Doping an optimized resonance-valence-bond state: A picture of spin-charge separation

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A systematic ''loop-gas'' formalism is developed for a general study of the resonance-valence-bond (RVB) states of a quantum antiferromagnet. At half-filling, we obtain analytic, parameter-free RVB amplitudes which reproduce virtually exact ground-state energy and spin excitation spectrum. A doped hole is then modeled by a holon-spinon pair moving on this optimized RVB background. Its energy is in excellent agreement with other estimates on the finite lattice for $t/J \leqslant 1$. Such a pair wave function shows a finite amplitude even at infinite separation. Spin-charge separation and vanishing quasiparticle spectral weight are discussed in this framework.

I. INTRODUCTION

The idea that a resonance-valence-bond (RVB) state of spin-liquid type[1] may be a precise picture of the two-dimensional quantum antiferromagnet was once the most attractive topic soon after the discovery of the high-T_c superconductivity. Despite numerous forms of wave functions were proposed (some of them are not quite RVB), there has always been a lack of systematic methods to carry out the analysis. In addition, subsequent numerical results have concluded with the long-range magnetic ordering (LRMO) for the ground state of the Heisenberg model, contrary to the naive short-range picture of the spin liquid. Nevertheless, what has been less emphasized in the literature is that even RVB states can possess LRMO if the bonds decay sufficiently slow. The optimized states are in fact such kind, as was first found on a square lattice by Liang, Doucot, and Anderson,[2] and recently found even on the triangular lattice by one of the authors.[3] Furthermore, a class of optimized RVB amplitudes were derived which reproduce virtually everything exactly:[4] Not only its ground-state energy and the staggered magnetization are identical to the exact values (as cited by Ref. 5), the low-lying spin-flip spectrum also agrees precisely with the best numerical result obtained by supercomputer.[6] These successes, we believe, should have strong impact on the original idea once a suitable generalization to the doped regime is found.

In this article, we sketch out an approach for a general analysis of the RVB states in terms of a loop-gas formalism.[7] It is based on the fact that an overlap between two given (generally different) realizations of the RVB bonds can be mapped onto a configuration of a self-avoiding loop gas. Various physical quantities may be then calculated in terms of the loop gas and Monte Carlo technique. We also develop a simple but powerful way of deriving the best RVB state. It is amazing that such a simple wave function gives a complete account of the whole energy.

Our main goal is to understand and provide a precise picture of holes moving on the optimized RVB background. In fact, it turns out to be simple enough for general audiences: We show that a doped hole may be accurately modeled by a holon-spinon pair for at least $t/J \leqslant 1$. A static hole is in an s-state relative to the background, in the sense that its counter part, the spin, carries completely the before-doping RVB phase. This is a peculiar two-body problem in which spin states at different sites are not orthogonal. Now it is energetically unfavorable for the spin to stay nearby the hole in the absence of the binding force, i.e., the superexchange energy between them. It thus escapes to infinity, giving rise to spin-charge separation. Hopping, on the other hand, is found to induce additional short-range p-wave component for the holon-spinon pair in order to gain coherent motion over the lattice. The energy of such kind of states agrees well with other accurate estimates on finite lattices (especially at $t/J \leqslant 1$). Both the s wave and the p wave lead to vanishing spectral weight as the lattice size increases once the effect of long-range spin-flip fluctuations is included. This means that a perturbation starting with the undoped state cannot account correctly for the coherent motion of the hole (in fact holon-spinon pair). A rigorous proof of this point on a general basis will be given elsewhere.[8]

The outline of the paper is as follows. In the next section we present the general formalism of using the loop gas as a computational tool. Then we show in Sec. III how an analytic self-consistency approximation can be used to derive the optimized set of RVB amplitudes. Section IV explains the use of the Monte Carlo technique in details, along with the main achievements at the half-filling limit. Section V applies the loop-gas formalism to the one-hole problem. The question of phase separation and vanishing quasiparticle weight is finally explored in Sec. VI. Section VII concludes the paper with some discussions and speculations on future work.

II. GENERAL SCHEME

We start with the so-called t-J model which is written as $H = H_t + H_J$. In terms of the Schwinger bosons $\{b_{i\sigma}^{\dagger}, b_{i\sigma}\}$ and slave fermions $\{f_i^{\dagger}, f_i\}$,

$$H_t=-t\sum_{\langle ij\rangle,\sigma}[f_i f_j^\dagger b_{i\sigma}^\dagger b_{j\sigma}+\text{H.c.}],$$
$$H_J=-\frac{J}{2}\sum_{\langle ij\rangle}A_{ij}^\dagger A_{ij}, \tag{1}$$

where

$$A_{ij}=b_{i\uparrow}b_{j\downarrow}-b_{i\downarrow}b_{j\uparrow}, \tag{2}$$

$$f_i^\dagger f_i+\sum_{\sigma=\uparrow\downarrow}b_{i\sigma}^\dagger b_{i\sigma}=1$$

and H_J includes the reference term $-(J/4)\Sigma_{\langle ij\rangle}n_i n_j$. Solving (1) in two dimensions is not yet possible. But the spin part of the Hamiltonian suggests that at *half-filling* one may look at the RVB type of trial wave function for the ground state:

$$|\Psi\rangle=\sum\prod_{k=1}^{N/2}[W_{i_k j_k}A_{i_k j_k}^\dagger]|0\rangle;$$
$$W_{ij}=-W_{ji}. \tag{3}$$

Here i_k, j_k are not necessarily nearest neighbors and the summation is over all possible pair configurations with $i_k\neq j_m$, and $i_k\neq i_m$ for $k\neq m$. Note that the Marshall sign is built into A_{ij}. How precise this state is depends on how one chooses the RVB amplitudes W_{ij}. We shall see that using optimized bond amplitudes one could virtually describe the exact ground state and the low-lying excitations within the RVB context.

