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Variational RVB wavefunctions for the spin-1/2 J_1–J_2 Heisenberg antiferromagnet on the triangular lattice

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Abstract. 'Resonating-valence-bond' (RVB) variational wavefunctions are numerically investigated in order to describe the ground state and the singlet low-lying excited states of the spin-1/2, J_1–J_2 Heisenberg antiferromagnet with $1/8 \lesssim J_2/J_1 \lesssim 1$ on triangular lattices of $N = 4p$ sites compatible with the classical Néel orders. Comparison with previous exact diagonalization results indicates that the singlet eigenstates associated with collinear Néel order, among which the ground state is found, can be accurately described with appropriate superpositions of two-sublattice RVB trial states, while the other singlet low-lying eigenstates associated with four-sublattice Néel order can be well approximated from the four-sublattice RVB *trial states*.

The spin-1/2, J_1–J_2 Heisenberg antiferromagnet on the triangular lattice has attracted attention, in particular, since quantum fluctuations could lift the degeneracy of the classical ground-state manifold, selecting a specific order [1–5]. This Hamiltonian reads

$$\mathcal{H} = 2J_1 \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + 2J_2 \sum_{\langle\langle i,k \rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_k \tag{1}$$

where J_1 and $J_2 = \alpha J_1$ are positive and the first and second sums respectively run over the first and second neighbours. In the classical limit ($S \to \infty$), its ground state is, when $1/8 < \alpha < 1$, a degenerate continuous manifold of four-sublattice Néel states (figure 1). The selection by quantum fluctuations of a two-sublattice collinear Néel state (figure 1) in this manifold of four-sublattice Néel states was first suggested from spin-wave calculations [1–3] and has recently received strong support from the exact diagonalization calculations of Lecheminant *et al* [5] on finite spin-1/2 systems. Analysing the symmetry properties of the eigenstates, these authors identified the set of eigenstates $\{^4\tilde{E}\}$ which enable one to construct any four-sublattice Néel state, and showed that the eigenstates with the lowest energies for every value of the total spin S form a subset $\{^2\tilde{E}\}$ of the set $\{^4\tilde{E}\}$, which includes all the eigenstates required to build any collinear state, and has the finite-size scaling property characteristic of the existence of collinear long-range order in the thermodynamic limit.

The purpose of this article is not to improve over the diagonalization results but to show that, for the J_1–J_2 model with $1/8 \lesssim \alpha \lesssim 1$, on samples of $N = 4p$ sites with periodic boundary conditions, compatible with classical orders, one may accurately approximate both the states in the $S = 0$ singlet subspace $\{^2\tilde{E}\}_{S=0}$, which include the ground state and the other states of the singlet subspace $\{^4\tilde{E}\}_{S=0}$ of $\{^4\tilde{E}\}$, by variationally optimizing singlet

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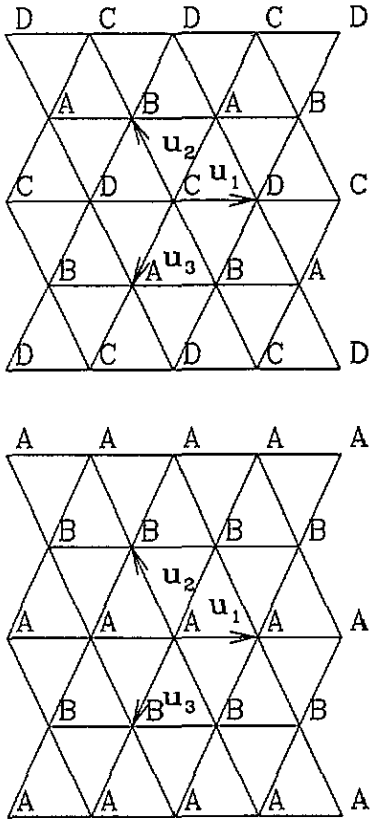

Figure 1. Top: the four-sublattice classical ground state. The classical spins on the same sublattice are parallel to each other with the sole constraint that the sum of four spins sited on different sublattices is zero. Bottom: one collinear classical ground state (in this case, classical spins in sublattices A and B are antiparallel). The two others have the ferromagnetic directions parallel to u_2 and u_3 respectively.

