

Superexchange mechanism and *d*-wave superconductivity

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We have formulated an auxiliary-boson mean-field theory consistent with the SU(2) symmetry of the Heisenberg model. At half filling, we find an infinite number of solutions related by the symmetry. Away from half filling the kinetic energy, acting as a symmetry-breaking field, selects a superconducting state of *d*-wave symmetry. The mean-field theory describes bosons and fermions with finite kinetic energy close to half filling. We derive self-consistent equations for the superconducting transition temperature T_c . We find that T_c vanishes at large and small filling factors.

The discovery of superconductivity in the rare-earth-based copper oxides,¹ followed by Anderson's suggestion of the relevance of the large- U limit of the Hubbard model to this problem,² has triggered a renewed interest in strongly correlated electron systems. Hirsh³ and Gros, Joynt, and Rice⁴ have shown that, in the large- U limit, the Hubbard model is equivalent to the model Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (f_{i,\sigma}^\dagger f_{j,\sigma} + f_{j,\sigma}^\dagger f_{i,\sigma}) + J \sum_{\langle ij \rangle} (\sigma_i \cdot \sigma_j - n_i n_j) - \mu_0 \sum_{\sigma} f_{i,\sigma}^\dagger f_{i,\sigma}, \quad (1)$$

acting on the subspace of empty and single occupied sites. σ_i is the spin of electron, $\langle ij \rangle$ denotes the summation over the nearest neighbors, and $J = 2t^2/U$.

Anderson² suggested that the ground state of the rare-earth copper oxides can be described by a correlated wave

$$H = -t \sum_{\langle ij \rangle, \sigma} (f_{i,\sigma}^\dagger b_j^\dagger f_{j,\sigma} + f_{j,\sigma}^\dagger b_i^\dagger f_{i,\sigma}) - \mu_0 \sum_{i,\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} + J \sum_{\langle ij \rangle} (\sigma_i \cdot \sigma_j) - (1 - b_i^\dagger b_i)(1 - b_j^\dagger b_j) + \sum_i \lambda_i \left(\sum_{\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} + b_i^\dagger b_i - 1 \right). \quad (3)$$

In this formalism, one introduces a boson operator b_i to keep track of the empty sites. The inequality constraint $\sum_{\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} \leq 1$ is replaced by an equality constraint $\sum_{\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} + b_i^\dagger b_i = 1$ enforced by the Lagrange multiplier λ_i . Kotliar and Ruckenstein⁸ have shown that in a certain auxiliary-boson formulation of the Hubbard model, treating the auxiliary-boson Hamiltonian in the mean-field theory is equivalent to evaluating matrix elements of the Hamiltonian in projected wave functions using the Gutzwiller approximation, suggesting the connections between the Gutzwiller and the auxiliary-boson approach. It is important to emphasize however that the auxiliary-boson provides a systematic treatment of the problem. Its mean-field theory can be improved by including the fluctuations around it.⁹ The first mean-field theory of the RVB due to Baskaran, Zou, and Anderson¹⁰ factorized the particle-particle channel by introducing an order parameter $\Delta_k = \Delta(\cos(k_x a) + \cos(k_y a))$, which describes a RVB phase with no gap to spin excitations (Δ_k vanishes

function of the form

$$|\Phi\rangle = P_G \prod_k (u_k + v_k f_{k,\sigma}^\dagger f_{k,-1}^\dagger) |0\rangle. \quad (2)$$

P_G is a Gutzwiller projection operator, and $N(1 - \delta) = \sum_{k\sigma} \langle f_{k,\sigma}^\dagger f_{k,\sigma} \rangle$ is the average number of electrons. At half filling i.e., $\delta = 0$, $|\Phi\rangle$ describes a disordered phase of the quantum Heisenberg antiferromagnet, e.g., the resonating valence bond (RVB) state. At finite δ , $|\Phi\rangle$ describes a superconducting state that evolves smoothly from the insulating state at $\delta = 0$.