To find the overlap between two sets of pair realizations, say, $\langle\psi_L|\psi_R\rangle$, let us start with site j_0 from $|\psi_R\rangle$, which could have either $b_{j_0\uparrow}^\dagger$ or $b_{j_0\downarrow}^\dagger$. This $b_{j_0\uparrow}^\dagger$ is then annihilated off by a bond from $\langle\psi_L|$, and is transferred to $b_{j_1\downarrow}$ at a new site. $b_{j_1\downarrow}$ is again transferred to $b_{j_2\uparrow}^\dagger$ at a next site by a bond from $|\psi_R\rangle$. This procedure can be continued after n steps when it reaches $b_{j_n\downarrow}^\dagger$, the latter is bonding with $b_{j_0\uparrow}^\dagger$. That is, we end up with a loop weighted by the product of W_{ij}'s along the loop. The remaining part of the lattice can be similarly treated, thus forming a loop gas. The problem can be most conveniently handled by using a 2×2 transfer matrix of the form

$$\mathbf{G}_{ij}=\begin{pmatrix}0 & W_{ij}\\ -W_{ij} & 0\end{pmatrix}, \tag{4}$$

which acts in the following way:

$$\begin{pmatrix}b_{i\uparrow}\\ b_{i\downarrow}\end{pmatrix}=\mathbf{G}_{ij}^*\begin{pmatrix}b_{j\uparrow}^\dagger\\ b_{j\downarrow}^\dagger\end{pmatrix};\quad \begin{pmatrix}b_{i\uparrow}^\dagger\\ b_{i\downarrow}^\dagger\end{pmatrix}=\mathbf{G}_{ij}\begin{pmatrix}b_{j\uparrow}\\ b_{j\downarrow}\end{pmatrix}.$$

The weight of the loop is simply

$$w(\{j_k\})=\text{Tr}[\mathbf{G}_{j_0 j_n}\mathbf{G}_{j_n j_{n-1}}^*\cdots\mathbf{G}_{j_2 j_1}\mathbf{G}_{j_1 j_0}^*]. \tag{5}$$

Note that the loop is direction dependent. Being definite, we always start loops (i.e., take j_0) at even sites. Let us denote $\langle\Psi|\Psi\rangle$ of an N-site lattice by Y_N. It is simply the partition function of the loop gas. To illustrate the calculation, one can decompose Y_N at a given j_0 into (all j_k's below are self-avoiding)

$$Y_N=\sum_{n=0}^{N-1}\left\{\sum_{\{j_k;k\neq 0\}}Y_{N-n-1}(\{j_k\})\times w(\{j_k\})\right\}. \tag{6}$$

The arguments of Y_{N-n-1} represent the sites excluded for the $(N-n-1)$-site partition function.

It is then straightforward to evaluate $\langle\Psi|\mathbf{S}_i\cdot\mathbf{S}_j|\Psi\rangle$. One simply performs the operation $\mathbf{S}_i\cdot\mathbf{S}_j$ at sites i and j *before* connecting them to other sites. The order of operations are relevant here: a given operator acts on $b_{i\sigma}^\dagger$'s ($b_{i\sigma}$'s) from the left (right) hand side. This results in modified transfer matrices at i and j: One inserts simultaneously to the loop(s) at sites i and j,

$$\tfrac{1}{4}(\sigma_z)_i(\sigma_z)_j+\tfrac{1}{2}[(\sigma_+)_i(\sigma_+)_j+(\sigma_-)_i(\sigma_-)_j]\qquad i-j=\text{odd};$$
$$\tfrac{1}{4}(\sigma_z)_i(\sigma_z)_j+\tfrac{1}{2}[(\sigma_+)_i(\sigma_-)_j+(\sigma_-)_i(\sigma_+)_j]\qquad i-j=\text{even}.$$

It turns out that there are nonzero matrix elements only when i and j are on the same loops. More precisely,

$$\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle=\frac{1}{Y_N}\sum_{n=1}^{N-1}\frac{3}{4}\left\{\sum_{\{j_k\}}Y_{N-n-1}(\{j_k\})\times\sum_{m=1}^{n}\text{Tr}[\sigma_z\mathbf{G}_{j_0 j_m}^{(2)}\sigma_z\mathbf{G}_{j_m j_0}^{(1)}]\delta_{ij_0}\delta_{jj_m}\right\}, \tag{7}$$

$$\mathbf{G}_{j_m j_0}^{(1)}\equiv\mathbf{G}_{j_m j_{m-1}}^*\cdots\mathbf{G}_{j_2 j_1}\mathbf{G}_{j_1 j_0}^*,$$
$$\mathbf{G}_{j_0 j_m}^{(2)}\equiv\mathbf{G}_{j_0 j_n}\cdots\mathbf{G}_{j_{m+2}j_{m+1}}^*\mathbf{G}_{j_{m+1}j_m}. \tag{8}$$

The two σ_z's in (7) simply transpose one of the $\mathbf{G}$'s, leading to a minus sign for odd distance between i and j. The ground-state energy follows the simple rule: If the two sites of a randomly picked bond are found to be in the same loop, its energy is $-(3/4)J$, otherwise it is 0. Figure 1 presents a typical case of the above picture. Then one sums over all the configurations.

