Doping dependence of antiferromagnetic correlations in high-temperature superconductors

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We have studied the single-band Hubbard model on a two-dimensional square lattice slightly below half filling. Using the canonical transformation and a form of variational wave function that allows an expansion in terms of hole concentration δ with respect to half filling, we find that a nonzero δ results in a frustration of the antiferromagnetic (AF) order favored by the superexchange interaction. Use of a variational Monte Carlo calculation enables us to construct a phase diagram in the t/U-δ plane in which the AF order disappears at $\delta \approx 0.06$ for a typical value of $t/U = \frac{1}{4}$.

Since the discovery of high-T_c superconductors,[1] there has been a significant theoretical effort to understand the properties of these materials both in the superconducting and nonsuperconducting states. Although it is becoming clear that at least a two-band Hubbard model will be needed to capture the physics of the copper perovskite compounds, it is important to understand the physics of the low-lying excitations of the doped Mott insulators within as simple a framework as possible. For this purpose, we study the two-dimensional single-band Hubbard model[2] in order to clarify the dependence of its antiferromagnetic (AF) long-range order on the hole concentration δ with respect to half filling where we identify each site of the model with a copper site in a CuO_2 plane of superconductors. Use of the canonical transformation appropriate for small t/U and subsequent application to a particular form of variational wave functions allows us to construct an effective spin Hamiltonian that shows increasing frustration of AF order with δ. With the help of a variational Monte Carlo calculation, where different trial wave functions are used to represent ordered and disordered phases, we obtain a semiquantitative phase diagram in t/U-δ plane.

Consider the single-band Hubbard Hamiltonian

$$H = -t \sum_{\substack{i,j,\sigma \\ i \leftarrow j}} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} , \tag{1}$$

where indices connected by an arrow under the summation indicate the sum over all possible nearest neighbors with the direction of electron motion taken into account. Thus, the first term of (1) is equal to $-t\sum_{\langle i,j\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})$ where $\langle i,j\rangle$ indicates the sum over bonds. For small t/U, we can use the canonical transformation[3] that eliminates the mixing of doubly occupied and singly occupied sites to $O(t/U)$. In our problem, the transformed *states* have no doubly occupied sites, and, hence, the transformed Hamiltonian may be written as

$$H = -t \sum_{\substack{i,j,\sigma \\ i \leftarrow j}} b_i c_{i\sigma}^{\dagger} c_{j\sigma} b_j^{\dagger} + \frac{2t^2}{U} \sum_{\substack{i,j,\sigma \\ i \leftarrow j}} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right) - \frac{t^2}{U} \sum_{\substack{i,j,k,\sigma \\ i \leftarrow j \leftarrow k}} b_i c_{i\sigma}^{\dagger} c_{j\sigma} c_{j-\sigma}^{\dagger} c_{k-\sigma} b_k^{\dagger} - \frac{t^2}{U} \sum_{\substack{i,j,k,\sigma \\ i \leftarrow j \leftarrow k}} b_i c_{i\sigma}^{\dagger} n_{j-\sigma} c_{k\sigma} b_k^{\dagger} . \tag{2}$$

Here, b_i is a slave boson keeping track of hole motion and satisfies the constraint $b_i^{\dagger}b_i + n_i = 1$, $\mathbf{S}_i = \frac{1}{2} c_{i\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta}$, and $n_i = n_{i\uparrow} + n_{i\downarrow}$. It is easy to see that the first and third terms can reduce the AF order favored by the second (superexchange) term since the hole motion in these terms results in the displacement of electrons by one lattice spacing without flipping spins (Fig. 1). Also, the last term of (2) indicates a possible exchange between next-nearest neighbors, and this may result in frustration of the system.

To make this idea more concrete, we attempt to separate the hole degrees of freedom from the spin degrees in the spirit of the Born-Oppenheimer approximation. We consider the above Hamiltonian operating on a

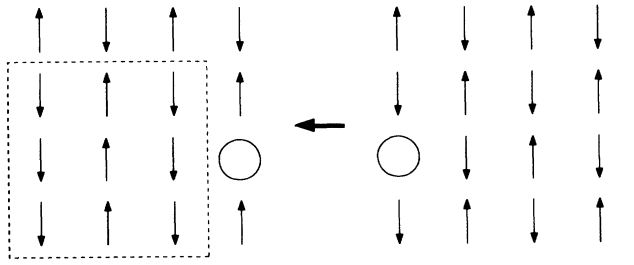

FIG. 1. Qualitative picture showing how a hole motion can destroy antiferromagnetic order in the Ising limit. The horizontal motion of a hole (indicated by an open circle) leaves misaligned spins in the box.

