Energy of the nearest neighbor RVB state by systematic loop expansion

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We present an approximation scheme for the calculation of the norm and energy of the nearest-neighbor-RVB state for the Heisenberg antiferromagnet on the 2D square lattice. The approximation leads to a systematic expansion of norm and energy, with the ‘expansion parameter’ being the maximum length of loops taken into account in the calculation of energy and norm. The expansion converges well, the best estimate for the ground state energy/site is $-0.434473J$.

The ‘RVB spin liquid’ is a frequently occurring phrase in connection with cuprate superconductors. It is supposed to describe a state with strong short range singlet correlations, but no long range magnetic order whatsoever. Despite its frequently being referred to in the literature, up to now the ‘RVB spin liquid’ is a rather elusive concept. For example, there exists to date no simple and manageable trial wavefunction for the 2D Heisenberg Antiferromagnet which would describe such a state, nor is the precise nature of its low lying elementary excitations known to any degree of certainty (as opposed e.g. to the antiferromagnetic state, where linear spin-wave theory gives an excellent approximation to the ground state wave function and allows a quantitative discussion of its excitation spectrum). Perhaps the best-defined ‘RVB spin liquid’ is the nearest neighbor RVB state $\bar{\psi}$ - at least this wave function can be written down in compact form. We introduce the singlet generation operator on the bond $i, \bar{j}$

$$s^\dagger_{i,\bar{j}} = \frac{1}{\sqrt{2}} \left( c^\dagger_{i,\bar{j}} c^\dagger_{\bar{i},\bar{j}} - c^\dagger_{i,\bar{j}} c^\dagger_{\bar{i},\bar{j}} \right),$$

where $c^\dagger_{i,\sigma} = c^\dagger_{i,\sigma} c^\dagger_{\bar{i},\bar{\sigma}}$, and the operator

$$S = \sum_i (s^\dagger_{i,\bar{i}+\bar{x}} + s^\dagger_{i,\bar{i}+\bar{y}}),$$

where $i + \bar{x}$ denotes the nearest neighbor of sites $i$ in $x$-direction. The nearest neighbor RVB state on a 2D square lattice with $N$ sites then is defined as

$$|\Psi\rangle = \frac{S^{N/2}}{(N/2)!} |vac\rangle = \sum_\phi |\phi\rangle.$$

In other words, the state consists of a superposition of all possible distributions of $N/2$ singlets over the plane, $\phi$, with equal phase. The total number of different singlet configurations corresponds to the number of dimer coverings of the plane, $N_c$. The calculation of $N_c$ is a well-known exactly solvable problem from statistical mechanics $[1,2]$ - however, knowledge of this number is not really necessary to estimate the ground state energy. As will be seen below, the energy of the state $\bar{\psi}$ is significantly higher than that of the antiferromagnetically ordered ground state - the nearest-neighbor RVB state itself therefore is no candidate for the ground state wave function. On the other hand, and this is the main motivation for the present work, it has recently been demonstrated for Heisenberg ladders $[3]$ that by starting from a ‘singlet vacuum’ a theory for triplet-like fluctuations ‘on top of’ this vacuum can be constructed, which in fact compares very well to numerical results. While for ladders the topology of the system rather uniquely determines one specific singlet covering, the nearest-neighbor RVB state would be an appealing candidate for a generalization of this approach to an isotropic and translationally invariant state of a planar system. In trying to do so, however, one encounters an as yet prohibitive technical obstacle: the fact that singlet configurations corresponding to different dimer coverings are not orthogonal $[4]$. More precisely, whenever we can draw a closed loop which passes through both sites of each dimer it touches, it is possible to shift the ‘train of dimers’ along the loop by one lattice spacing, so as to obtain a different covering. Then, the ‘Néel components’ in the two dimer coverings along the loop are identical, so that there is a nonvanishing overlap. Each ‘Néel component’ has the prefactor $2^{-l/2}$, where $l$ is the number of sites in the loop, so that the overlap originating from the loop is $2^{-(l/2-1)}$. Clearly the most important contributions thus come from states which differ only by short loops. First, the overlap due to short loops is larger, and second, a long loop ‘blocks’ more possibilities for drawing other loops. In the following, we want to make these considerations more quantitative.