III. OPTIMIZING THE AMPLITUDES

Rigorous analytic evaluation of the RVB expectation values appears problematic. But a simple self-consistency approach yields surprising accuracy. One can first approximate, in (6) and (7), $Y_N/Y_{N-n-1}\to y^{n+1}$. This replaces the complicated "environment" of a loop of $(n+1)$ sites by a uniform weight $1/y^{n+1}$. Let us try to ignore the self-avoiding restriction in the first place, and denote the corresponding y by y_0. The correct y is then obtained by properly identifying the overcounting. The matrix after summing over the paths connecting i to j reads [$i\neq j$; see (8)],

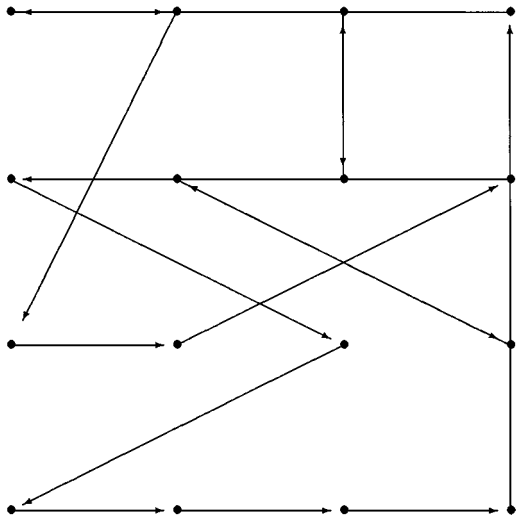

FIG. 1. A typical configuration of the loop gas on a 4×4 lattice, starting $(-1,-1)$ at the left-bottom corner. The sites (0,0) and (1,0) happen to be on the same loop, thus contributing $-3/4$ to the ground-state energy.

$$\mathbf{R}_{ij}=\frac{1}{N}\sum_{\mathbf{k}}\frac{\exp(-i\mathbf{k}\cdot\mathbf{r}_{ij})}{1-|W_{\mathbf{k}}/y_0|^2}\begin{pmatrix}1 & W_{\mathbf{k}}^*/y_0\\ -W_{\mathbf{k}}^*/y_0 & 1\end{pmatrix}. \quad (9)$$

y_0 is determined, from (6), by the total probability of finding the paths, $\mathrm{Tr}(\mathbf{R}_{ii}-1)=1$ [see (14) below]. Now y can be recovered by grouping the extra winding at a given site (say i) into $1/y$ (recovering the self-avoiding loops) which gives, approximately,

$$y^{-1}=\mathrm{Tr}(\mathbf{R}_{ii}/2)\times y_0^{-1}=(3/2)\times y_0^{-1}. \quad (10)$$

For the spin-spin correlations, we now have one path starting from i to j and the other from j to i. Ignoring again the overlap between the two paths, the result of the summation is simply $\mathbf{R}_{ij}$ and $\mathbf{R}_{ji}^*$. But, taking two independent paths results in an additional over-counting of a factor 3/2 [see (10)] which should be deducted. We end up with the expression (dropping y_0 as $W_{\mathbf{k}}$ is variational)

$$E_{\mathrm{bond}}=\left|\frac{1}{N}\sum_{\mathbf{k}}\frac{\gamma_{\mathbf{k}}}{1-|W_{\mathbf{k}}|^2}\right|^2-\left|\frac{1}{N}\sum_{\mathbf{k}}\frac{\Gamma_{\mathbf{k}}W_{\mathbf{k}}}{1-|W_{\mathbf{k}}|^2}\right|^2, \quad (11)$$

where

$$\gamma_{\mathbf{k}}=\frac{1}{2}(\cos k_x+\cos k_y), \quad (12)$$

$$\Gamma_{\mathbf{k}}=\frac{1}{2}(\sin k_x+\sin k_y). \quad (13)$$

Equation (11) is subject to $W_{\mathbf{k}}=-W_{-\mathbf{k}}$ and the normalization constraint

$$\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{1-|W_{\mathbf{k}}|^2}=\frac{3}{2}. \quad (14)$$