variational wave function

$$|\Psi\rangle=\prod_{k,\sigma}P_{k\sigma}|\nu\rangle\,, \tag{3}$$

where $P_{\mathbf{k}\sigma}=u_{\mathbf{k}}+v_{\mathbf{k}}c_{\mathbf{k}\sigma}c_{-\mathbf{k}-\sigma}$ injects holes with momentum $\pm\mathbf{k}$, and $|\nu\rangle$ represents a half-filled state with exactly one electron per site (and, therefore, it has only spin degrees of freedom). Due to the latter constraint on $|\nu\rangle$, the electrons in $|\nu\rangle$ are highly correlated in $\mathbf{k}$ space. The minimization of the energy expectation value $\langle\Psi|H|\Psi\rangle$ is done through the optimization of $|\nu\rangle$ rather than treating $|\Psi\rangle$ in full. Thus, we simplify the expression for the energy expectation value by approximating

$$\langle H\rangle\approx\langle\nu|H_{\rm eff}|\nu\rangle\,,$$

where we have defined an effective Hamiltonian that will only operate on spins of $|\nu\rangle$,

$$H_{\rm eff}=\left(\prod_{\mathbf{k},\sigma}P_{\mathbf{k}\sigma}\right)^{\dagger}H\left(\prod_{\mathbf{k},\sigma}P_{\mathbf{k}\sigma}\right). \tag{4}$$

In effect, we approximate the minimization of $\langle H\rangle$ in the complete Hilbert space by the minimization of $\langle H_{\rm eff}\rangle_{\nu}$ within the subspace spanned by $\{|\nu\rangle\}$. This is possible, since the operator $P_{\mathbf{k}\sigma}$ fixes the way holes are introduced to the system and eliminates their degrees of freedom from our trial wave function. The normalization of $|\Psi\rangle$ is guaranteed if $u_{\mathbf{k}}^2+v_{\mathbf{k}}^2/4=1$.

In general, we are interested in the expectation value of an operator $\hat{O}$ given by

$$\langle\Psi|\hat{O}|\Psi\rangle=\left\langle\nu\left|\left(\prod_{\mathbf{k},\sigma}P_{\mathbf{k}\sigma}\right)^{\dagger}\hat{O}\left(\prod_{\mathbf{k},\sigma}P_{\mathbf{k}\sigma}\right)\right|\nu\right\rangle. \tag{5}$$

Using the operator identity

$$\hat{O}P_{\mathbf{k}\sigma}=P_{\mathbf{k}\sigma}\hat{O}+[\hat{O},P_{\mathbf{k}\sigma}]\,, \tag{6}$$

we find, after repeated applications,

$$\left\langle\nu\left|\left(\prod_{\mathbf{k},\sigma}P_{\mathbf{k}\sigma}\right)^{\dagger}\hat{O}\left(\prod_{\mathbf{k},\sigma}P_{\mathbf{k}\sigma}\right)\right|\nu\right\rangle=\langle\nu|\hat{O}|\nu\rangle+\sum_{\mathbf{k},\sigma}\langle\nu|P_{\mathbf{k}\sigma}^{\dagger}[\hat{O},P_{\mathbf{k}\sigma}]|\nu\rangle+\sum_{\mathbf{k},\sigma,\mathbf{k}',\sigma'}\langle\nu|P_{\mathbf{k}\sigma}^{\dagger}P_{\mathbf{k}'\sigma'}^{\dagger}[[\hat{O},P_{\mathbf{k}'\sigma'}],P_{\mathbf{k}\sigma}]|\nu\rangle+\cdots\,. \tag{7}$$

This expansion is valid if $P_{\mathbf{k}\sigma}$'s commute with each other and this is the case with our choice. Applying Eq. (7) to the total number operator $\sum_i n_i$, we find

$$\left\langle\nu\left|\sum_i n_i\right|\nu\right\rangle=N-\sum_{\mathbf{k}}v_{\mathbf{k}}^2\,, \tag{8}$$

where we have used $[[\sum_i n_i,P_{\mathbf{k}'\sigma'}],P_{\mathbf{k}\sigma}]=0$, and N is the number of sites in the system. Equating this to the total number of electrons $N(1-\delta)$ gives the expression for δ in terms of $v_{\mathbf{k}}$,

$$\delta=\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}^2}{N}\,. \tag{9}$$

