# Generating-function approach to the resonating-bond state on the triangular and square ladders

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We calculate the energy of a resonating-valence-bond (RVB) state for the Heisenberg antiferromagnet Hamiltonian on the triangular and square ladders as  $N \rightarrow \infty$ . We take the RVB state to be a linear combination of all states in which all spins are bonded pairwise into nearest-neighbor singlets. The amplitude of each such state in the RVB wave function is proportional to  $\gamma^{n/2}$ , where  $\gamma$  is a variational parameter, and *n* is the number of horizontal bonds in the state. The optimal  $\gamma$  is very close to 1, when all states have equal amplitude. We compare our results to Anderson's finite-size calculation for the triangular ladder and to spin-wave theory for the twodimensional lattices.

## I. INTRODUCTION

The existence or nonexistence of long-ranged antiferromagnetic order (LRAO) has long been a fundamental issue in condensed-matter physics.<sup>1</sup> While there is no rigorous proof of a finite sublattice magnetization in the ground state of the Heisenberg antiferromagnet and, in fact, the exact Bethe-ansatz solution in one dimension says otherwise, it is widely believed that LRAO exists in higher dimensions. This belief is based on the stability of the Néel state with respect to spin-wave fluctuations for d > 1. However, Anderson has pointed out that the Néel state may just be locally stable in frustrated lattices. In particular, he suggests the resonating-valencebond (RVB) state as the ground state of the Heisenberg antiferromagnet on the two-dimensional (2D) triangular lattice.<sup>2</sup> The underlying structure of this state is that of "resonating" local singlet pairs. Recently, Anderson has further postulated the RVB state as the explanation of high- $T_c$  superconductivity.<sup>3,4</sup> To suppress the LRAO on the square lattices of these materials, Anderson invokes possible frustration due to further-neighbor interactions and/or additional quantum fluctuations due to a finite Hubbard U (Ref. 5).

The intuition for RVB states comes from the fact that on a chain the state with neighboring spins paired into singlets has an energy per spin  $E_s$  lower than that of the Néel state  $E_N$ :

$$E_N = -J/4 , \qquad (1.1)$$

$$E_s = -3J/8$$
 (1.2)

While  $E_S$  is independent of the underlying lattice,  $E_N$  is highly sensitive to it. On the 2D square and triangular lattices, we have  $E_N = -J/2$  and -3J/8, respectively, the last being the classical energy of the well-known 120° structure. The energy of the Néel state is lowered by quantum fluctuations, assuming the antiferromagnetic (AF) state remains stable. The singlet energy is also lowered by forming the RVB state, a linear combination of the different singlet states. Since  $E_N = E_S$  on the triangular lattice, it is quite possible that  $E_{RVB} < E_{AF}$ . The problem is that while  $E_{AF}$  is probably adequately approximated by the spin-wave theory,<sup>1</sup>  $E_{RVB}$  is much harder to calculate due to the nonorthogonality of the singlet states. Fazekas and Anderson<sup>6</sup> showed that the ground state is a RVB-like state close to the Ising  $(J \ll J_z)$  limit, and argued that it remains so for  $J = J_z$ . Also, Anderson,<sup>2</sup> using a singlet-only basis, calculated the lowest energies for N=2,4,6,8 on the triangular ladder [Fig. 1(a)], and extrapolated these to  $N = \infty$ , giving an energy per spin lower than the spin-wave theory on the entire triangular lattice.

The rationale behind Anderson's extrapolation is not entirely clear.<sup>7</sup> Here we present a calculation for the  $N = \infty$  ladder. The price we pay is that we are restricted to a nearest-neighbor singlet basis and, more importantly, to assigning equal amplitude to all such singlet states, except for one variational parameter. Thus the energy obtained is not as good as the extrapolated one. On the other hand, it is a real calculation and does give an energy slightly better than the spin-wave energy for the 2D triangular lattice.



FIG. 1. (a) Triangular and (b) square ladders with periodic boundary conditions. Periodic boundary conditions were not used in Anderson's finite-size calculation.