It can be minimized via the method of Lagrangian multiplier. For simplicity, we assume here real $W_{\mathbf{k}}$'s. It is now a simple exercise to find (picking up the right solution satisfying $|W_{\mathbf{k}}|\leqslant1$)

$$W_{\mathbf{k}}=\frac{d_2\Gamma_{\mathbf{k}}}{1+\sqrt{(1+d_1\gamma_{\mathbf{k}})^2-(d_2\Gamma_{\mathbf{k}})^2}}, \quad (15)$$

with

$$\frac{d_1}{d_2}=\frac{\Sigma_{\mathbf{k}}[\gamma_{\mathbf{k}}/(1-W_{\mathbf{k}}^2)]}{\Sigma_{\mathbf{k}}[\Gamma_{\mathbf{k}}W_{\mathbf{k}}/(1-W_{\mathbf{k}}^2)]} \quad (16)$$

and d_2 is the Lagrangian multiplier corresponding to (14). In the present case, it is always possible to get a consistent solution with $d_1\equiv0$. Note that W_{ij} so obtained connects between those sites with odd distances. Here $d_2=1$ in order to satisfy (14) [still, a condensation at $\mathbf{k}=\pm(\pi,\pi)/2$ is required, related to LRMO of the state[3,4]]. Nevertheless, $d_2<1$ gives a set of amplitudes which all have quite low energies but finite correlation lengths. In addition, finite d_1 corresponds to having spiral twist on the RVB bonds. They may be used as trivial wave functions at finite temperature or finite doping where LRMO is absent.

IV. MONTE CARLO SIMULATION

Analytic approach is useful for finding the right amplitudes. In addition, the structure of (7) allows as well a direct evaluation via Monte Carlo simulation. It amounts to sampling over the configurations of the loop gas. The rule to calculate the spin-spin correlations is particularly simple as mentioned in Sec. II. In the simulation, a common phase $\exp[i\mathbf{k}_0\cdot(\mathbf{r}_i-\mathbf{r}_j)]$, $\mathbf{k}_0=(\pi,\pi)/2$ can be taken out, leading to positive weights for all loops. Thus the standard Metropolis algorithm applies.

Our ground state has rotational invariance so that $\langle\Psi|\mathbf{S}_j|\Psi\rangle=0$. The states $|\phi_{j,\alpha}\rangle=S_{j,\alpha}|\Psi\rangle$, $\alpha=x,y$ or 1,2, form the spin-flip excited states of the system ($S_z=2iS_yS_x$ is a two-flip process). Out of them one can construct the Bloch states

$$|\phi_{\mathbf{k},\alpha}\rangle=\frac{1}{N^{1/2}}\sum_j\exp(i\mathbf{k}\cdot\mathbf{r}_j)|\phi_{j,\alpha}\rangle, \quad (17)$$

$$\epsilon_{\mathbf{k},\alpha}=\frac{\langle\phi_{\mathbf{k},\alpha}|H|\phi_{\mathbf{k},\alpha}\rangle}{\langle\phi_{\mathbf{k},\alpha}|\phi_{\mathbf{k},\alpha}\rangle}-E_0.$$

The evaluations of the matrix elements $\langle\phi_{k,\alpha}|\phi_{l,\alpha}\rangle$, $\langle\phi_{k,\alpha}|\mathbf{S}_i\cdot\mathbf{S}_j|\phi_{l,\alpha}\rangle$ can again be done using the transfer matrix (4) and can be mapped to a loop-gas statistics. Extreme care has to be taken with the orders of the operators on the loop, sometimes, the loop direction. The relevant loops[9] are listed in Fig. 2. Some techniques of avoiding the sign oscillations are discussed in Ref. 4.

We briefly report the main results at half-filling. The optimized state on 48×48 lattice has an energy $-0.3344J$/bond, virtually identical to commonly accepted $-0.3346(1)J$/bond for the ground-state energy. The staggered magnetization is 0.311, agreeing with 0.31(2) of the most reliable estimates.[5] On 4×4 lattice it is -0.3509 vs

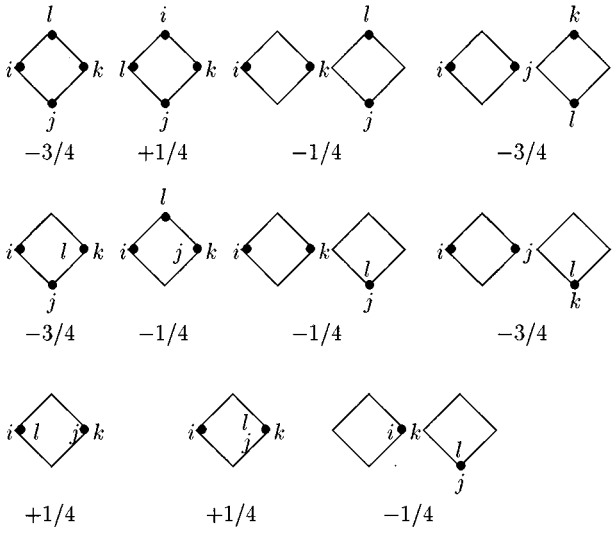

FIG. 2. A list of loop configurations and the associated weights in evaluating $\langle \phi_{k,\alpha}|\mathbf{S}_i\cdot\mathbf{S}_j|\phi_{l,\alpha}\rangle$. There is, in addition, a common factor $(-1)^{k-l}$ for all graphs.

-0.35089, which can then serve as an exact reference wave function. Figure 3 plots the spin-flip spectrum, calculated on a 12×12 lattice. It turns out to fit the renormalized spin-wave result $\epsilon_{\mathbf{k}}=2JZ_r\sqrt{1-\gamma_{\mathbf{k}}^2}$, with $Z_r\cong1.22$, in excellent agreement with the result of Ref. 6 done on a supercomputer. To summarize, this optimized, parameter-free RVB state, with full rotational and translational symmetry, is virtually identical to the exact one for any practical purposes. It provides a solid ground for the following analysis.