Now it is straightforward to show that the nth-order term of the expansion (7) is $O(\delta^n)$:

$$\sum_{\{\mathbf{k}_i,\sigma_i\}}\langle\nu|P_{\mathbf{k}_1\sigma_1}^{\dagger}\cdots P_{\mathbf{k}_n\sigma_n}^{\dagger}[\cdots[[\hat{O},P_{\mathbf{k}_n\sigma_n}],P_{\mathbf{k}_{n-1}\sigma_{n-1}}],\ldots,P_{\mathbf{k}_1\sigma_1}]|\nu\rangle\sim\sum_{\{\mathbf{k}_i\}}\frac{v_{\mathbf{k}_1}^2v_{\mathbf{k}_2}^2\cdots v_{\mathbf{k}_n}^2}{N^n}\sim O(\delta^n)\,, \tag{10}$$

so long as $\hat{O}$ conserves the particle number. Therefore the expansion (7) is in fact an expansion in terms of the hole concentration δ. Since we are interested in a small δ regime, we will keep only the first two terms of (7). Applying this truncated form to the Hamiltonian (2), we find that $H_{\rm eff}$ defined in (4) is effectively (assuming that there are $N/2$ up spins),

$$H_{\rm eff}=2t\sum_{i\leftarrow j}J_{ij}(\mathbf{S}_i\cdot\mathbf{S}_j+\tfrac{1}{4})+\frac{2t^2}{U}\sum_{i\leftarrow j}(1-2J_{ii})(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4})+\frac{2t^2}{U}\sum_{i\leftarrow j\leftarrow k}J_{ik}[-(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4})+\tfrac{1}{2}(\mathbf{S}_i\cdot\mathbf{S}_k-\tfrac{1}{4})] \tag{11}$$

with

$$J_{ab}=J(\mathbf{R}_a,\mathbf{R}_b)=\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}^2}{N}\cos\mathbf{k}\cdot(\mathbf{R}_a-\mathbf{R}_b)\,, \tag{12}$$

which only operates on spins. Now, the minimization of $\langle H\rangle$ is converted to that of $\langle H_{\rm eff}\rangle_{\nu}$ for a given form of $P_{\mathbf{k}\sigma}$.

To go further, we must specify $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. To do this, we use the result of $t/U\rightarrow 0$ limit where we have some knowledge of how the system behaves. First, by Nagaoka's theorem,[4] we expect the system to become a ferromagnet for small δ. Second, if we polarize all spins in one direction, we can compute the exact energy expectation value for given δ. These two points can be compared to our $H_{\rm eff}$ and made consistent by choosing appropriate $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. We make the assumption that (11) is a good representation of the magnetic states so that the resulting values of the coupling constants may be applied for arbitrary spin configurations. The consistent choice is to take $v_{\mathbf{k}}$ to be nonzero only near the "corners" of Brillouin zone, i.e., near $\mathbf{k}=\pm(\pi/a)(e_x\pm e_y)$ with a being the lattice constant. Assuming that this remains valid away from $t/U\rightarrow 0$ limit, we replace $\cos\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)$ and $\cos\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_k)$ in (12) by -1 and $+1$, respectively, for nearest neighbors and next-nearest neighbors. Note that, in the strong correlation limit, this assumption does not necessarily violate the symmetry imposed by the underlying spin configuration. For instance, though it is clear that if the AF long-range order exists then the *quasiholes* must reside below the Fermi surface defined by $|\mathbf{k}_x|+|\mathbf{k}_y|=\pi/a$, the *actual holes* themselves need not be at the Fermi surface and may be found at the "corners" as we have conjectured here. One can see in the

study of Gutzwiller wave functions[5] and quantum Monte Carlo calculations[6] that the particle density is nonzero over the entire Brillouin zone for large-U Hubbard model, making it at least possible to take out electrons at the corners of the zone.

