinant, the matrix structure helps in the symmetrization of the wave function, but here it is necessary for proper combinatorics of the paired states in the RVB wavefunction.

The Pfaffian of a $2n \times 2n$ antisymmetric matrix A with elements a_{ij} is defined as

$$Pf(A) = \sum_P \delta_P a_{p_1 p_2} a_{p_3 p_4} \dots a_{p_{2n-1} p_{2n}},$$

$$p_{2i-1} < p_{2i+1}, \text{ and } p_{2i-1} < p_{2i}, \quad \forall i \quad (1)$$

where the summation is over all allowed permutations p_1, p_2, \dots, p_{2n} of the integers $(1, 2, \dots, 2n)$, δ_P being the parity of the permutation. An operational definition is $[Pf(A)]^2 = \det(A)$ which also sets the Pfaffian of an odd ordered antisymmetric matrix as zero. Several decomposition formula for Pfaffians can be found, though in a different context, in Ref. 6.

The RVB wavefunction is defined in terms of the paired states ϕ_{ij} for sites i and j . A valence bond state is defined as $\phi_\alpha = \prod \phi_{ij}$ where the product is over the

pairings of the sites (each site is paired with one and only one other site). A linear combination of these valence bond states will then be an RVB state:

$$\Psi_{\text{RVB}} = \sum_\alpha c_\alpha \phi_\alpha. \quad (2)$$

The form of the wave function that has been most widely used or used as the starting point is the nearest neighbor RVB (NNRVB) wavefunction [1–4, 7] for which $c_\alpha = 1$ and the pairing is over the nearest neighbours only. The pairings then constitute the dimer coverings of the lattice. In the simplest situation, ϕ_{ij} is taken as the singlet $\phi_{ij} = (|\uparrow_i \downarrow_j\rangle - |\downarrow_i \uparrow_j\rangle) / \sqrt{2}$ where $|\uparrow_i\rangle$ and $|\downarrow_i\rangle$ are the up and down eigenstates at site i with the convention that the first up spin is always on the same sublattice. More general ϕ_{ij} as, e.g., in Ref. 2, can be considered in our approach without any modification.

The Pfaffian construction requires a properly oriented lattice (i.e., each bond has an arrow) such that every closed loop of even number of bonds has an odd number of arrows in the opposite direction. This “clockwise-odd” condition can be ensured for $2-d$ Bravais lattices by enforcing the same for the smallest loop (2×2 square) on the lattice [8, 9]. The sites are numbered such that the odd numbered sites are on one sublattice and the even numbered on another (Fig. 1). The arrows go always in the direction of increasing site labels. Any larger square lattice can be built up by translating the basic 2×2 block of Fig. 1. For the 2×2 case with free boundary condition (FBC), we construct a 4×4 antisymmetric matrix A whose ij element is ϕ_{ij} with the sign determined by the arrow from i to j as follows:

$$A = \begin{pmatrix} 0 & \phi_{12} & 0 & \phi_{14} \\ -\phi_{12} & 0 & \phi_{32} & 0 \\ 0 & -\phi_{32} & 0 & \phi_{34} \\ -\phi_{14} & 0 & -\phi_{34} & 0 \end{pmatrix} \quad (3)$$

Note that the sign convention of the previous paragraph requires that the odd index comes first (i.e., ϕ_{32} and not ϕ_{23}). The Pfaffian (=square root of determinant) of this matrix is $Pf(A) = \phi_{12} \phi_{34} + \phi_{14} \phi_{32}$ which is precisely the NNRVB wavefunction [7]. The proper arrow choices guarantee that all the dimer coverings appear

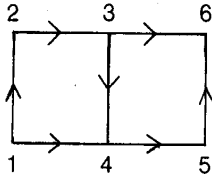


Fig. 1. An oriented 2×3 lattice. The ij arrow goes from i to j if $i < j$. The 2×2 part of it is used in (3)

with the same sign as is required by Marshall's sign criterion [1, 2]. Generalization to bigger and other lattices is straightforward.

The above construction is valid for the wavefunction with $c_\alpha = 1$. If the coefficients are factorizable so that c_α can be written as a product of weights x_{ij} of the bonds present in the α valence bond state, then the matrix representation would require an additional factor x_{ij} for the corresponding matrix element, i.e. $[A]_{ij} = \pm x_{ij} \phi_{ij}$ with the sign determined by the orientation of the ij bond. The Pfaffian, as before, gives the correct wavefunction.