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#### **II. PRELIMINARIES**

In this section we introduce our wave function and outline the approach. We are interested in calculating  $E_{\rm RVB}$  for the Heisenberg Hamiltonian, with the coupling constant J equal to 1,

$$H = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j , \qquad (2.1)$$

where the sum is over nearest-neighbor pairs. For two spins the ground state is the singlet

$$|(i,j)\rangle = (1/\sqrt{2})(|i\uparrow\rangle | j\downarrow\rangle - |i\downarrow\rangle | j\uparrow\rangle). \quad (2.2)$$

To simplify the discussion let us first consider the square ladder [Fig. 1(b)]. As a zeroth-order approximation, we take a singlet state, in which all spins are bonded pairwise into a nearest-neighbor singlet. We call such states nearest-neighbor singlet states (NNSS's), a subset of general singlet states (SS's) where any spin forms a singlet with some other (not necessarily nearest-neighbor) spin. The definition of the RVB state is somewhat vague, ranging from a linear combination of all SS's to just NNSS's. In part, this is due to the lack of orthogonality of such states. Since a SS which is not a NNSS has a gap of at least  $\frac{3}{2}J$ , it would seem that the more restrictive definition should suffice. This is partly borne out by Anderson's finite-size calculation.

Restricting ourselves to NNSS's only, we still cannot say what the ideal linear combination is. For a start we can simply assign them all equal amplitude. Our approach allows a trivial improvement. First note that horizontal bonds always occur in pairs, i.e., if (2i + 1, 2i + 3), then also (2i, 2i + 2). We introduce a variational parameter  $\gamma$  such that our RVB wave function is

$$|\Psi\rangle = \sum_{\alpha} {}_{\gamma} n_{\alpha} |\Psi_{\alpha}\rangle = \sum_{\alpha} |\alpha\rangle , \qquad (2.3)$$

where the sum is over all NNSS's, and  $n_{\alpha}$  is the number of pairs of horizontal bonds. The inadequacy of this wave function and possible improvement will be discussed with the results in Sec. V.

Our aim is to calculate and minimize  $\langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$ . For convenience we will use a periodic boundary condition (PBC). We will adopt a convention such that if i, j forms a singlet, then it occurs as (i, j) for i to the left or on top of j. A general NNSS is composed of blocks of vertical bonds separated by blocks of horizontal pairs. A sum over state index  $\alpha$ is equivalent to a sum over all possible bond configurations. The total number of bonds is  $N_b = N$ , for 2N spins. Our approach is to sum over all  $N_h$  and calculate the matrix elements, which will serve as generating functions. From these we can perform the appropriate differentiation to obtain the physical  $(N_h = N)$  answers. We now introduce the generating functions for repeated vertical bonds and horizontal pairs, respectively,

$$v(x) = \sum_{n=1}^{\infty} x^n = x/(1-x) , \qquad (2.4)$$

$$h(x) = \sum_{n=1}^{\infty} (\gamma x)^{2n} = (\gamma x)^2 / [1 - (\gamma x)^2] . \qquad (2.5)$$

Their meaning will become clear below.

#### **III. CALCULATIONS**

A. 
$$\langle \Psi | \Psi \rangle$$

A principal difficulty in dealing with a RVB state is the nonorthogonality of the  $|\alpha\rangle$ 's. Let us separate  $\langle \Psi | \Psi \rangle$  into diagonal,  $\sum_{\alpha} \langle \alpha | \alpha \rangle$ , and off-diagonal,  $\sum_{\alpha,\beta} \langle \alpha | \beta \rangle$ , terms. For two different states  $\alpha$  and  $\beta$ , some spins are bonded identically and some differently. We now introduce the concept of the diagonal block (DB) and the off-diagonal loop (ODL). A diagonal block is an uninterrupted sequence of spins identically bonded in  $\alpha$  and  $\beta$ . Similarly we can define the off-diagonal block, where all bonds are different. This last can be subdivided into ODL's, a sequence of off-diagonal horizontal pairs bounded by OD vertical bonds on both sides (see Fig. 2). For example, if  $\alpha = (1,2),(3,4)$ ,  $(5,6),\ldots$ , and  $\beta = (1,2),(3,5),(4,6),\ldots$ , then 1,2 form a DB and 3,4,5,6 an ODL. Between two consecutive ODL's, there may or may not be a DB.