Combining this conjecture with (9), we find for given δ (up to some constant)

$$H_{\text{eff}}=\frac{2t^2}{U}\left\{\left[1-\left(\frac{U}{t}+5\right)\delta\right]\sum_{\substack{i,j\\ i\leftarrow j}}\mathbf{S}_i\cdot\mathbf{S}_j+\tfrac{1}{2}\delta\sum_{\substack{i,j,k\\ i\leftarrow j\leftarrow k}}\mathbf{S}_i\cdot\mathbf{S}_k\right\}. \tag{13}$$

We caution the reader that the last sum has two equivalent terms if i and k are second-nearest neighbors (i.e., diagonal from each other) since there are two possible paths from k to i, whereas there is only one if i and k are third-nearest neighbors (i.e., distance $2a$ away). The Hamiltonian (13) clearly shows that the hole (a) diminish the strength of AF coupling and (b) create frustration due to next-nearest-neighbor coupling. It is important to note that the frustration term originates in the last term of the Hamiltonian (2) which results from pair hopping that, together with the third term, is often dropped in the literature. The importance of this term has also been noted by Yokoyama and Shiba.[7]

The Hamiltonian (13) can be written in a concise manner:

$$H_{\text{eff}}=J_1\sum_{\substack{i,j\\ i\leftarrow j}}\mathbf{S}_i\cdot\mathbf{S}_j+J_2\sum_{\substack{i,j,k\\ i\leftarrow j\leftarrow k}}\mathbf{S}_i\cdot\mathbf{S}_k\,. \tag{14}$$

So, we have reduced our original problem to obtaining the ground state of the spin Hamiltonian (14). To this end, we will use a small cluster calculation and the variational Monte Carlo method.

The calculation on a small number of spins is done on ladder shape configurations, as shown in Fig. 2, with a variational state corresponding to linear combination of singlet pairs. [This is like Anderson's resonating-valence-bond (RVB) state.[8]] Comparing the energy found in this calculation to the one obtained for the AF state using the spin-wave theory[9] allows us to determine which one of these is more likely to be the ground state. To simplify the calculation, we limit the $i\leftarrow j\leftarrow k$ sum in (14) to the diagonal neighbors (i.e., we exclude those pairs with distances $2a$). We have computed up to eight spin sites and extrapolated to infinite size. We find that the AF state that is stable at $J_2/J_1=0$ loses its stability above $J_2/J_1=0.12$ where the RVB-like state attains a lower ground-state energy. This indicates that the crossover from the AF to the RVB state exists at a considerably lower value of J_2/J_1 than that of the classical ($S\rightarrow\infty$) case $J_2/J_1=0.25$.

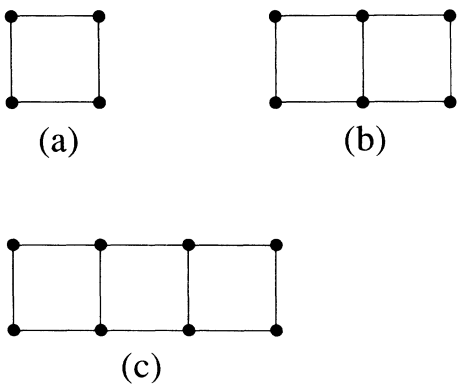

FIG. 2. The ladder configuration considered in the small cluster calculation of the Hamiltonian (14) corresponding to (a) four sites, (b) six sites, and (c) eight sites.

In order to further investigate size dependence of the above results for the Hamiltonian (14), we have also performed a variational Monte Carlo calculation. We compare the energy expectation values of trial wave functions representing AF- and RVB-like states.[10] After transforming the Hamiltonian to that of a lattice Bose gas with hard core,[11] where each boson indicates an up spin, we have chosen the boson wave functions for AF and RVB states in the following form:

$$\Psi_{\text{AF}}\propto\prod_{\substack{i,j\\ i<j}}\exp[-V(r_{ij})],\quad V(r_{ij})=\begin{cases}\infty, & r_{ij}=0,\\ p, & r_{ij}=a,\\ 0, & \text{otherwise},\end{cases} \tag{15}$$

and

$$\Psi_{\text{RVB}}\propto\prod_{\substack{i,j\\ i<j}}(r_{ij})^{q^2}\prod_i\exp\left(-\frac{\pi}{2}q^2\rho r_i^2\right), \tag{16}$$

where the products are taken over the number of bosons ($N/2$ in our case), $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$ and $\rho=\frac{1}{2}$. The variational parameters are p and q^2 for Ψ_{AF} and Ψ_{RVB}, respectively. The latter function is similar to the form used by Kalmeyer and Laughlin in a study of an RVB state on a triangular Heisenberg model.[12] We have, however, chosen a variable power of q^2, and discarded the phase factors. This modification, in turn, results in the destruction of rotational invariance and other properties that are believed to hold for the wave function studied by Kalmeyer and Laughlin.[13] We show elsewhere[10] that Ψ_{RVB} has an algebraically decaying AF correlation function. The way we have implemented the periodic boundary conditions for Ψ_{RVB} is discussed in the Appendix.