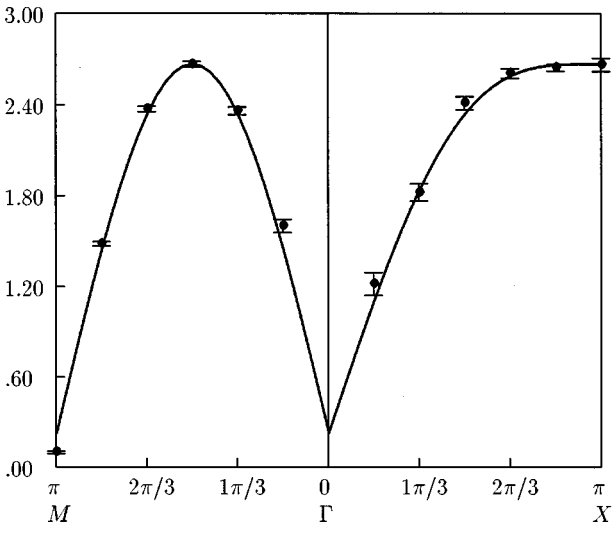

FIG. 3. The spin-flip excitation spectrum in ● and in units of J, calculated on a 12×12 lattice, along the (1,0) (right-hand side) and the (1,1) axes. The curve corresponds to the renormalized spin-wave result with $Z_r=1.22$ and an up-shift $\cong0.22$ (presumably due to the finite lattice size).

V. SINGLE HOLE MOVING ON THE RVB BACKGROUND

How does a doped hole vary the RVB wave function? Since all the spins are paired in the ground state (3), creating a hole by removing one spin at a given site i will leave its spin partner unattended. Prior to doping, the latter spin can be at any site j which is connected to the first one by the RVB amplitude W_{ij}. If one maintains such an RVB amplitude after the removal of site-i spin, the static-hole energy would be just $4\times(0.3344+1)J=2.3376J$ relative to the undoped state. This is considerably higher than, e.g., $2.193(7)J$ estimated in Ref. 10 at $t=0$ limit. The reason is that, by removal of the spin, it is no longer energetically favorable for its former spin partner to stay nearby. In other words, one should find a different amplitude F_{ij}, in place of W_{ij}, for the hole-spin pair. The unattended spin may be properly called spinon,[11] as it carries spin-1/2 surrounded by other spin-singlet pairs. Accordingly, the hole here may be called holon as no spin is associated with it. This holon-spinon pair are mobile with respect to the antiferromagnetic RVB background just like their parental spin pair. If they form a bound state, it means a spin-charge confinement and the dopant carries both spin and charge. But once the holon and the spinon have a finite amplitude of being infinitely far away, a spin-charge separation is realized. We note that as the holon moves around, more RVB spin pairs in the background may be broken. Nevertheless, breaking an additional nearby RVB pair would cause much higher energy when $t/J\ll1$. Thus, at least in this limit, one may focus on the holon-spinon pair and safely neglect the pair-breaking effect in the RVB background.

Let us define an operation which projects out the bond W_{ij} in $|\Psi\rangle$ but preserves the phase (for the mere sake of convenience),

$$P_{ij}|\Psi\rangle=\sum\frac{W_{ij}}{|W_{ij}|}\prod_{k=1}^{N/2-1}[W_{i_kj_k}A_{i_kj_k}^{\dagger}]|0\rangle\Big|_{i_k,j_k\neq i,j}. \quad (18)$$

Now imagine the spin as an ''electron'' surrounding the hole, a ''nucleus,'' thus forming an atom with wave function $\psi_\sigma(\mathbf{r}_s-\mathbf{r}_h)$ under the set of bases $\{|s,\sigma;h\rangle=b_{s\sigma}^{\dagger}f_h^{\dagger}P_{hs}|\Psi\rangle\}$. The phase of ψ_σ is relative to the RVB background. Different bases are not orthogonal. Instead, their inner products should be calculated using

$$\langle s',\sigma';h'|s,\sigma;h\rangle=\delta_{\sigma',\sigma}\delta_{h',h}\times\mathcal{M}, \quad (19)$$

where

$$\mathcal{M}=\sum_{n=1}^{N-1}\left\{\sum_{\{j_k\}}Y_{N-n-1}(\{j_k\})\times\frac{\mathrm{Tr}[\mathbf{G}_{j_0j_1}^{*}\cdots\mathbf{G}_{j_nj_0}]}{2|W_{j_0j_1}^{*}W_{j_nj_0}|}\right\}_{j_0=h,j_1=s',j_n=s}, \quad (20)$$

which forms a second kind of loop gas to be illustrated below. In the presence of hole hopping, the Bloch state of a given $\mathbf{k}$ is

$$|\mathbf{k}\sigma\rangle=\frac{1}{N}\sum_{s,h=1,N}\psi_{\mathbf{k}\sigma}(\mathbf{r}_s-\mathbf{r}_h)\exp(i\mathbf{k}\cdot\mathbf{r}_h)|s,\sigma;h\rangle. \quad (21)$$