# 1. Diagonal overlap $\sum_{\alpha} \langle \alpha | \alpha \rangle$

The overlap between a singlet and itself is, of course, 1. On top of that we associate a factor x for each vertical bond and a factor  $\gamma^2 x^2$  for each pair of horizontal bonds. Consider the spins 1,2. They can be in the configuration (1,2) or (1,3),(2,4) or (2N-1,1),(2N,2), contributing to the overlap x,  $\gamma^2 x^2$ , and  $\gamma^2 x^2$ , respectively. These need to be multiplied by the sum of overlaps between all possible DB's. This is easily seen to be given by

$$d(x) = 1 + 2 \sum_{n=1}^{\infty} (vh)^n + (h+v) \sum_{n=0}^{\infty} (vh)^n$$
$$= [1 - x - (\gamma x)^2]^{-1}, \qquad (3.1)$$

where the second term, for example, indicates that the rest of the spins cover the lattice by an arbitrary number of repeated units of a vertical block followed by a horizontal block, or the other way, around. The factor 1

FIG. 2. Some examples of diagonal blocks (DB's) and offdiagonal loops (ODL's). A bond is indicated by a line and  $\alpha$  or  $\beta$  denotes the state the bond is in. From left to right, we have ODL, ODL, DB, ODL, and DB.

implies that there are no other spins in the system and will give 0 upon differentiation, but it is included for later convenience. The diagonal contribution to the overlap is

$$\langle \Psi | \Psi \rangle_{\mathrm{D}} = W_a(x) + W_b(x)$$
,

with

$$W_a(x) = xd(x), \quad W_b(x) = 2\alpha^2 x^2 d(x)$$
 (3.2)

# 2. Off-diagonal overlap $\langle \alpha | \beta \rangle$

Off-diagonal overlaps are decoupled into overlaps of DB's and of ODL's. The overlap of a DB has already been obtained as d(x). The overlap of an ODL composed of 2n spins can be analyzed as follows (see Fig. 3):

(a) The *n* bonds from  $|\alpha\rangle$  (or  $\langle\beta|$ ) give  $x^n$ .

(b) The combined n-1 pairs of horizontal bonds give  $\gamma^{n-1}$ .

(c) The overlap is nonzero only if we decompose the singlets into the alternating up-down-up-down configuration as we go around the loop. This gives  $2(\frac{1}{2})^n = (\frac{1}{2})^{n-1}$ , the factor 2 coming from an overall spin flip. In this decomposition a bond carries a positive (negative) sign if its configuration is up-down (down-up) from left to right or top to bottom. In any loop the number of negative signs is even and so the overall sign is always positive.

(d) A factor of 2 since the loop can arise from  $\langle \alpha | \beta \rangle$  or  $\langle \beta | \alpha \rangle$ .

Combining the above and summing over all possible loop sizes implies that the ODL overlap is

$$L(x) = \sum_{n=2}^{\infty} \left[ 2(\gamma/2)^{n-1} \right] x^n = \gamma x^2 / (1 - \gamma x/2) .$$
 (3.3)

Again let us consider the configuration of spins 1,2. The possibilities are the following.

(a) Diagonal and (1,2). The contribution is

$$U_{a}(x) = xd^{2}L \sum_{n=0}^{\infty} (dL)^{n}$$
  
=  $\gamma x^{3}d / [1 - (1 + \gamma/2)x - (\gamma^{2} + \gamma/2)x^{2} + (\gamma x)^{3}/2]$ 

$$\equiv \gamma x^{3} d / C(x) . \qquad (3.4)$$

FIG. 3. (a) One of two decompositions which contribute to the overlap between states  $\alpha$  and  $\beta$  in an ODL of eight spins. The other decomposition is given by an inversion of all the spins in the loop. (b) Decomposition in an ODL of ten spins.

The significance of the 1 in d(x) is revealed here since between two ODL's, there may or may not be a DB.

(b) Diagonal and not (1,2). The only difference is that x in (3.4) should be replaced by  $2\gamma^2 x^2$ ,

$$U_b(x) = 2\gamma^3 x^4 d / C(x) . (3.5)$$

(c) Off diagonal. If this ODL contains 2n spins, 1,2 can be in one of the *n* positions. Thus this special loop contributes

$$L_{s}(x) = \sum_{n=2}^{\infty} [2(\gamma/2)^{n-1}]nx^{n}$$
$$= (-2 + \gamma x/2)x^{2}/(1 - \gamma x/2)^{2}, \qquad (3.6)$$

which implies a contribution to the overlap of the whole lattice of

$$U_{c}(x) = L_{s}d \sum_{n=0}^{\infty} (dL)^{n}$$
  
= [(2-\gamma x/2)\gamma x^{2}]/[(1-\gamma x/2)C(x)]. (3.7)

Combining the diagonal and off-diagonal contributions, we see that

$$\langle \Psi | \Psi \rangle = \langle \Psi | \Psi \rangle_{\rm D} + \langle \Psi | \Psi \rangle_{\rm OD}$$
  
=  $W_a + W_b + U_a + U_b + U_c$  . (3.8)

More precisely,  $\langle \Psi | \Psi \rangle$  is given by taking the coefficient of  $x^n$  of (3.8).