In Fig. 3, we show the lowest-energy expectation value per boson for trial wave functions Ψ_{AF} and Ψ_{RVB} vs frustration J_2/J_1 obtained for a 50×50 lattice. (Energies are practically independent of the sizes above 14×14.) The crossover occurs at $(J_2/J_1)_c\approx0.066$ above which the AF phase becomes less favorable compared to the RVB phase. This value is roughly consistent with the small cluster calculation in that by scaling the result of the cluster calculation by the numbers of next nearest neighbors taken, we find $0.12(\frac{8}{12})=0.08$ that is close to the value found in our Monte Carlo calculation.

Using the value $(J_2/J_1)_c\approx0.066$, we can draw a phase diagram[14] in $t/U-\delta$ plane using (11). The boundary between AF and RVB phases is given by the relation

$$\frac{\delta/2}{1-(U/t+5)\delta}=\left(\frac{J_2}{J_1}\right)_c=0.066\,. \tag{17}$$

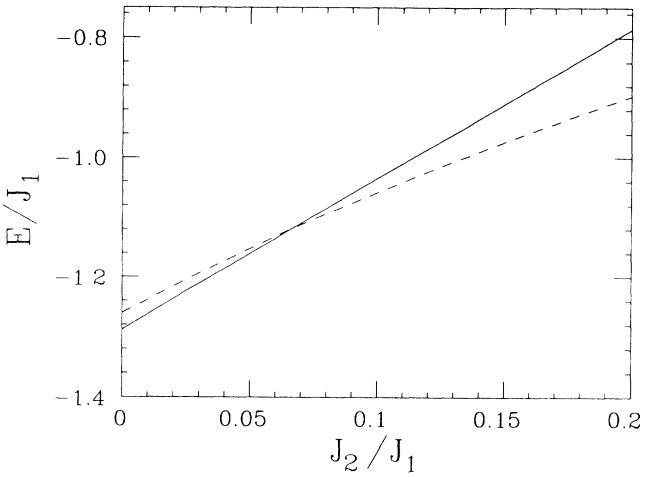

FIG. 3. The plot of energy per site in units of J_1 vs J_2/J_1 for variational trial wave functions Ψ_{AF} (solid line) and Ψ_{RVB} (dashed line). They cross each other at $J_2/J_1 \approx 0.066$.

The resulting diagram is shown in Fig. 4. As t/U is increased, the boundary approaches the asymptotic value of $\delta \approx 0.08$, and for a typical value of $t/U = \frac{1}{4}$, we find the AF-RVB transition to occur at $\delta \approx 0.06$.

To compare our result with experiments on high-T_c superconductor materials, we must, in addition, give consideration to the three-dimensional coupling between CuO_2 planes since the Néel temperature T_N of a two-dimensional Heisenberg system is zero.[15] The introduction of interlayer coupling, however, must be done carefully since our choice of RVB wave function has an algebraically decaying correlation. A mean-field-type coupling will result in a three-dimensional AF order in both AF and RVB phases discussed above. It must therefore be assumed that the true ground state in the region indicated