The main difficulty in the investigation of these wave functions is the evaluation of the Gutzwiller projection. The exact calculation of observable matrix elements in the states described by Eq. (2) can only be done numerically using Monte Carlo technique.⁴⁻⁶ Alternatively, one can transform (1) into an equivalent auxiliary-boson Hamiltonian⁷

along a line called the pseudo-Fermi surface). Their results were independently derived and extended by Ruckenstein, Hirshfeld, and Appel.¹¹ Kotliar¹² found that the stable solutions of the mean-field theory at half filling is a mixture state describing a coherent superposition of *s*- and *d*-wave order parameters. Affleck and Marston¹³ developed a different mean-field theory by decoupling in the particle-hole channel and found a flux phase as a stable solution at half filling. The equivalence between Kotliar's mixed phase and Affleck and Marston's flux phase has been clarified by using a hidden SU(2) local gauge symmetry by Affleck, Zou, Hsu, and Anderson.¹⁴ A related approach, derived by Anderson, Baskaran, Zou, and Hsu;¹⁵ Zou and Anderson;¹⁶ Isawa, Maekawa, and Elisawa;¹⁷ and Suzumura, Hasegawa, and Fukuyama¹⁸ emphasized the importance of treating the boson and the fermion degrees of freedom in the same footing.

In this Rapid Communication, we explore a complete Hartree-Fock-Bogolubov factorization of Hamiltonian

(3). The motivation for this work is twofold. First, in the previous treatment,^{10–12} the bosons and the fermions in (3) have very little kinetic energy close to half filling, since the hopping amplitude turned out to be proportional to δ . As has been emphasized by Anderson¹⁹ and Zou and Anderson,¹⁶ in the RVB state the holes represented by the boson operators here should gain kinetic energy of order t . The spin degrees of freedom should also have a kinetic energy of order J . These results should come from the mean-field theory. Second, it is well known that at half filling, the large- U Hubbard model is equivalent to the Heisenberg model, which has a global SU(2) particle-hole symmetry.²⁰ The mean-field theory of factorization in the particle-particle channel violates such symmetry.

In the paper, we do a consistent Hartree-Fock-Bogolubov factorization of (3). The resulting mean-field

Hamiltonian has the SU(2) symmetry of the original model and the kinetic energy of the bosons and the fermions are finite close to half filling, resolving the difficulty of previous mean-field theory.

In the mean-field approximation, λ_i are replaced by its static value λ . At first approximation, we assume that $b_i^\dagger b_j = |b|^2 = \delta$. Introducing the order parameters

$$\kappa_x = 3J \langle f_{i,\sigma}^\dagger f_{i+x,\sigma} \rangle / 2, \quad (4a)$$

$$\kappa_y = 3J \langle f_{i,\sigma}^\dagger f_{i+y,\sigma} \rangle / 2, \quad (4b)$$

$$\Delta_x = 3J \langle f_{i,1} f_{i+x,-1} - f_{i,-1} f_{i+x,1} \rangle / 2,$$

$$\Delta_y = 3J \langle f_{i,1} f_{i+y,1} - f_{i,-1} f_{i+y,1} \rangle / 2,$$

we obtain from (3) the mean-field Hamiltonian

$$H_0 = - \sum_{i\sigma} [(\kappa_x f_{i,\sigma}^\dagger f_{i+x,\sigma} + \kappa_y f_{i,\sigma}^\dagger f_{i+y,\sigma}) + \text{c.c.}] + \sum_i [\Delta_x (f_{i,1}^\dagger f_{i+x,-1}^\dagger - f_{i,-1}^\dagger f_{i+x,1}^\dagger) + \text{c.c.}] \quad (5)$$

$$+ \sum_i [\Delta_y (f_{i,1}^\dagger f_{i+y,-1}^\dagger - f_{i,-1}^\dagger f_{i+y,1}^\dagger) + \text{c.c.}] - \delta t \sum_{(ij)\sigma} (f_{i,\sigma}^\dagger f_{j,\sigma} + \text{c.c.}) - \mu \sum_{i\sigma} f_{i,\sigma}^\dagger f_{i,\sigma}$$

and the corresponding Landau-Ginzburg free energy

$$F = -2T \sum_k \ln \cosh(\beta E_k / 2) - \mu N + 2N (|\kappa_x|^2 + |\kappa_y|^2 + |\Delta_x|^2 + |\Delta_y|^2) / (3J), \quad (6)$$