trial states describing two-sublattice and four-sublattice 'resonating-valence-bond' (RVB) states. To this end, a class of two-sublattice RVB trial states, denoted $|\psi_2\rangle$, and several classes of four-sublattice RVB trial states, noted $|\psi_4\rangle$, which are computationally convenient, were investigated using Monte Carlo calculations. In what follows, we describe these trial states and then compare their energy and spin–spin correlation values with the exact results available for $N = 12, 16, 28$ from [5]. The comparison shows that, when optimized, the $|\psi_2\rangle$ states have energy and spin–spin correlation values very close to those of the (nearly degenerate) eigenstates of $\{^2\tilde{E}\}_{S=0}$, whereas similar agreement is found between the properties of certain $|\psi_4\rangle$ states and those of the eigenstates of $\{^4\tilde{E}\}_{S=0}$ not in $\{^2\tilde{E}\}_{S=0}$. Results obtained for $N = 36$, with the two-sublattice RVB trial state and a four-sublattice RVB trial state describing a tetrahedral state, are also reported.

The two-sublattice $|\psi_2\rangle$ trial states which were investigated are superpositions of valence-bond states $|\beta\rangle$, built from singlet bonds connecting opposite sublattices A and B (see figure 1), weighted by the product $\omega(\beta)$ of the weights associated with individual bonds:

$$|\psi_2\rangle = \sum_{\beta} \omega(\beta)|\beta\rangle \tag{2a}$$

$$|\beta\rangle = \prod_{i=1}^{N/2}(A_i B_{\beta_i}) \qquad \omega(\beta) = \prod_{i=1}^{N/2} h(A_i B_{\beta_i}) \tag{2b}$$

where the A_i (B_i) label the $N/2$ A (B) sites, $(ij) = |\uparrow_i\downarrow_j - \downarrow_i\uparrow_j\rangle$ denotes a singlet bond between the two sites i and j, the sum is over all permutations β of the set $i = \{1, 2, \ldots, N/2\}$ and $h(i, j)$ is a real positive function of the distance between sites i and j whose values will be variationally determined. These trial states are similar to those considered previously for the Heisenberg antiferromagnet on the square lattice by Liang, Douçot, and Anderson [6] who found that using such a factorized form for the weights enables one to obtain an excellent variational energy for this model. We recall briefly some of their general properties. If $h(i, j)$ is constant $\forall$ i, j, then $|\psi_2\rangle$ represents a classical collinear Néel state projected on the singlet subspace: the total spin on a sublattice is then a maximum, $S_A = S_B = N/4$, with $\langle S_i \cdot S_j\rangle = 1/4$ if i and j are two different sites on the same sublattice and $\langle S_i \cdot S_j\rangle = -(1/4)(1 + 2/N)$ if i and j are on different sublattices. This state would be the ground state for a Hamiltonian with infinite-range antiferromagnetic coupling of the spins on the A and B sublattices, but is not energetically optimal if antiferromagnetic interactions are short ranged [7]. Then one expects to find the lowest energy for values of the $h(i, j)$ which decay with the distance. The optimum $|\psi_2\rangle$ state will still display collinear long-range order in the thermodynamic limit ($N \to \infty$) provided that h decays sufficiently slowly. In this study, we did not attempt to confirm the existence of collinear order from variational calculations. In fact, since the amount of Néel long-range order in $|\psi_2\rangle$ depends on the long-range behaviour of h while the energy is mostly sensitive to the short-range part of h, one will presumably find ordered and disordered $|\psi_2\rangle$ states very close in energy. A variational approach will not allow one to assess conclusively the amount of long-range order.