B. 
$$\langle \Psi | H | \Psi \rangle$$

Again we separate out the diagonal

$$(\langle H \rangle_{\mathrm{D}} = \sum_{\alpha} \langle \alpha | H | \alpha \rangle)$$

and off-diagonal

$$(\langle H \rangle_{\mathrm{OD}} = \sum_{\alpha, \beta \alpha \neq \beta} \langle \alpha | H | \beta \rangle)$$

contributions. We also retain the definitions of DB and ODL with respect to the  $\alpha$ 's. First, consider matrix elements of the form  $C = \langle \alpha | \mathbf{S}_i \cdot \mathbf{S}_j | \beta \rangle$ , where both  $| \alpha \rangle$  and  $| \beta \rangle$  contain (i,m). If m = j,  $\mathbf{S}_i \cdot \mathbf{S}_j(i,j) = -\frac{3}{4}(i,j)$ , and so

$$C = -\frac{3}{4} \langle \alpha | \beta \rangle . \tag{3.9}$$

If  $m \neq j$ ,  $\mathbf{S}_i \cdot \mathbf{S}_j$  changes (i,m) from a singlet into a triplet, which is, of course, orthogonal to (i,m), and so

$$C = 0$$
 . (3.10)

1.  $\langle H \rangle_{\rm D}$ 

From Eq. (3.9),

$$\langle H \rangle_{\rm D} = -\frac{3}{4} N \left[ W_a(x) + W_b(x) \right] . \tag{3.11}$$
  
2.  $\langle H \rangle_{\rm OD}$ 

Because of the periodic boundary condition, we need only  $N\langle \mathbf{S}_1, \mathbf{S}_2 \rangle_{\text{OD}}$  and  $2N\langle \mathbf{S}_1, \mathbf{S}_3 \rangle_{\text{OD}}$ . The matrix ele-

ments depend on the bonding situation of 1,2 for the former and 1,2,3,4 for the latter. Below we state the different cases and the answers.

For case (i),  $\mathbf{S}_1 \cdot \mathbf{S}_2$ , we have the following.

(a) 1,2 diagonal and paired. Using (3.9), calculating this is no different from calculating the overlap for the same condition:

$$M_a(x) = -\frac{3}{4}U_a(x) , \qquad (3.12)$$

where  $U_a$  is given by (3.4).

(b) 1,2 diagonal and unpaired. This gives zero according to (3.10).

(c) 1,2 off diagonal. This gives

$$M_{c}(x) = -\frac{3}{4}U_{c}(x) . \qquad (3.13)$$

To obtain this it suffices to show that  $S_1 \cdot S_2$ , acting on the ODL that 1,2 are in, just gives  $-\frac{3}{4}$ . Recall that in calculating ODL's only a decomposition of the singlets into alternating  $\uparrow \downarrow \uparrow \downarrow \cdots$  (or  $\downarrow \uparrow \downarrow \uparrow \cdots$ ) configurations contributes. It is clear that for any loop containing 1,2 such a decomposition always leads to 1,2 having opposite spins. Thus,

$$\langle S_{1z}S_{2z}\rangle_{ODL} = -\frac{1}{4}\langle \rangle_{ODL}$$
.

By symmetry,

$$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle_{\text{ODL}} = -\frac{3}{4} \langle \rangle_{\text{ODL}}$$
.

For case (ii),  $2\mathbf{S}_1 \cdot \mathbf{S}_3$ , we have the following.

(a) 1,2,3,4 diagonal and paired as (1,3),(2,4). Again from (3.9) this is not any different from calculating the overlap,

$$P_a(x) = -\frac{3}{4}U_b(x) . (3.14)$$

(b) 1,2,3,4 diagonal, but 1,3 are not bonded. From (3.10), this gives zero.

(c) 1,2,3,4 are part of the same ODL. In this case 1,3 is either bonded in the bra or in the ket.  $2\mathbf{S}_1 \cdot \mathbf{S}_3$  acting on this bond gives  $-\frac{3}{2}$ . If this loop contains 2n spins, 1,2,3,4 can be in any n-1 position [cf. the analysis above Eq. (3.5)]. Thus this special loop contributes:

$$L'_{s}(x) = \sum_{n=2}^{\infty} [2(\gamma/2)^{n-1}](n-1)x^{n}$$
$$= \gamma x^{2}/(1-\gamma x/2)^{2} . \qquad (3.15)$$

Taking the factor  $-\frac{3}{2}$  and the rest of the spins into account, we have

$$P_{c}(x) = -\frac{3}{2}L'_{s}d\sum_{n=0}^{\infty} (dL)^{n}$$
  
=  $-(\frac{3}{2}\gamma x^{2})/[(1-\gamma x/2)C(x)]$ . (3.16)

(d) 1,2 and 3,4 belong to different ODL's. This gives zero. To see this it is simplest to consider the action of  $S_{1+}S_{3-}$ . This operator flips spin 1 from down to up in the ket without affecting any other spins in the ODL that it is in. This forces an up-up-up configuration in the ODL decomposition which is nonexistent.