with the notations $\kappa_x = |\kappa_x| \exp(i\alpha_x)$, $\kappa_y = |\kappa_y| \exp(i\alpha_y)$, $\Delta_x = |\Delta_x| \exp(i\beta_x)$, $\Delta_y = |\Delta_y| \exp(i\beta_y)$, $\theta = \beta_y - \beta_x$,

$$E_k = \{(\varepsilon_k - \varepsilon_{-k}) + [(\varepsilon_k + \varepsilon_{-k} - 2\mu)^2 + 4|\Delta_k|^2]^{1/2}\} / 2, \quad (7a)$$

$$\varepsilon_k = -\delta t K(k) - 2[|\kappa_x| \cos(k_x a - \alpha_x) + |\kappa_y| \cos(k_y a - \alpha_y)], \quad (7b)$$

$$\Delta_k = 2[\Delta_x \cos(k_x a) + \Delta_y \cos(k_y a)], \quad (7c)$$

and $K(k) = 2[\cos(k_x a) + \cos(k_y a)]$. The chemical potential μ is determined by $1 - \delta = \sum_{i\sigma} \langle f_{i,\sigma}^\dagger f_{i,\sigma} \rangle$.

We find numerically that the minimum of the free energy (6) is at $\alpha_x = \alpha_y = 0$, $\kappa_x = \kappa_y$, $|\Delta_x| = |\Delta_y|$, and $\theta = \pi$. The order parameter κ_x and Δ_x as functions of δ are shown in Fig. 1. Notice that $\kappa_x \sim J/2$ close to half filling, and, hence, the effective boson hopping amplitude $2t\kappa_x/3J$

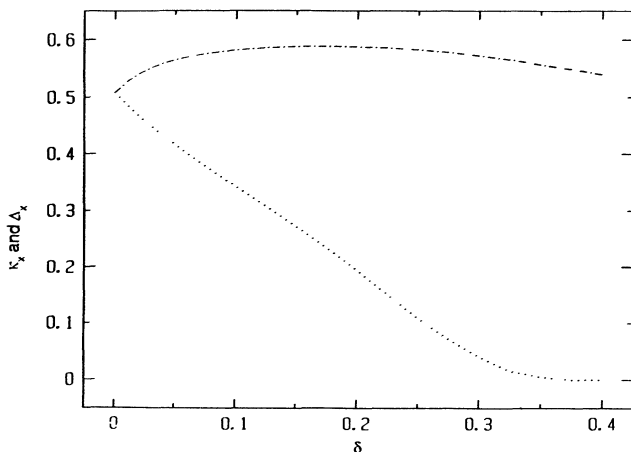


FIG. 1. $\kappa_x(\delta)$ (dot-dashed line) and $\Delta_x(\delta)$ (dotted line) in units of J at $T=0$ for $t=10J$.

is of order $t/3$. At half filling, we find an infinite number of solutions. In these solutions, the excitation spectrum has four point zeros, even away from half filling.

These results can be understood by using a Landau expansion of the free energy (6). When $\delta=0$, the free energy (6) has a global SU(2) symmetry,²⁰ i.e., defining as in Ref. 14, $U_{ij} = 3J \langle \psi_i \psi_j^\dagger + \phi_i \phi_j^\dagger \rangle / 2$, with $\psi_i^\dagger = (f_{i,1}^\dagger, f_{i,-1}^\dagger)$ and $\phi_i^\dagger = (f_{i,-1}^\dagger, -f_{i,1}^\dagger)$, we find that $F(U_x, U_y) = F(gU_x g^{-1}, gU_y g^{-1})$ for an arbitrary SU(2) element g . The infinite number of solutions that we found are all the SU(2) rotations from the mixed phase ($\kappa_x = \kappa_y = 0$, $\Delta_x = 1$, $\Delta_y = i$). Here we address the question which of these state is selected as one moves away from half filling. The hopping term induces a term linear in the order parameters κ_x and κ_y

$$\Delta F = -\delta A (\kappa_x + \kappa_y), \quad (8)$$

where A is a temperature-dependent positive factor. This term acts as a symmetry-breaking field in the SU(2) space and selects the direction $U_x = 1/\sqrt{2}(\sigma_x - \sigma_z)$ and $U_y = -1/\sqrt{2}(\sigma_x + \sigma_z)$. This corresponds to $\kappa_x = \kappa_y = 1$, $\Delta_x = -\Delta_y = 1$, i.e., a d -wave solution with finite hopping. This is in agreement with the Monte Carlo calculations of Gros,⁶ which indicate that the d -wave state has the lowest energy.