The above approach generalizes to an n-sublattice structure [7, 8]. The four-sublattice $|\psi_4\rangle$ trial states we have considered are the superpositions of all the valence-bond states $|\beta\gamma\delta\rangle$ having the same numbers n_{ab}, n_{ac}, n_{ad}, n_{bc}, n_{bd}, n_{cd} of AB, AC, AD, BC, BD, CD singlet bonds connecting the different sublattices A, B, C, D (see figure 1). Their weights $\omega(\beta\gamma\delta)$ are the products of the weights $h(i, j)$ of the individual bonds. Here too, the $h(i, j)$ are functions of the distance between sites i and j and will be the variational parameters. These trial states read

$$|\psi_4\rangle = \sum_{\beta\gamma\delta} \omega(\beta\gamma\delta)|\beta\gamma\delta\rangle \tag{3a}$$

$$|\beta\gamma\delta\rangle = \prod_{i=1}^{n_{ab}}(A_i B_{\beta_i}) \prod_{j=1}^{n_{ac}}(A_{n_{ab}+j} C_{\gamma_{(n_{cd}+j)}}) \prod_{k=1}^{n_{ad}}(A_{(n_{ab}+n_{ac}+k)} D_{\delta_k}) \times \prod_{l=1}^{n_{bc}}(B_l C_{\gamma_{(n_{ac}+n_{cd}+l)}}) \prod_{m=1}^{n_{bd}}(B_{\beta_{(n_{bc}+m)}} D_{\delta_{(n_{ad}+m)}}) \prod_{n=1}^{n_{cd}}(C_{\gamma_n} D_{\delta_{(n_{ad}+n_{bd}+n)}}) \tag{3b}$$

$$\omega(\beta\gamma\delta) = \prod_{i=1}^{n_{ab}} h(A_i B_{\beta_i}) \prod_{j=1}^{n_{ac}} h(A_{n_{ab}+j} C_{\gamma_{n_{cd}+j}}) \prod_{k=1}^{n_{ad}} h(A_{n_{ab}+n_{ac}+k} D_{\delta_k}) \times \prod_{l=1}^{n_{bc}} h(B_l C_{\gamma_{n_{ac}+n_{cd}+l}}) \prod_{m=1}^{n_{bd}} h(B_{\beta_{n_{bc}+m}} D_{\delta_{n_{ad}+m}}) \prod_{n=1}^{n_{cd}} h(C_{\gamma_n} D_{\delta_{n_{ad}+n_{bd}+n}}) \tag{3c}$$

where the A_i, B_j, C_k, D_l label the sites of the A, B, C, D sublattices respectively, while the β_i, γ_j, δ_k are elements of three whole sets of permutations of $\{1, 2, \ldots, N/4\}$: the

$|\beta\gamma\delta\rangle$ are obtained by permuting the ends of the bonds on the same sublattice. Therefore, those states where $h(i, j)$ is constant have maximal values of the total spins on each of the sublattices, $S_A = S_B = S_C = S_D = N/8$, since they are symmetric under the interchange of any two spins in a given sublattice, and are the RVB formulations of projections of a classical Néel state onto the singlet subspace, as first shown by Ma [7]. Every $|\psi_4\rangle$ state relates to a projected four-sublattice Néel state, just like the $|\psi_2\rangle$ do to a projected collinear state. Here, however, one has several projected four-sublattice Néel states, one for each allowed set of values of the $n_{\mu\nu}$ ($\mu, \nu = \{a, b, c, d\}$). Note that the six numbers $n_{\mu\nu}$ will be completely determined by the values of two of them since all sites are connected to a bond. This implies that $n_{bd} = n_{ac}$, $n_{cd} = n_{ab}$, $n_{ad} = n_{bc} = N/4 - n_{ab} - n_{ac}$ with $n_{ab} + n_{ac} \leqslant N/4$. The different types of $|\psi_4\rangle$ state will later be specified via the values of n_{ab} and n_{ac}. As pointed out by Ma, two types of projected four-sublattice Néel state can be easily pictured. One is the state where all $n_{\mu\nu} = N/12$ (note that N must then be an integer multiple of 12). Then $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = -1/12 - 2/3N$ between spins on any two different sublattices. This state is the projection of the classical Néel state which has the spins on the four sublattices pointing in a tetrahedral configuration. The others, allowed for $N = 4p$, are those having only two non-zero $n_{\mu\nu}$, for instance $n_{ab} = n_{cd} = N/4$. Then $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = -1/4 - 2/N$ if $i \in A$ and $j \in B$ or if $i \in C$ and $j \in D$; otherwise $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = 0$ if i and j are on different sublattices. The associated classical Néel states have the spins on the A, B sublattices antiparallel and the spins on the C, D sublattices antiparallel in a perpendicular direction, forming a cross. The energies of all the projected two-sublattice and four-sublattice Néel states are equal: $E_\psi = -(J_1/4)(1 + \alpha)(1 + 8/N)$ per site. In the case of accidental degeneracy, $\alpha = 0.5$ for $N = 12$, $\alpha = 1$ for $N = 16$, they are possible ground states. Otherwise, the $|\psi_4\rangle$ are energetically optimized with a function h decaying with the lengths of the bonds and will display Néel long-range order in the thermodynamic limit if h decays sufficiently slowly, like the $|\psi_2\rangle$ states.