To that end we write the norm as

$$\langle \Psi | \bar{\psi} \rangle = N_c \left( 1 + \sum_{\phi \neq \psi} \langle \phi | \psi \rangle \right),$$

where $\bar{\psi}$ denotes the statistical average over all configurations $|\psi\rangle$. As a first step we restrict the sum over $\phi$ to those configurations which can be obtained from $|\psi\rangle$ by ‘rotating’ a certain number of $l=4$-loops. We denote the number of these 4-site loops by $\nu$, and start with the case $\nu=1$. If there are $N$ sites in the system, we can obviously draw $N$ different 4-site loops in the plane. However, in most cases the dimers of $|\psi\rangle$ will not ‘fit’ into the drawn loop. Let us assume that we have drawn a 4-site loop somewhere in the plane, and consider the lower left cor-
Next, if the dimers fit into the loop we can create a new stick to our simple estimate. As will be seen below, a situation happens that the relevance for the infinite system may be questionable. Since the difference is not too large anyway, we replace it by an approximation. Numerical calculations on 4 \times 4 and 6 \times 6 lattices with periodic boundary conditions indicate that the probability is higher, i.e. one should replace 1/(z-1) = 0.33333 \rightarrow 0.47. On the other hand the values of \( N_c \) obtained for these systems differ strongly from the ones expected in the thermodynamical limit, so the relevance for the infinite system may be questionable. Since the difference is not too large anyway, we stick to our simple estimate. As will be seen below, a change of the probability can be incorporated easily.

Next, if the dimers fit into the loop we can create a new state \(|\phi\rangle\) by rotating the dimers along the drawn loop, and have \(|\phi\rangle|\psi\rangle = 1/2\). The total contribution to the overlap from all states which can be obtained by rotating one 4-site loop in \(|\psi\rangle\) therefore is \( N_1 \) with

\[
\lambda_1 = \frac{1}{z(z-1)} = \frac{1}{12}.
\]

Next, let us assume that we have drawn \( \nu \) different 4-site loops in the plane. The first question then is: in how many different ways can we do that? There are \( N \) ways to draw the first loop and since the second loop should not intersect the first one, a number of positions for the second loop are blocked. More precisely, the number of ways to draw the second loop is only \( N-b_{11} \), where \( b_{11} = 9 \). If the first two loops are far from each other they will block \( 2b_{11} \) possible positions, so that the number of ways to draw the third loop is \( N-2b_{11} \). Continuing we estimate the number \( n_\nu \) of different ways to draw \( \nu \) loops as

\[
N(N-b_{11})(N-(2b_{11}))(N-(3b_{11}))\ldots(N-(\nu-1)b_{11})
\]

\[
= b_{11}^\nu \left( \frac{N}{b_{11}} \right)^\nu.
\]

The factor of 1/\( \nu! \) is due to the fact that by drawing one loop after the other, each configuration of loops is generated in \( \nu! \) different ways. We have assumed that each loop blocks precisely \( b_{11} \) following loops, which is only an approximation; deviations will occur if a loop is placed ‘close’ to a previously drawn loop. The probability for this to happen is proportional to the ‘average density’ of loops squared, and we will have to check later on that this is small.

Assuming that (3) is a reasonable approximation for the number of different loop configurations, we can now repeat the considerations for the single loop for each of the \( \nu \) loops. In this way we find that the total overlap of \(|\psi\rangle\) with all states which differ by rotating \( \nu \) 4-site loops is simply \( n_\nu \lambda_1^\nu \), whence the contribution to the overlap of \(|\psi\rangle\) with all states which differ by rotating an arbitrary number of 4-site loops is

\[
N_4 = N_c \sum_{\nu>1} \left( \frac{N/b_{11}}{\nu} \right)^\nu (\lambda_1 b_{11})^\nu
\]

\[
= N_c \left[ (1 + \lambda_1 b_{11})^{N/b_{11}} - 1 \right].
\]