The critical temperature T_{RVB} of the pairing field Δ_k is

determined by solving numerically the self-consistent equations

$$\kappa_x = -\frac{3J}{8N} \sum_k K(k) \tanh \left(\frac{\varepsilon_k - \mu}{2T_{\text{RVB}}} \right), \quad (9a)$$

$$1 = \frac{3J}{8N} \sum_k g_\alpha(k)^2 / (\varepsilon_k - \mu) \tanh \left(\frac{\varepsilon_k - \mu}{2T_{\text{RVB}}} \right), \quad (9b)$$

$$\delta = \frac{1}{N} \sum_k \tanh \left(\frac{\varepsilon_k - \mu}{2T_{\text{RVB}}} \right), \quad (9c)$$

where $g_\alpha(k) = 2[\cos(k_x a) - \cos(k_y a)]$ for d wave and $g_\alpha(k) = K(k)$ for s wave. We find that only the d wave has nonzero T_{RVB} , and the results for T_{RVB} and κ_x at T_{RVB} as functions of δ are shown in Fig. 2. The s -wave solution has vanishing T_{RVB} and, therefore, the mixture of s and d wave does not exist away from half filling. This can be understood in the light of previous work which factorized the particle-particle channel. It was shown in Ref. 12 that the s -wave transition temperature vanishes as soon as the effective hopping δt is of order J . In the present SU(2) invariant approach, the effective hopping is of order $J + \delta t$, and, therefore, the s -wave state is completely suppressed.

The physical meaning of the critical temperature calculated above is the temperature below which there is a significant singlet pair formation. To obtain a superconducting state, one has to establish phase coherence between the singlet pairs, and this is determined by a different characteristic temperature T_{BC} , which is significantly lower than T_{RVB} , very close to half filling. This idea appears naturally in the auxiliary-boson formalism.¹⁷ The physical electron is represented by the operator $f_i^\dagger b_i$, and the superconducting order parameter is given by $\langle b_i f_{i+1}^\dagger b_j f_{j+1}^\dagger \rangle \approx \langle b_i b_j \rangle \langle f_{i+1}^\dagger f_{j+1}^\dagger \rangle$. The superconducting state is a state with both $\langle b_i b_j \rangle \neq 0$ and $\langle f_{i+1} f_{j+1} \rangle \neq 0$. The nonvanishing $\langle b_i b_j \rangle$ can be obtained either by one boson condensation ($\langle b_i \rangle \neq 0$), or by boson pair condensation. Here we investigate the first possibility. Performing a Hartree-Fock-Bogolubov factorization for both the boson and the fermion degrees of freedom in (3),

we obtain a set of self-consistent equations

$$t_f = \frac{t}{4N} \sum_p K(p) \langle b_p^\dagger b_p \rangle + \frac{3J}{8N} \sum_{k\sigma} K(k) \langle f_{k\alpha}^\dagger f_{k\sigma} \rangle, \quad (10a)$$

$$t_b = \frac{J}{4N} \sum_p \langle b_p^\dagger b_p \rangle + \frac{t}{4N} \sum_{k\sigma} K(k) \langle f_{k\alpha}^\dagger f_{k\sigma} \rangle, \quad (10b)$$

$$\Delta_k = \frac{3J}{2N} \sum_{k'} K(k-k') \langle f_{k',1} f_{-k',-1} \rangle, \quad (10c)$$

$$1 - \delta = \frac{1}{N} \sum_{k\sigma} \langle f_{k\alpha}^\dagger f_{k\sigma} \rangle, \quad (10d)$$