Several others features of the set of $|\psi_2\rangle$ and $|\psi_4\rangle$ trial states must also be noticed. First, for a given h function, there are three degenerate $|\psi_2\rangle^{u_i}$ states corresponding to the three possible ferromagnetic directions u_1, u_2, u_3 (see figure 1) on the triangular lattice and these states are non-orthogonal because of the non-orthogonality of the valence-bond states, although they are linearly independent: as $|\psi_2\rangle^{u_i} \neq |\psi_2\rangle^{u_j}$ if $i \neq j$ the 3×3 overlap matrix is non-singular. Similarly, for a given h function, there are several degenerate non-orthogonal $|\psi_4\rangle$ states corresponding to the permutations of the three numbers n_{ab}, n_{ac}, n_{ad}, except when all the $n_{\mu\nu}$ are equal, i.e. for the $|\psi_4\rangle(n_{ab} = n_{ac} = N/12)$ states derived from the classical tetrahedral Néel state. Yet, the $|\psi_4\rangle$ states are non-orthogonal even if they are not related by a permutation of the $n_{\mu\nu}$ and the $|\psi_4\rangle$ states may overlap with the $|\psi_2\rangle^{u_i}$ states. With three $|\psi_2\rangle^{u_i}$ and all the possible $|\psi_4\rangle(n_{ab}, n_{ac})$ states, one has a number of different trial states which is larger than the dimension of $\{^4\tilde{E}\}_{S=0}$, i.e. the number of linearly independent singlet states associated with a four-sublattice structure, which is $1 + N/4$ [5]. One has an overcomplete set of non-orthogonal trial states. Unlike the exact eigenstates, neither the $|\psi_2\rangle^{u_i}$ nor the $|\psi_4\rangle(n_{ab}, n_{ac})$ states (except the $|\psi_4\rangle(n_{ab} = n_{ac} = N/12)$ states) have a definite symmetry under the action of the space group. Obviously it would have been preferable to work with an orthogonalized set of trial states of definite symmetry which may be obtained from a superposition of the trial states having the mandatory properties under the space group symmetries, but for computational convenience we worked with the above trial states. Fortunately, this did not prevent a comparison with the exact results on the small samples investigated—but if the exact eigenstates were not known, one would have to devise an orthogonalized set of trial states from group symmetry analysis.

The values of the spin–spin correlation and the energies of the $|\psi_2\rangle$ and $|\psi_4\rangle$ states

were computed using the Monte Carlo algorithm described in [6, 8] which consists in the sampling of pair of valence-bond states with a probability proportional to the product of their weights and the absolute value of their overlap. The method is very effective for the $|\psi_2\rangle$ states and for the $|\psi_4\rangle$ states with almost four kinds of bond where the overlaps of every pair of valence-bond states are all positive (this is the advantage of the present trial states), but becomes time consuming on large samples for the $|\psi_4\rangle$ states with six kinds of bond where the overlaps are then of both signs [8]. In the first case, this algorithm can deal with very large samples, even with the workstations we used, but in the second case, an alternative algorithm would have been required for samples larger than those studied here, focusing on the comparison with exact results available for $N = 12, 16, 28$ at $\alpha = 0.7$. Variational calculations were carried out with the $|\psi_2\rangle$ states and with the $|\psi_4\rangle$ states with all possible sets of values of the $n_{\mu\nu}$ for the $N = 12$ and $N = 16$ lattices and with the $|\psi_2\rangle$ states for $N = 28$. On the $N = 36$ lattice we compare the $|\psi_2\rangle$ states and the $|\psi_4\rangle$ states corresponding to the tetrahedral Néel state (all $n_{\mu\nu}$ equal). There is only one variational parameter for $N = 12, 16$: $h(\sqrt{3})$, the value of the weight function for second-nearest-neighbour bonds at distance $\sqrt{3}$ but three: $h(\sqrt{3})$, $h(\sqrt{7})$ and $h(3)$ for $N = 28, 36$.