The form with bond weightfactors, though may not be the most general NNRVB wave function, has the potentiality of gauging the importance of a subclass of bonds. Such a scheme is necessary if there are certain static defect sites like holes. If the effect of the hole is to produce a local change in the interaction, then the corresponding wavefunction can be discussed by putting in the weight factors for the bonds that emanate from the defect site. If, on the other hand, the effect of the hole is to prevent pairing, then the corresponding matrix elements are zero. For odd number of holes, the Pfaffian is zero. This merely reflects the fact that perfect pairing is not possible with odd number of sites. Two or more even number of holes pose no such problem.

An interesting situation would be to take the weightfactors for different bonds in such a way that a particular valence bond state is stabilized. The transition to the RVB state can then be studied by varying these weights. Incidentally, the corresponding classical dimer models show rich critical behaviors [9]. It remains to be seen what one can learn about the quantum system from the classical problem. Another intriguing feature is the connection between the dimer states and the spanning trees on a subset of a sublattice of the square lattice [10]. This would mean that for the NNRVB wavefunction only a subset of bonds are really important, others are determined by them. What can be the significance of that?

Long range paired states (as in Ref. 1) can also be represented in this matrix form though one would lose the control on the sign of these "long ranged" states in the total wavefunction. Nevertheless, the Pfaffian expansion still guarantees that only the perfectly paired states appear in the wavefunction. As an example we consider the 2×3 lattice (Fig. 1) with (1, 6) and (2, 5) pairings and with FBC. With the same arrow convention as before, the Pfaffian of this 6×6 matrix is

$$\Psi_{\text{RVB}} = \phi_{12} \phi_{34} \phi_{56} + \phi_{12} \phi_{36} \phi_{54} + \phi_{14} \phi_{32} \phi_{56} - \phi_{14} \phi_{52} \phi_{36} + \phi_{16} \phi_{32} \phi_{54} + \phi_{16} \phi_{52} \phi_{34}. \quad (4)$$

Although one configuration enters with a wrong sign, but still all the valence bond states are present. Factorizable weights as in Ref. 1 can be handled as discussed after (3). Incorporating long ranged dimers (which makes a lattice nonplanar) in a Pfaffian description (so that all states appear with the same sign) remains an open problem.

Just to show that one can handle these matrices, we have calculated the normalization \aleph_N of NNRVB wavefunction with singlet ϕ_{ij} 's for $2 \times N$ lattices (with FBC) using REDUCE upto $N=7$. The difficulty with the Pfaffian approach, at present, is the nonavailability of numerical procedures for evaluating Pfaffians. The normalization can be calculated easily because it is actually the square root of the determinant of A^2 . From graph theory, it is known that the ij element of A^2 contains the weights for going from j to i in all possible ways. Therefore, for a bipartite lattice, A^2 can be written in block diagonal form with elements only in the odd-odd and even-even blocks. Since the determinant of the two are the same, the normalization requires evaluation of the determinant of an $N \times N$ (instead of $2N \times 2N$) matrix.

By extrapolating the results we have for N upto 7, we get, for large N , $\aleph_N \approx \exp(0.738 N)$. We now postulate that $\aleph_N \approx (\Omega_N)^\alpha$ for large N , where Ω_N is the number of dimer coverings. Since Ω_N on this ladder lattice forms a Fibonacci sequence with N ($\Omega_N \approx \tau^N$ for $N \rightarrow \infty$, τ being the golden mean), we obtain $\alpha = 1.53$. Taking α to be universal, we estimate for an $M \times N$ lattice $\aleph = (2.44)^{MN}$.

In summary, we have shown how a Pfaffian representation can be used to describe exactly the RVB wavefunction. This representation is capable of handling wavefunctions with different bond weight factors and also long range pairings. In the later case, however, a few "long range" states appear with a different sign. Fixing the sign of these states in this approach remains a problem that deserves further studies. We also suggest that, given the importance of this problem and the relevance of Pfaffians in other problems [6, 9], numerical procedures be developed for direct computation of Pfaffians.

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