$$\delta = \frac{1}{N} \sum_p \langle b_p^\dagger b_p \rangle, \quad (10e)$$

where $t_f(t_b)$ is the effective hopping amplitude of the fermions (bosons) which determine the kinetic energy $\varepsilon_k = -t_f K(k)$ [$\varepsilon_p = -t_b K(p)$] of the fermions (bosons). We solved (10) by assuming a small interlayer hopping term in the z direction^{20,21} $K(k) = 2[\cos(k_x a) + \cos(k_y a) + r_x \cos(k_z a)]$ to obtain a finite boson condensation temperature T_{BC} and T_{RVB} . As expected from the $T=0$ study, the pairing has d -wave symmetry. The corresponding T_{RVB} and T_{BC} as functions of δ are shown in Fig. 3, we find that for small δ , $T_{\text{BC}} < T_{\text{RVB}}$, and $T_c = T_{\text{BC}}$ increases almost proportional to δ . For large δ , $T_{\text{RVB}} < T_{\text{BC}}$, and $T_c = T_{\text{RVB}}$ decreases as δ increases. The boson condensation temperature is not very sensitive to the value of small interlayer hopping amplitude since it depends on r_z logarithmically.

In conclusion, we formulated a mean-field theory which has all the symmetries of the original Hamiltonian at half filling. Away from half filling, the ground state has a d -wave symmetry. Both bosons and fermions have finite kinetic energy close to half filling. The hopping amplitude for the bosons is of order $t/3$ while that of the fermions is of order $J/2$. In the language of wave functions, our approach is equivalent to studying states (2) with three variational parameters. Finding a minimum of the free energy at half filling optimizes the exchange energy, while minimizing the free energy in the manifold of states related by an SU(2) operation is equivalent to optimizing the

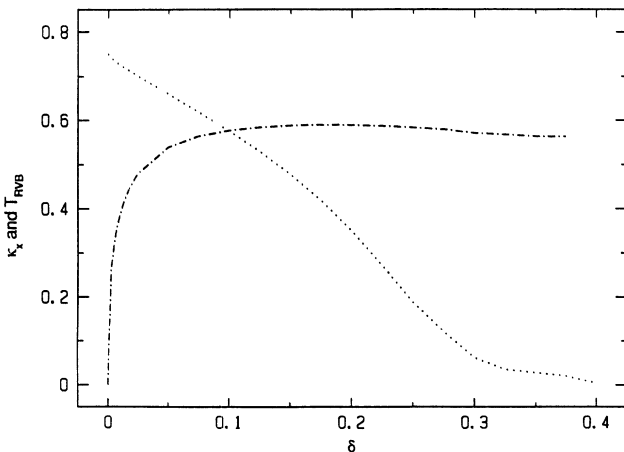


FIG. 2. $\kappa_x(\delta)$ (dot-dashed line) and $T_{\text{RVB}}(\delta)$ (dotted line) in units of J at T_{RVB} for $t=10J$.

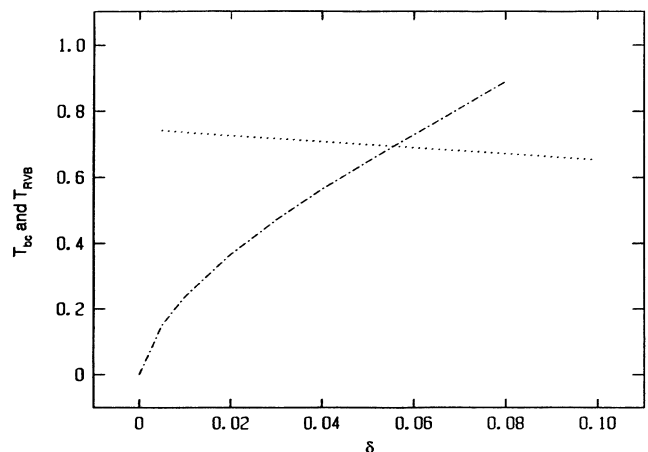


FIG. 3. $T_{\text{BC}}(\delta)$ (dot-dashed line) and $T_{\text{RVB}}(\delta)$ (dotted line) in units of J for $t=5J$.

kinetic energy of the holes. We calculated the Bose condensation temperature self-consistently, and found a superconducting critical temperature which vanishes for large and small filling factors. In this paper, we restrict ourselves to translationally invariant solutions. We are currently investigating possible solutions which break the translational invariance. In our view, it is important to clarify the stability of the different mean-field solutions as

a first step to understanding the effect of fluctuations around the mean-field theory.

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