Table 1. Energy values E_ψ of the optimized trial states investigated, $|\psi_2\rangle$ and $|\psi_4\rangle(n_{ab}, n_{ac})$, and those of the exact low-lying kth eigenstates E_k for lattices of N sites when $\alpha = J_2/J_1 = 0.7$. The exact ground state labelled 0 has the energy E_0. n_k is the degeneracy of the eigenstate k. The numbers in brackets are the estimated errors on the last digits of the variational energies E_ψ. The $|\psi_4\rangle$ states with six types of bond (all $n_{\mu\nu} \neq 0$) are indicated with an asterisk (*). Among these, the $|\psi_4\rangle(1, 1)$ and $|\psi_4\rangle(3, 3)$ for $N = 12$ and $N = 36$, respectively, derive from tetrahedral Néel states.

N	$\|\psi\rangle$	E_ψ	k	E_k	n_k	
12	$\|\psi_2\rangle$	−0.718 81 (8)	0	−0.719 49	2	Γ_3
12	$\|\psi_4\rangle(2, 1)$	−0.718 35 (5)	1	−0.717 07	1	Γ_1
12	$\|\psi_4\rangle(3, 0)$	−0.717 13 (5)				
12	$\|\psi_4\rangle(1, 1)$*	−0.714 37 (6)	2	−0.713 39	1	Γ_2
16	$\|\psi_2\rangle$	−0.646 12 (16)	0	−0.646 35	1	Γ_1
16	$\|\psi_4\rangle(2, 2)$	−0.645 73 (10)	1	−0.645 82	2	Γ_3
16	$\|\psi_4\rangle(3, 1)$	−0.644 36 (10)				
16	$\|\psi_4\rangle(4, 0)$	−0.643 23 (10)				
16	$\|\psi_4\rangle(2, 1)$*	−0.642 41 (13)	2	−0.642 22	2	Γ_3
28	$\|\psi_2\rangle$	−0.631 17 (16)	0	−0.631 58	2	Γ_3
28			1	−0.631 57	1	Γ_1
28			2	−0.618 83	1	Γ_1
28			3	−0.617 93	2	Γ_3
28			4	−0.613 46	2	Γ_3
36	$\|\psi_2\rangle$	−0.619 97 (10)				
36	$\|\psi_4\rangle(3, 3)$*	−0.582 20 (179)				

Results obtained at $\alpha = 0.7$ for the energy values E_ψ of the optimized trial states considered here, on samples of $N = 12, 16, 28, 36$ sites, are displayed in table 1 together with the energy values E_k obtained by Lecheminant *et al* [5] on samples with $N = 12, 16, 28$ sites, for the $1 + N/4$ lowest-lying exact eigenstates. The spin–spin correlations $S_0 \cdot S_r$ between a spin at the origin and a spin in the rth shell of the exact eigenstates computed on samples of $N = 12, 16$ sites are reported in table 2 together with the $S_0 \cdot S_r$ averaged

over the rth shell of the trial states. The authors of [5] have shown that these $1 + N/4$ exact eigenstates form the set $\{^4\tilde{E}\}_{S=0}$ of singlet states which enter into the construction of any four-sublattice Néel state, since they transform, under the operations of the space group of the triangular lattice, like the irreducible representations, $\Gamma_1, \Gamma_2, \Gamma_3$, of the group S_4 of permutations of four elements, and the number of $\Gamma_1, \Gamma_2, \Gamma_3$ in this set is exactly the one that is mandatory for that. We recall that Γ_1 is the trivial representation, Γ_2 is the one-dimensional representation that is even under a rotation $\mathcal{R}_{2\pi/3}$ of $2\pi/3$ around an axis perpendicular to the plane of the lattice and odd in a reflection σ_x around the axis u_1, whereas the two-dimensional Γ_3 is non-trivial under $\mathcal{R}_{2\pi/3}$. The authors of [5] have also shown that within $\{^4\tilde{E}\}_{S=0}$ the three states lowest in energy may be identified as the subset $\{^2\tilde{E}\}_{S=0}$ of singlet states associated with a collinear structure, since $\{^2\tilde{E}\}_{S=0}$ should consist of one Γ_1 state and two degenerate Γ_3 states.