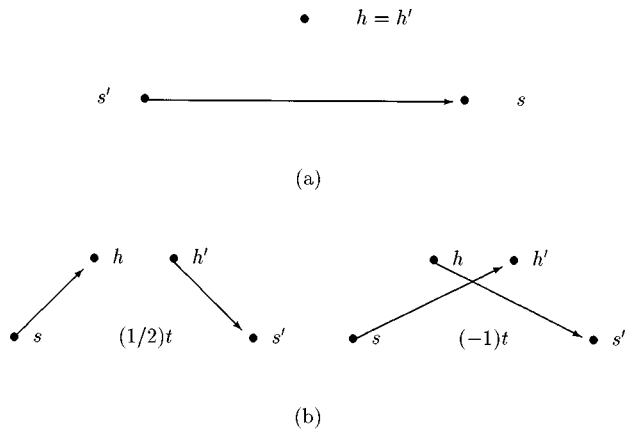

FIG. 4. A schematical representation of the loop gas used to calculate the hole energy. (a) Loop gas of the second kind in which the hole site $h=h'$ is isolated with an open chain running from s to s'. (b) Loop gas of the third kind and the weights used in the calculation of the hopping matrix elements.

The energy of $|\mathbf{k}\sigma\rangle$ is computed using the expression

$$E_{\mathbf{k}\sigma}=\mathcal{N}^{-1}\sum_{s',s;h',h}\psi^{*}_{\mathbf{k}\sigma}(\mathbf{r}_{s'}-\mathbf{r}_{h'})\psi_{\mathbf{k}\sigma}(\mathbf{r}_{s}-\mathbf{r}_{h}) \times\{T_1\delta_{h',h}+T_2\eta_{h',h}\,e^{i\mathbf{k}\cdot(\mathbf{r}_h-\mathbf{r}_{h'})}\}, \tag{22}$$

$$\mathcal{N}=\sum_{h}\psi^{*}_{\mathbf{k}\sigma}(\mathbf{r}_{s'}-\mathbf{r}_{h})\langle s',\sigma;h|s,\sigma;h\rangle\psi_{\mathbf{k}\sigma}(\mathbf{r}_{s}-\mathbf{r}_{h}). \tag{23}$$

In (22),

$$T_1=\langle s',\sigma;h|H_J|s,\sigma;h\rangle,\quad T_2=\langle s',\sigma;h'|H_t|s,\sigma;h\rangle,$$

and $\eta_{h',h}$ sets the nearest neighbor constraint between h' and h. Once the holon-spinon wave function is obtained, the spectral weight can be easily calculated using the same loop gases via the definition

$$Z_{\mathbf{k}}=\frac{|\langle\Phi|c^{\dagger}_{\mathbf{k}\sigma}|\mathbf{k}-\sigma\rangle|^2}{\langle\Phi|\Phi\rangle\langle\mathbf{k}-\sigma|\mathbf{k}-\sigma\rangle}, \tag{24}$$

where $c^{\dagger}_{\mathbf{k}\sigma}$ is the usual electron creation operator. (More details on this are given in the next section.)

We perform numerical diagonalization on finite lattices to find the eigenstates and eigenenergies (which give also information of excited states). The evaluation of the matrix elements for the normalization and the spin part is almost the same as before. But we now use a loop gas in which hole site h is isolated while an open chain connects s to s'. For the hopping term, a third kind of loop gas with two open chains is employed: If the chain starting at s connects to the nearest neighbor hopping site h' (also an open end), the configuration contributes $(-1)t$; otherwise when s connects back to h (the hole it belongs to) it is $(1/2)t$. The two additional "loop gases" are illustrated in Fig. 4. Note that there is an overall ratio between the two kinds of loop gas, which can be computed by referring to the original loop gas.

Selected results on the ground-state energy $E_{\mathbf{k}\sigma}$ for a one-hole problem as a function of t/J are shown in Table I, along with some best numerical results[12,13] for comparison. The corresponding quasiparticle weight is presented in Table II. Note that the RVB ground state is taken as the reference state, whose energy differs negligibly from that of the true ground state on the 4×4 and 8×8 lattices. Clearly the holon-spinon pair wave function so constructed, free from adjustable parameters once the rigid RVB background is chosen, is able to yield accurately the superexchange energy and the major part of the kinetic energy. It is, as a matter of fact, an excellent approximation for $t/J\leqslant1$ as noted above and virtually exact at $t/J\to0$. Further improvement on the approximation at $t/J\geqslant1$ will be discussed in Sec. VII.

TABLE I. The ground-state energy (in units of J) of the holon-spinon pair vs the exact (Ref. 12) or the variational (Ref. 13) results on finite lattices when available. The errors in the data are negligible for small t/J, but have not been systematically analyzed.