(e) 1,2 diagonal and 3,4 off diagonal or vice versa. This also gives zero. The total is

$$\langle H \rangle = 2N(-\frac{3}{8}\langle \Psi | \Psi \rangle + \frac{1}{2}P_c) . \qquad (3.17)$$

## **IV. GROUND-STATE AND RESONANCE ENERGY**

Before we use the results from Sec. III to obtain the energy, we show how the corresponding expressions for the triangular ladder can be obtained with minor modifications. On the triangular ladder there are two types of "vertical" bonds, the 60° bonds [e.q., (1,2)] or the 120° bonds [e.g., (1,4)]. It is easy to see that no NNSS can contain both 60° and 120° bonds. Furthermore the overlap between a NNSS containing 60° bonds and one containing 120° bonds is at most  $(\frac{1}{2})^{N/2}$ . Thus, in spite of the PBC, it is possible to include only one type of vertical bond; choosing the 60° one makes the notation consistent with the square ladder. Calculations of the various matrix elements are identical except now we have to include the term  $S_1 \cdot S_4$  in the Hamiltonian. The only place this has a nonzero contribution is (c) of Sec. III B 2, giving a value equal to  $-\langle S_1 \cdot S_3 \rangle$ . So for this case (3.16) becomes

$$P_{c}(x) = -(\frac{3}{4}\gamma x^{2})/[(1-\gamma x/2)C(x)]. \qquad (3.16')$$

To obtain  $\langle \Psi | \Psi \rangle$  and  $\langle H \rangle$ , we should take the coefficient of  $x^N$  in (3.8) and (3.17). The easiest way to do this is to use partial fractions and take the Taylor expansion. When  $N = \infty$ , only the root with the smallest magnitude survives. We first formally write

$$E = \frac{1}{2N} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{:-\frac{3}{8}(W_a + W_b + U_a + U_b + U_c) + \frac{1}{2}P_c:}{:W_a + W_b + U_a + U_b + U_c:} ,$$
(4.1)

where : : denotes taking the coefficient of  $x^N$ . The first term is just the singlet energy  $-\frac{3}{8}$ , thus identifying the second term as the resonance energy  $\Delta E$ . Note that  $\Delta E(\text{square}) = 2\Delta E(\text{triangle})$ .  $\Delta E$  should be minimized with respect to  $\gamma$ .

The polynomials that appear in the denominators of the various generating functions are  $f_1(x)=1-x$  $-\gamma^2 x^2$ ,  $f_2(x)=1-\gamma x/2$ , and C(x). Superficially  $\langle \Psi | \Psi \rangle$  contains all three, while  $P_c(x)$  only has the last two. However, the various terms in Eq. (3.8) for  $\langle \Psi | \Psi \rangle$  can actually be organized to give

$$\langle \Psi | \Psi \rangle = : \frac{\gamma x^2 (2 - \gamma x/2)}{(1 - \gamma x/2)C(x)} : + : \frac{(x + 2\gamma^2 x^2)(1 - \gamma x/2)}{C(x)} : ,$$
(3.8)



FIG. 4. The Hamiltonian causes a resonance between these two degenerate states.

which indicates that  $f_1$  is absent from  $\langle \Psi | \Psi \rangle$  also. The root of  $f_2$  is

$$x_1 = -2/\gamma \ . \tag{4.2}$$

Let  $x_0$  be the smallest root of C(x). We find that  $|x_0| < |x_1|$ . The result for the energy is the following.

(a)  $\gamma = 0$ . Only the NNSS's with all vertical bonds remain.  $\Delta E = 0$ .

(b)  $\gamma < 0$ . This is the situation of antiresonance. Resonant states are out of phase with each other and  $\Delta E > 0$ .