Table 2. Spin–spin correlations $S_0 \cdot S_r$ between a spin at the origin and a spin in the rth shell in the trial states $|\psi_2\rangle$, $|\psi_4\rangle(n_{ab}, n_{ac})$ and in the exact low-lying kth eigenstates for the $N = 12$ and $N = 16$ lattices when $\alpha = J_2/J_1 = 0.7$. The variational values are the average values of the spin–spin correlations within the rth shell.

N	$\lvert\psi\rangle$	r	$S_0 \cdot S_r$	k	r	$S_0 \cdot S_r$
12	$\lvert\psi_2\rangle$	1	−0.119 99(2)	0	1	−0.118 65
		2	−0.170 86(2)		2	−0.173 11
		3	0.241 28(2)		3	0.240 63
12	$\lvert\psi_4\rangle(2, 1)$	1	−0.122 39(1)	1	1	−0.122 72
		2	−0.167 27(1)		2	−0.166 14
		3	0.243 03(1)		3	0.242 39
12	$\lvert\psi_4\rangle(3, 0)$	1	−0.122 07(1)			
		2	−0.167 10(2)			
		3	0.241 87(2)			
12	$\lvert\psi_4\rangle(1, 1)$	1	−0.126 52(2)	2	1	−0.128 04
		2	−0.159 41(2)		2	−0.156 79
		3	0.243 70(2)		3	0.244 31
16	$\lvert\psi_2\rangle$	1	−0.141 99(3)	0	1	−0.142 98
		2	−0.104 82(4)		2	−0.103 51
		3	0.243 62(4)		3	0.243 01
16	$\lvert\psi_4\rangle(2, 2)$	1	−0.141 06(2)	1	1	−0.141 72
		2	−0.105 98(3)		2	−0.105 06
		3	0.244 07(3)		3	0.243 58
16	$\lvert\psi_4\rangle(3, 1)$	1	−0.138 64(1)			
		2	−0.108 78(2)			
		3	0.244 82(2)			
16	$\lvert\psi_4\rangle(4, 0)$	1	−0.136 30(1)			
		2	−0.111 60(2)			
		3	0.245 79(2)			
16	$\lvert\psi_4\rangle(2, 1)$	1	−0.134 65(3)	2	1	−0.134 88
		2	−0.113 53(3)		2	−0.113 13
		3	0.246 38(3)		3	0.246 02

As seen in table 1, the energies of the $|\psi_2\rangle$ are always very close to the ground-state energies and smaller than the energies of the first excited states, i.e. between those of the Γ_1, Γ_3 states of $\{^2\tilde{E}\}_{S=0}$ which are close in energy. Besides, the $S_0 \cdot S_r$ of the $|\psi_2\rangle$ states are also close to those of the Γ_1, Γ_3 states of $\{^2\tilde{E}\}_{S=0}$ (see table 2). This suggests that the states in $\{^2\tilde{E}\}_{S=0}$ will very likely be well described with a superposition of the $|\psi_2\rangle$ states with appropriate symmetry, like $|\psi_2\rangle^{u_1} + |\psi_2\rangle^{u_2} + |\psi_2\rangle^{u_3}$ for the Γ_1