		4×4		8×8	
k	t/J		Exact		Variation
	0.0	2.361	2.349	2.215	2.232
	0.2	2.251	2.248	2.081	2.111
$(\pi,\pi)/2$	0.5	1.811	1.764	1.591	1.594
	1.0	0.830	0.656	0.571	0.447
	2.5	-2.416	-3.305	-2.717	-3.552
	5.0	-7.950	-10.49	-8.296	-10.448

It is important to observe that the ground state of the holon-spinon pair after diagonalization can be well approximated to all range of t/J by $[\mathbf{k}=(\pi,\pi)/2]$

$$\psi_{\mathbf{k}\sigma}(\mathbf{r}_s-\mathbf{r}_h)\cong\frac{1-(-1)^{h-s}}{2}+C_{\mathbf{k}}\eta_{s,h}\,\exp[i\mathbf{k}\cdot(\mathbf{r}_s-\mathbf{r}_h)]. \tag{25}$$

Namely, it consists of a uniform s-wave (the first term) and a nearest neighbor p-wave component (with magnetic number $m=\pm1$). The coefficient $C_{\mathbf{k}}$ is determined by minimizing the energy. The resulting energy and spectral weight are shown in Table III. They are essentially the same as the previous results of the numerical diagonalization. The agreement does not vary much with lattice sizes. The physical

TABLE II. The spectrum weight corresponding to Table I.

		4×4		8×8	
k	t/J		Exact		Variation
	0.0	0.98		0.91	
	0.2	0.92	0.91	0.84	0.831
$(\pi,\pi)/2$	0.5	0.79		0.71	0.684
	1.0	0.67	0.59	0.61	0.553
	2.5	0.57	0.40	0.54	0.388
	5.0	0.54	0.28	0.52	0.348

TABLE III. The energy (in units of J) and the spectral weight of the trivial wave function (25) as a function of t/J. The point is that they are extremely close to those of the direct diagonalization presented in Tables I and II.

		4×4		8×8	
k	t/J	Energy	Weight	Energy	Weight
	0.0	2.361	0.97	2.219	0.90
	0.2	2.253	0.91	2.097	0.85
$(\pi,\pi)/2$	0.5	1.816	0.78	1.624	0.69
	1.0	0.842	0.66	0.633	0.58
	2.5	-2.379	0.56	-2.562	0.50
	5.0	-7.870	0.52	-7.971	0.47

picture here is rather simple. The main process of hopping goes like this: When the pair is in the p-wave bound state, the holon hops by placing the spinon in front of it and then exchanging their sites. After that the spinon relaxes to infinity to lower the superexchange energy, forming the s wave. When the pair is in the latter state, the hole first breaks the RVB pair of one of its nearest-neighbor spins, and then exchanges its site with the spin's to form the p wave. The remaining two spins form a new RVB pair which condenses back into the background.

VI. SPIN-CHARGE SEPARATION AND VANISHING SPECTRAL WEIGHT

We have shown that the holon-spinon pair description can very accurately account for the one-hole ground state, at least for $t/J \leqslant 1$. An important consequence is that the holon and spinon do not always bind together and there is a finite amplitude for the spinon running away from the holon, in favor of its superexchange energy. This is a clear indication of the spin-charge separation. With the increase of t/J, additional broken RVB pairs or spin-flip processes may be dynamically created by hopping, but including these corrections should not change the conclusion of the spin-charge separation because a bound state of the holon and spinon does not favor the hopping energy either, which becomes increasingly important at large t/J.

The spin-charge separation has an interesting implication for the spectral weight $Z_{\mathbf{k}}$ of the bare-hole state $c_{k\sigma}|\Phi\rangle$. As defined in (24), $Z_{\mathbf{k}}$ measures the overlap of $c_{k\sigma}|\Phi\rangle$ with the plane-wave state $|\mathbf{k}-\sigma\rangle$ of the doped system. To actually compute it, one can use the Wannier states. Namely, one calculates the overlap of $c_{h-\sigma}|\Phi\rangle \propto \Sigma_s W_{sh}|s,\sigma;h\rangle$ and $|\psi_{h\sigma}\rangle = \Sigma_s \psi_{\mathbf{k}\sigma}(\mathbf{r}_s - \mathbf{r}_h)|s,\sigma;h\rangle$ [according to (21)]. Thus the pair wave function $\psi_{\mathbf{k}\sigma}$ basically determines the overlap. It follows immediately that, in terms of the analytical form of (25), the bound-state component of $|\psi_{h\sigma}\rangle$ at $\mathbf{k}=(\pi,\pi)/2$ has no contribution to the overlap or the spectral weight due to its p-wave symmetry. Now in the bare-hole state $c_{h-\sigma}|\Phi\rangle$ the unattended spinon stays nearby the holon for the amplitude $W_{sh}\to 0$ at $|\mathbf{r}_{sh}|\to\infty$. On the other hand, the spinon in $|\psi_{h\sigma}\rangle$ can be infinitely separated from the holon with a finite amplitude as shown in (25). Generally speaking, one would expect to get zero overlap between these two states on an infinite lattice, and thus $Z_{\mathbf{k}}=0$. Nevertheless, with the presence of LRMO, things become a little bit tricky. In this case, W_{ij} falls off in its marginal form (power-law decay, r_{ij}^{-2}) to give a long-range order, and we find a finite $Z_{\mathbf{k}}$ instead, for both analytic and numerical $\psi_{\mathbf{k}\sigma}$. It is due to the fact

$$\lim_{|\mathbf{r}_s-\mathbf{r}_{s'}|\to\infty}\langle s',\sigma;h|s,\sigma;h\rangle \neq 0. \tag{26}$$

[In terms of Monte Carlo simulation, the chain in Fig. 4(a) has a finite probability of being infinitely long.] This effect is marginal in the sense that once W_{ij} falls slightly faster than it is here at large r_{ij} [for example, using $d_2<1$ in (15)], one would have $Z\equiv 0$. However, in the following, we shall emphasize that even in the presence of the long-range order the spin-charge separation should still lead to a vanishing spectral weight, due to some nonlocal phase effect.