The extra 1 on the r.h.s. is negligible and will be dropped henceforth. Note that we have extended the upper limit of the sum up to \( N/b_{11} \), where our above estimate certainly is invalid. As mentioned above, our derivation will be valid only if the ‘average density’ of loops is small, and our next objective is to check this assumption. To be more precise, we want to find out which order \( \nu \) in the expansion (3) gives the dominant contribution. Approximating the factorials by Stirling’s formula and nominally differentiating with respect to the number of loops, \( \nu \), we find that the maximum contribution to the sum comes from terms with

\[
\nu_0 = \frac{\lambda_1 N}{1 + b_{11} \lambda_1} = \frac{N}{21}.
\]

Moreover, in the neighborhood of \( \nu_0 \) we find \( n_\nu \lambda_1^\nu \propto \exp(-N(\nu - \nu_0)^2) \). On the average, each drawn loop thus has 20 ‘free squares’ around it, and terms which significantly different loop density give a negligible contribution. This implies first that our approximation of neglecting correlations between the loops is probably reasonably justified for the terms which give the dominant contribution to the norm, and second that extending the sum in (3) up to \( N/b_{11} \) is justified as well.

Having obtained a first estimate for the norm of the RVB state we proceed to compute the expectation value of \( H \) to the same approximation. To that end we introduce
the projection operator $P = \langle \psi | \psi \rangle$ and $Q = 1 - P$. We find

$$
\langle \phi | H | \psi \rangle = \langle \phi | (P + Q)H | \psi \rangle = \langle \phi | \psi \rangle E + \langle \phi | QH | \psi \rangle
$$

(6)

where $E$ denotes the expectation value of the Hamiltonian in the state $| \psi \rangle$. We now write the expectation value of the Hamiltonian as

$$
\langle \Psi | H | \Psi \rangle = N_c \left( \frac{3NJ}{8} + \sum_{\phi \neq \psi} \langle \phi | H | \psi \rangle \right),
$$

(7)

and again restrict the summation to those states which can be obtained from $| \psi \rangle$ by rotating an arbitrary number of 4-site loops. The first term on the r.h.s. in (6) then simply gives the energy of one dimer covering, $-3NJ/8$, multiplied by the approximate norm. The second term is more involved and represents the ‘true off-diagonal’ contribution. Let us assume that we act with the exchange term along a bond $(i, j)$ connecting two sites covered by two different singlets in $| \psi \rangle$. Then one has

$$
h_{ij} s_i^{+} s_j^{+} = \frac{J}{4} \sum_{\alpha=x, y, z} t_i^{+} \alpha t_j^{+} \alpha,
$$

where $t_i^{+} \alpha$ creates the $\alpha$-component of the 3-vector of triplets on the bond $(i, i')$. Next, a singlet and a triplet have opposite time reversal parity, and a necessary condition for a nonvanishing overlap along one loop is that both states have equal time reversal parity ‘along the loop’. We can conclude that only those states $| \phi \rangle$ can have a nonvanishing matrix element with $| \psi \rangle$ which differ from $| \psi \rangle$ along a loop covering both bonds, $(i, i')$ and $(j, j')$. Let us assume that we have a dimer configuration

\[ \begin{array}{cccc}
\cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots \\
-1/2 & x & J/2 & x & 1/2 = -J/8
\end{array} \]

**FIG. 2.** A contribution to $h' = \langle \phi | QH | \psi \rangle$: starting two singlets in $x$-direction (left state) and acting with the transverse Heisenberg exchange along the indicated bonds one obtains two states which are orthogonal to the initial state, but correspond to singlets in $y$-direction. Each of these channels gives a total contribution of $-J/8$ to $h'$.