state, $|\psi_2\rangle^{u_1} + \omega|\psi_2\rangle^{u_2} + \omega^2|\psi_2\rangle^{u_3}$ and $|\psi_2\rangle^{u_1} + \omega^2|\psi_2\rangle^{u_2} + \omega|\psi_2\rangle^{u_3}$ where $\omega = e^{i2\pi/3}$ for the Γ_3 states. In all cases the $|\psi_2\rangle$ states yield lower variational energies than the $|\psi_4\rangle$ states. Slightly higher in energy above the $|\psi_2\rangle$ states one finds, however, the $|\psi_4\rangle(n_{ab}, n_{ac})$ states with four kinds of bond, $|\psi_4\rangle(2, 1)$ for $N = 12$, $|\psi_4\rangle(2, 2)$, $|\psi_4\rangle(3, 1)$ for $N = 16$. Their energy and spin–spin correlation values are also close to those of the Γ_1, Γ_3 states of $\{^2\tilde{E}\}_{S=0}$ (see tables 1 and 2), although closer to those of the first excited states. Thus, superpositions of these trial states with Γ_1, Γ_3 symmetry may also describe the states of $\{^2\tilde{E}\}_{S=0}$, but perhaps not as well as the states formed out of the $|\psi_2\rangle$ states. As seen in tables 1 and 2, it is the $|\psi_4\rangle(n_{ab}, n_{ac})$ states with six kinds of bond, $|\psi_4\rangle(1, 1)$ for $N = 12$, $|\psi_4\rangle(2, 1)$ for $N = 16$, which have energies and spin–spin correlations close to those of the eigenstates of $\{^4\tilde{E}\}_{S=0}$ not included in $\{^2\tilde{E}\}_{S=0}$ (which are well separated in energy from the states in $\{^2\tilde{E}\}_{S=0}$). In particular there is a good agreement for $N = 12$ between the values obtained for the $|\psi_4\rangle(1, 1)$ state, which derive from a tetrahedral Néel state, and those of the Γ_2 state. Here the trial state also has the same symmetry properties as the Γ_2 state. This suggests that the Γ_2 states may be described with the tetrahedral $|\psi_4\rangle$ trial states if N is a multiple of 12 whereas, if N is not an integer multiple of 12, the states of $\{^4\tilde{E}\}_{S=0}$ not in $\{^2\tilde{E}\}_{S=0}$ will be well described by superposition of the $|\psi_4\rangle$ states with six kinds of bond with appropriate symmetry. For N larger than 16, several states of $\{^4\tilde{E}\}_{S=0}$ not in $\{^2\tilde{E}\}_{S=0}$ have similar symmetry properties. The construction of an orthogonal set of $|\psi_4\rangle$ states will then be necessary. The variational energy of the tetrahedral $|\psi_4\rangle$ state for $N = 36$ is reported in table 1 together with the energy of the $|\psi_2\rangle$ state. The variational values suggest that the two families of states may be even better separated in energy for $N = 36$ than for smaller samples. By contrast, the $|\psi_4\rangle$ states with two kinds of bond, $|\psi_4\rangle(3, 0)$ for $N = 12$ and $|\psi_4\rangle(4, 0)$ for $N = 16$, have energies intermediate between those of the states in $\{^2\tilde{E}\}_{S=0}$ and the other eigenstates of $\{^4\tilde{E}\}_{S=0}$, and spin–spin correlations somewhat different from those of these eigenstates.

To summarize, the results presented here suggest that the singlet states $\{^4\tilde{E}\}_{S=0}$ of the tower of states $\{^4\tilde{E}\}$ which built any four-sublattice Néel state in the thermodynamic limit can be accurately described with simple RVB trial states with factorized weights. In particular, superposition of the RVB trial states $|\psi_2\rangle$ built in connecting two sublattices by singlet bonds may accurately describe the singlet states $\{^2\tilde{E}\}_{S=0}$ of $\{^4\tilde{E}\}_{S=0}$ which are associated with a collinear structure and among which one finds the ground state. On the other hand, the others states $\{^4\tilde{E}\}_{S=0}$ not in $\{^2\tilde{E}\}_{S=0}$ may be described starting from the four-sublattice $|\psi_4\rangle$ trial states having six kinds of bond, with a tetrahedral $|\psi_4\rangle$ trial state for the Γ_2 state or by superposition of the $|\psi_4\rangle$ trial states in the case of the Γ_1 and Γ_3 states. This provides a picture of the $\{^4\tilde{E}\}_{S=0}$ states. The results suggest also that one could, using a variational approach, corroborate the conclusion drawn in [5] from exact diagonalizations on a small system that the collinear state is selected by quantum fluctuations for the J_1–J_2 model with $1/8 \lesssim \alpha \lesssim 1$. The availability of good trial states is also important in calculations with stochastic projection methods, like the Green function Monte Carlo method, which enable one to obtain exact results on a large system, and the present trial states may be useful for this purpose, provided that one overcomes the well-known numerical difficulties encountered in such methods in the case of frustrated systems.

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