As far as $Z_{\mathbf{k}}$ is concerned, there is a crucial ingredient missing in the preceding section's discussion. Recall that we are confined in a sub-Hilbert space where only a holon-spinon pair is considered while the rest spins are still in the RVB ground state. But a careful examination shows that the bases $|s,\sigma;h\rangle$ are actually not completely orthogonal to those states where some background spins are flipped as excitations. Note that the overlap is finite no matter how far a flip is from the hole site. This nonorthogonal effect is due to many-body effects in the RVB wave function (3) after the removal of the spin at hole site, but its correction to the energy $E_{\mathbf{k}\sigma}$ and other short-range properties seems negligible. However, it could profoundly affect the long-distance behavior of the wave function $\psi_{\mathbf{k}\sigma}$ in (25). The argument goes as follows.

There is a simple rule in the loop-gas formalism to consider the overlap between RVB states with these "zero-point" spin flips due to the presence of a hole. A loop must contain an even number of flip sites. More precisely, a flip must be repaired by the next flip as one goes on the loop. The hole site can be considered as either a flip or a regular one. A pair of flips having odd distance between them acquires a (-1) factor. Thus, as one walks from a given s to s' in $\langle s',\sigma;h|s,\sigma;h\rangle$ [cf. Fig. 4(a), but now the RVB background containing spin flips] and as the distance between s to s' increases, there are more and more flips adding to the path. Even though such effect is negligible locally, the total sign of the weight will be accumulated at long distance and will effectively cause the overlap vanishing. In other words, the s-wave component in (25) actually involves some phase-string correction at large length scale, which always leads to vanishing spectral weight. In fact, based on a different approach, $Z=0$ has been rigorously shown in Ref. 8 for the one hole problem, due to a similar unrepairable phase string induced by doping.

VII. DISCUSSION

In this paper, we have developed a general scheme for studying RVB states of quantum antiferromagnet, and the optimized RVB state is shown to be virtually identical to the exact ground state as well as excitation states. We have then extended the approach to the doped regime and demonstrated

that a one-hole problem may be modeled, accurately at small t/J and reasonably at large t/J, by a holon-spinon pair moving on the optimized RVB background. The spin-charge separation and vanishing quasiparticle spectral weight were revealed, which is consistent with a general proof of zero spectral weight in this kind of system.[8]

Why has the discussion of the spectral weight problem in the literature been inconclusive and why is our zero-weight result not evident in finite-size calculations? We believe that the key issue here is the failure to take into account the spin distortion over a long range, where the associated U(1) phase fluctuations are particularly important (cf. Ref. 8). A direct diagonalization can only be done on a system of 20 sites or so where the spin-flip energy gap is still too large to play a role. Perturbation theories based on the usual spin-string picture do not really let the string be long. A next-nearest-neighbor string theory already yields accurate energies over the entire range t/J. The basic argument is that the energy cost of the string will be linearly increased with its length so that the string cannot be too long. However, it has been shown[8] that besides such a conventional spin string, there is a hidden U(1) phase string which has been neglected in the usual slave-fermion approach and in contrast to the former it causes less energy and is not repairable by low-lying spin fluctuations. Therefore, in order to capture correctly the long-range properties of the system one has to consider the background distortion at sites far away from the hole. This would require the string to reach far away from a given polaron center, which is practically difficult. In addition, there is always a lack of precise wave function at the half-filling limit to start with. Having the nearly-exact half-filling wave function is in fact the unique advantage of the present approach.

In Tables I and II, the spectral weight of our result seems too large compared to others as t/J increases. This suggests that the same long-range fluctuation discussed in the preceding section might also be responsible for the kinetic energy deficiency at $t/J \geqslant 1$ in our calculation. Another possibility is to have broken pairs in the RVB background. This would allow, among other things, the spinon to occupy the even sites with respect to the holon. In both cases, the effective pairing of the RVB background is weakened (cf. below). In the next order of approximation, one would extend the Hilbert space to include these effects. Also, it is interesting that the background fluctuations induce flipping of the spinon in the holon-spinon pair. A careful study of this ''Kondo effect'' may reveal physical properties of the system.

Things become simpler if the RVB background has no LRMO, for instance, in the presence of finite but dilute doping. The spin-flip spectrum would have a finite gap and therefore be less important. On the other hand, the right-hand side of (26) is readily zero. The spin-flip effect is no longer an essential ingredient of spin-charge separation. In fact we found that using an undoped state of (15) with $d_2 < 1$ can actually yield lower energies at large t/J (but the result is too primitive to be presented here). It is interesting that background spin flips play a similar role as the gauge fluctuations in the recent approach of Weng, Sheng, and Ting,[14] whose results agree with many experimental features of the high-T_c superconductors. Possible generalization of the present approach to finite doping is currently under study.

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