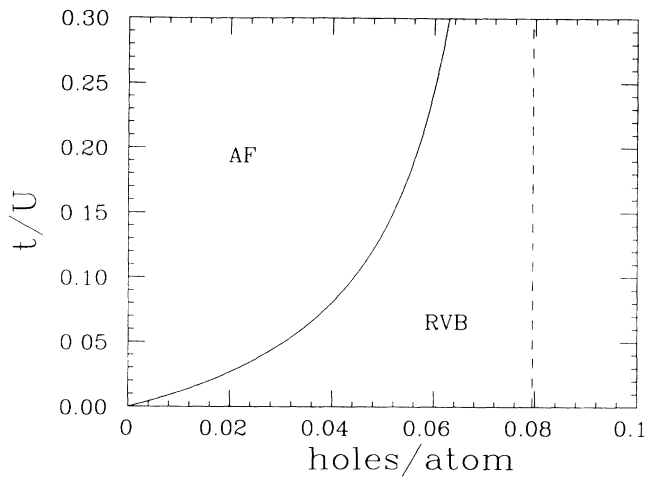

FIG. 4. Phase diagram obtained by comparing the Hamiltonians (13) and (14), with the crossover point $(J_2/J_1)_c \approx 0.066$. The solid line shows the phase boundary between AF and RVB phases. The boundary approaches the asymptotic value $\delta \approx 0.08$ holes/atom in the $t/U \rightarrow \infty$ limit indicated by the dashed line. (See, however, Ref. 14.)

by RVB in the phase diagram Fig. 4 has an exponentially decaying correlation function for this phase diagram to be meaningful in showing the upperbound of the critical-hole concentration. This is reasonable in view of the fact that the AF correlation function is likely to go through only a narrow region (maybe a line) of algebraically decaying phase (well described by our Ψ_{RVB}) before reaching exponential decay as doping is increased. This picture is supported by the study by Chakravarty, Halperin, and Nelson[16] of the nonlinear σ model where AF order at $T=0$ is found to disappear by going through a "point" in their parameter space where an algebraically decaying correlation is observed. With such a limitation in mind, we can compare the phase boundary of Fig. 4 with the experimentally found critical-hole concentration where T_N goes to zero. Our estimate of roughly 0.06 is consistent with available experimental values.[17] Though this agreement is rather encouraging, one must be conscious of the various limitations involved in our approach. (a) Our phase diagram, which assumes a mean-field-type interlayer coupling, can only hope to show the upper bound of the critical hole concentration. (b) The simple single-band Hubbard model only provides a first approximation to the correct physics of CuO_2 layers. (c) Our diagram itself relies on the validity of our variational wave functions for $|\nu\rangle$ as well as the conjecture that we can extrapolate results for the ferromagnetic limit where the mobile holes are found near the "corners" of the Brillouin zone to the general magnetic configuration [see Eq. (3)]. Another possibility that explains the rapid disappearance of AF order is that the nature of the interlayer coupling is more complex than that represented by a simple mean-field-type picture. The latter possibility has already been pointed out by Tranquada *et al.* for $YBa_2Cu_3O_{7-y}$ materials.[18]

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APPENDIX: IMPLEMENTATION OF PERIODIC BOUNDARY CONDITIONS FOR Ψ_{RVB}

The Bose gas wave function Ψ_{RVB} can be written as

$$\Psi_{RVB} \propto \exp\left\{-\frac{1}{2}\left[q^2\left[-2\sum_{\substack{i,j \\ i>j}}\ln r_{ij}\right]+\pi q^2\rho\sum_i r_i^2\right]\right\}. \tag{A1}$$

The exponent of the right-hand side of (A1) is nothing but one-half of the potential energy for two-dimensional one component plasma of charge q and density ρ. To write this in the Jastrow form, we consider the interaction of the

two charges with positive background and periodic boundary conditions. The system is placed on a square lattice of side L with one particle for every lattice site. In order to impose periodic boundary conditions, we consider the interactions of a particle at position $\mathbf{r}$ in the original square with a charge q at position $\mathbf{R}$ and the set of images located in periodic replicas of the square. Since the resulting potential will be a periodic function, the charge at $\mathbf{R}$ can without loss of generality be placed at the corner: $\mathbf{R}_0=(L/2)(\mathbf{e}_x+\mathbf{e}_y)$ leading to the sum of interactions with charges $\mathbf{R}_i=(2n_{ix}+1)(L/2)\mathbf{e}_x+(2n_{iy}+1)(L/2)\mathbf{e}_y$. The interaction potential of the charge q at $\mathbf{r}$ with this set of charges is

$$V_r=-2q^2\sum_i \ln|\mathbf{R}_i-\mathbf{r}| = -q^2\sum_i \ln(R_i^2+r^2-2rR_i\cos\theta_i),$$

where θ_i is the angle between $\mathbf{r}$ and $\mathbf{R}_i$. As a result of the square lattice structure, for each point $\mathbf{R}_i$ in the first quadrant, there are three other points at the same distance from the origin but with θ_i replaced by $\theta_i+(\pi/2)$, $\theta_i+\pi$, and $\theta_i+(3\pi/2)$, respectively. Summing these four contributions to the potential one finds