which fits onto a 4-site loop, and consider the matrix element of $H$ between this configuration and the ‘rotated’ dimer covering. Looking at Figure 2, one can read off that the total contribution of this loop to the matrix element is

$$
\langle \phi | QH | \psi \rangle = -2 \cdot 2 \cdot \frac{J}{8},
$$

where the additional factor of 2 comes from the ‘spin reversed’ processes. Recalling that the same configuration would have contributed a factor of $1/2$ to the overlap of the two states we find the total off-diagonal contribution is given by

$$
H_4 = -N_c J \sum_{\nu > 1} \left( \frac{N/ b_{11}}{\nu} \right) \nu (\lambda_1 b_{11})^\nu
$$

$$
= -\frac{NJ \lambda_1}{1 + \lambda_1 b_{11}}
$$

This is just the expectation value $\langle \phi | QH | \psi \rangle / \langle \phi | \psi \rangle$ for a single 4-site loop times the ‘most probable number’ of loops, compare (6). Dividing by the norm we obtain our first estimate for the expectation value of the energy:

$$
E = -NJ \left[ 3 + \frac{\lambda_1}{1 + \lambda_1 b_{11}} \right] = -0.422619NJ.
$$

(8)

Quite obviously, the correction due to off-diagonal processes to the energy is rather small.

We proceed to the second step. Whereas we restricted the sums in the norm and expectation value of $H$ to configurations which differed only by 4-site loops from $| \psi \rangle$, we now enlarge this subset to comprise all states differing by 4 or 6-site loops. Let us assume that we have drawn $\nu$ 4-site loops in the plane, and ask how many ways are there to draw $\nu_1$ additional 6-site loops. Putting the first 6-site loop we have to make sure that it does not intersect any of the 4-site loops and assuming that each of the 4-site loops blocks a total of $b_{12} = 15$ possible positions of 6-site loops, we find that the first 6-site loop can be drawn in $N_1 = N - b_{12} \nu$ ways. Now, we proceed precisely as for the 4-site loops: every 6-site loops that we draw blocks $b_{22} = 15.5$ other possible 6-site loops (a 6-site loop in $x$-direction blocks 15 6-site loops in $x$-direction and 16 6-site loops in $y$-direction), so that we estimate the number of ways in which the $\nu_1$ 6-site loops can be drawn as

$$
N_1(N_1 - b_{22})(N_1 - 2b_{22}) \cdots (N_1 - (\nu_1 - 1)b_{22})_{2\nu_1}^{\nu_1}
$$

$$
= (2b_{22})_{\nu_1}^{\nu_1} \left( \frac{(N_1 - b_{22})}{\nu_1} \right)_{\nu_1}^{\nu_1}.
$$

Thereby the extra factor of $2^{\nu_1}$ is due to the fact that there are two different types of 6-site loops (in $x$-direction and $y$-direction). By analogous considerations as for the 4-site loop, we now estimate that each drawn 6-site loop gives a contribution of

$$
\lambda_2 = \frac{2}{4z(z-1)^2} = \frac{1}{72}
$$

to the overlap. Proceeding as above we find that the total contribution to the norm from all states containing $\nu$ 4-site loops and an arbitrary number of 6-site loops is
The ‘most probable number’ of 4-site loops drops by \( \approx 15\% \) from \( N/21=0.0476N \) to 0.0403\( N \), whereas the most probable number of 6 loops is 0.0194\( N \). Enlarging the subset of states used for the computation of energy and norm does have only a moderate influence, i.e. our procedure is reasonably convergent.

In addition the procedure has an induction-like character: enlarging the sums in (3) and (7) the subset of states leads to additional prefactors in the norm, a renormalization of the preceding \( \lambda \)'s, additional terms in the expectation values of \( H \) and a renormalization of the exchange integrals in the preceding energy contributions. Repeating everything including also 8-site loops gives an estimate for the energy of \( E = -0.434473N J \), the number of 4-loops drops by only 8\%. The convergence thus is quite fast, with the difference between subsequent estimates dropping by an order of magnitude in each step (actually the dependence is not monotonous in that the estimate including 8-loops is higher than the the one from 6-site loops). We can conclude that taking into account only 4-site loops may be sufficient to get reasonably accurate results with little effort - this may be an important simplification in further applications of the state (1).

Comparing with results of numerical calculations which give an energy of \( \approx -0.6 J \) /site the agreement is obviously not too good. This is probably due to the fact that our simple estimates for the probability to find a given loop in an arbitrary dimer configuration are not too accurate.

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