(c)  $\gamma > 0$ . Here the resonant states are in phase and for all  $\gamma > 0$  and  $\Delta E < 0$ . For  $\gamma = 1$ , with all NNSS's given equal amplitude, the resonant energy on the triangular ladder is  $\Delta E = -0.0905$  (twice that on the square ladder). Slight improvement is obtained by taking the optimal  $\gamma = 1.17$ , with  $\Delta E = -0.0912$ .

A by-product of this calculation is the total number of NNSS's. This is just given by the diagonal overlap with  $\gamma = 1$ .

$$N_{\text{tot}} = \frac{1}{N!} \frac{d^{N}}{dx^{N}} [W_{a}(x) + W_{b}(x)]_{x=0}$$
$$= \frac{1}{N!} \frac{d^{N}}{dx^{N}} \frac{x + 2x^{2}}{1 - x - x^{2}} \Big|_{x=0}$$
$$= x^{-N}_{+} + x^{-N}_{-}, \qquad (4.3)$$

where  $x_{+,-} = 2/(1\pm\sqrt{5})$  are the roots of  $f_1(x)$  with  $\gamma = 1$ .

- <sup>1</sup>For a review, see D. C. Mattis, *The Theory of Magnetism I* (Springer-Verlag, Berlin, 1981).
- <sup>2</sup>P. W. Anderson, Mater. Res. Bull. 8, 153 (1973).
- <sup>3</sup>P. W. Anderson, Science 235, 1196 (1986).
- <sup>4</sup>G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. 63, 973 (1987).
- <sup>5</sup>J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985); Phys. Rev. Lett. **54**, 1317 (1985).
- <sup>6</sup>P. Fazekas and P. W. Anderson, Philos. Mag. 30, 432 (1974).
- <sup>7</sup>Anderson made a 1/N extrapolation using (2,6) or (4,8) spins. Previous exact finite-size calculations on 1D rings [J. C.

#### V. DISCUSSION

For the triangular ladder the present result gives  $\Delta E = -0.0912$  and a ground-state energy per spin of  $E_{\rm RVB} = -0.466$ . This is equal to or slightly better than spin-wave approximation for the entire 2D triangular lattice  $[E_{\rm SW} = -0.463 \pm 0.007$  (Ref. 2)], and is also equal to or slightly better than Anderson's result for eight spins. It is not comparable to Anderson's extrapolated value, with its questionable validity. Since our answer is variational for the 2D lattice, we do support the RVB state as being more stable than the antiferromagnetic state.

For the square ladder this calculation gives  $\Delta E = -0.182$  and  $E_{\rm RVB} = -0.557$ . This is better than spin-wave theory for the ladder  $[E_{\rm SW} = -0.553$  (Ref. 8)], but not for the 2D square lattice  $[E_{\rm SW} = -0.66$  (Ref. 9)]. Of course, this is mainly due to the Néel energy being so much lower than the singlet energy. The prevailing view seems to be that for 2D systems the RVB state is unlikely to be more stable than the AF state without the aid of frustration.

A brief discussion on how to improve on this calculation is in order. First, let us point out why within the present calculation the optimum  $\gamma$  cannot be very different from 1. The underlying physics behind RVB is that the Hamiltonian allows a transition from a pair of horizontal bonds to a pair of vertical bonds (see Fig. 4). Thus it is important that one takes a linear combination that includes a NNSS and its resonant state with similar amplitude.<sup>10</sup> For this reason vertical bonds and horizontal bonds cannot have very different weights. Most of the effort in taking a linear combination, however, merely serves to increase the overlap, and is counterproductive. This can be reduced by perhaps adjusting the phase of the different NNSS's, which brings us to the question of phase coherence. Anderson has raised the question of whether the RVB states in fact exhibit offdiagonal long-range order (ODLRO) in the form of long-range phase coherence (this is different from the superconducting RVB state recently proposed<sup>3</sup>). Our concept of the off-diagonal loop seems to be a useful way to think about this. We are currently investigating this aspect.

Bonner and M. E. Fisher, Phys. Rev. 135, A640 (1964)] and 2D square lattices [J. Oitmaa and D. D. Betts, Can. J. Phys. 56, 897 (1978)] indicate that larger-size systems are required for extrapolation. Also, while the 1/N extrapolation seems reasonable, Bonner and Fisher obtained a  $1/N^2$  result for their calculation.

- <sup>8</sup>Y. Fan (unpublished).
- <sup>9</sup>P. W. Anderson, Phys. Rev. 86, 694 (1952).
- <sup>10</sup>For this reason we consider it unlikely that the s-wave RVB state proposed in Refs. 3 and 4, with  $\gamma = -1$ , can be the lowest-energy state.