$$V_r=-q^2\sum_{i\in(\mathrm{I})}\ln\left[1+\left(\frac{r}{R_i}\right)^8-2\left(\frac{r}{R_i}\right)^4\cos4\theta_i\right] -2q^2\sum_{i\in(\mathrm{I})}4\ln R_i, \tag{A2}$$

where $i\in(\mathrm{I})$ denotes a sum restricted to angles in the first quadrant. It is worth stressing that expression (A2) is valid only when the entire system is symmetric about the origin. Given this symmetry, one can straightforwardly compute the potential contributed by the uniform positive background by integrating the force obtained from Gauss's law $V_b=(\pi q^2/L^2)+\text{const}$ where the constant $\to\infty$ and cancels the last term of (A2). Hence, the total potential between the particle at $\mathbf{r}$, the lattice replicas of $\mathbf{R}_0$ and the positive background is given by

$$V_p(\mathbf{r})=-q^2\sum_{i\in(I)}\ln\left[1+\left(\frac{r}{R_i}\right)^8-2\left(\frac{r}{R_i}\right)^4\cos4\theta_i\right] +\frac{\pi q^2}{L^2}r^2. \tag{A3}$$

The series converges reasonably fast and sufficient accuracy is obtained by summing over $0\le(n_{ix},n_{iy})\le200$. Using this result, we have expressed Ψ_{RVB} in Jastrow form on a lattice with periodic boundary conditions

$$\Psi_{\mathrm{RVB}}=\prod_{i>j}\exp[-\tfrac{1}{2}\tilde{V}_p(\mathbf{r}_i-\mathbf{r}_j)], \tag{A4}$$

where $\tilde{V}_p(\mathbf{r})=V_p(\mathbf{r}+\mathbf{R}_0)$. This is what we have used in our Monte Carlo calculation. One can verify that the form (A4) reduces to the form given in Eq. (A1) in the limit $L\to\infty$.

[1] J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).

[2] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963).

[3] A. B. Harris and R. V. Lange, Phys. Rev. **157**, 295 (1967); K. A. Chao, J. Spalek, and A. M. Oleś, J. Phys. C **10**, L271 (1977); J. E. Hirsch, Phys. Rev. Lett. **54**, 1317 (1985); C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B **36**, 381 (1987).

[4] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[5] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963); Phys. Rev. **134**, A923 (1964); **137**, A1726 (1965); H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 1490 (1987); also see C. Gross, R. Joynt, and T. M. Rice, in Ref. 3.

[6] J. E. Hirsch and D. J. Scalapino, Phys. Rev. B **29**, 5554 (1984).

[7] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 3570 (1987).

[8] P. W. Anderson, Science **235**, 1196 (1987).

[9] P. W. Anderson, Phys. Rev. **86**, 694 (1952).

[10] S. Doniach, M. Inui, V. Kalmeyer, and M. Gabay (unpublished).

[11] T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).

[12] V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987).

[13] V. Kalmeyer and R. B. Laughlin (unpublished).

[14] We have not considered the boundary to a ferromagnetic phase that is expected for small values of t/U and δ following Ref. 4.

[15] J. M. Kosterlitz and D. J. Thouless, Prog. Low Temp. Phys. **7B**, 373 (1978).

[16] S. Chakravarty, B. I. Halperin, and D. R. Nelson (unpublished).

[17] The relationship between the hole concentration in CuO_2 planes and the chemical composition of samples is yet unclear. In $La_{2-x}Sr_xCuO_{4-y}$ (or $La_{2-x}Ba_xCuO_{4-y}$) compounds, the doping is believed to be given by $\delta\approx x-2y$ and the critical concentration for the disappearance of AF order is estimated at 0.06–0.1. See D. C. Johnston *et al.*, Phys. Rev. B **36**, 4007 (1987); D. C. Johnston *et al.*, in *Proceedings of the International Conference on High-Temperature Superconductors: Materials and Mechanisms of Superconductivity, Interlaken, Switzerland, 1988,* edited by J. Müller and J. L. Olsen [Physica C (to be published)]; also see T. Fujita *et al.*, Jpn. J. Appl. Phys. **26**, L368 (1987). A different value of the critical δ was obtained by Y. Kitaoka *et al.* (unpublished) cited in A. Aharony *et al.* (unpublished).

[18] J. M. Tranquada *et al.* (unpublished).