Odd-Parity Singlet Pairing in the Positive-U Hubbard Model

Richard T. Scalettar and Rajiv R. P. Singh
Department of Physics, University of California, Davis, California 95616

Shoucheng Zhang
IBM Research Division, Almaden Research Center, 650 Harry Road, San Jose, California 95120
(Received 1 April 1991)

We consider the possibility of an odd-parity singlet pairing in the positive-U Hubbard model, which naturally incorporates short-ranged antiferromagnetic correlations in the ground state. In a quantum Monte Carlo simulation of a nearly half-filled Hubbard model, we find that the repulsive U enhances the tendency for this type of pairing more strongly than for other pairing channels considered earlier. We propose a BCS-type wave function for this pairing where the gap has no nodes over the Fermi surface, and discuss various experimental consequences in connection to high-T_c superconductivity.

PACS numbers: 74.65.+n, 71.20.Ad, 74.20.−z, 75.10.Lp

The newly discovered copper oxide materials exhibit antiferromagnetism at half filling and high-temperature superconductivity upon doping. In spite of their high transition temperatures, many properties of the superconducting state are similar to the BCS case [1]. There is strong evidence for a superconducting gap over the entire Fermi surface, although the magnitude and temperature dependence of such a gap has remained controversial. Among the novel features are the persistence of antiferromagnetic correlations in the superconducting state and the absence of the Hebel-Slichter peak in the nuclear relaxation rate. In contrast to the superconducting phase, the normal "metallic" phase shows many anomalous properties. The proximity of the superconducting phase to the antiferromagnetic one and the unusual normal-state properties have led to an extensive theoretical search for superconductivity in the repulsive-U Hubbard model. Among the proposed mechanisms are the resonating valence bond (RVB) [2], the spin-bag mechanism [3], paramagnon exchange [4], and anyon superconductivity [5].

In a different approach to superconductivity in the Hubbard model, Yang [6] recently discovered a class of eigenstates which had the property of off-diagonal long-range order (ODLRO). Yang and Zhang [7] showed that the Hubbard model has a pseudospin SU(2) symmetry in addition to the well-known SU(2) spin symmetry. Using these symmetries and the mapping between the positive- and negative-U models, it was shown by Singh and Scalettar [8] that Yang's superconducting states are mapped to ferromagnetic ones under the change in sign of U. Thus by exact mapping to the Nagaoka problem [9], these eigenstates become the ground states of the negative-U Hubbard model in the presence of a spin polarization. One of the most distinctive features of this new pairing is that the pairs have a net momentum $\boldsymbol{\pi}$.

In this paper, we explore momentum-$\boldsymbol{\pi}$ pairing in the positive-U Hubbard model by Monte Carlo simulations. Although previous numerical studies have examined pairing instabilities for various *relative* angular momentum channels, the center-of-mass momentum was restricted to zero. On-site s-wave pairing is strongly suppressed by the positive U, while the extended s-wave channel showed only a very weak, temperature-independent enhancement, consistent with the rigorous results of Zhang [10]. Only the $d_{x^2-y^2}$-wave pairing shows a substantial enhancement near half filling. To study pairing with total momentum $\boldsymbol{\pi}$, consider the operator

$$\Delta_x^\eta = \sum_r (-1)^r (c_{r\uparrow} c_{r+x\downarrow} - c_{r\downarrow} c_{r+x\uparrow}) = 2\sum_k \sin(kx) c_{k\uparrow} c_{-k+\pi\downarrow} \quad (1)$$

and similarly Δ_y^η. Both operators are spin singlets. Under the parity transformation $c_{r\sigma} \to c_{-r\sigma}$, they change sign. A state exhibiting ODLRO in Δ_x^η and Δ_y^η operators shall be called an odd-parity-singlet-pairing (OPSP) state. Note that the oddness under parity arises because of the (π,π) pair center-of-mass momentum; the relative-coordinate wave function remains even, consistent with the Pauli principle [11].

As we shall show, the pair function for the OPSP state is nonvanishing only when the up and down spins belong to different sublattices. An odd-parity momentum-π pairing state for spins on the same sublattice must necessarily be triplet. This gives the OPSP state a more extended antiferromagnetic character than the d-wave case. Furthermore, this pairing has a lower angular momentum. Thus we expect it to be most favorable near the antiferromagnetic phase. Such a pairing operator is implicitly used in the spin-bag mechanism of Schrieffer, Wen, and Zhang [3], who considered pairing of eigenstates in the presence of long-ranged spin-density-wave order which mixes k and $\pi - k$. It also arises in the theory of Kampf and Schrieffer [3], where the quasiparticle energies at k and $\pi - k$ are nearly degenerate due to the dressing of low-energy antiferromagnetic fluctuations [12].

We have used the determinant Monte Carlo method

[13] to compute the 9×9 susceptibility matrix [14]

$$M_{ab}^{\eta}=\int_0^{\beta}\langle\Delta_a(\tau)\Delta_b^{\dagger}(0)\rangle d\tau\,,$$
$$\Delta_a^{\eta}(\tau)=\frac{1}{\sqrt{N}}\sum_r(-1)^r c_{r\downarrow}(\tau)c_{r+\mathbf{a}\uparrow}(\tau)\,, \qquad (2)$$

where $\mathbf{a}$ takes on value $\mathbf{0},\pm\mathbf{x},\pm\mathbf{y},\pm\mathbf{x}\pm\mathbf{y}$. From M_{ab}^{η} we construct various pairing susceptibilities $P_\alpha(r)$ in the $\alpha=s$, p, and d angular momentum channels with r denoting the spatial structure of the pairing [13]. We compare these fully correlated susceptibilities with the uncorrelated ones $\bar{P}_\alpha$, which include only the self-energy dressing of the quasiparticles, to infer the enhancement of the effective interaction vertex Γ_α defined by [15]

$$\Gamma_\alpha=P_\alpha^{-1}-\bar{P}_\alpha^{-1}\,. \qquad (3)$$

In Fig. 1 we show $P_d(x^2-y^2)$, $\bar{P}_d(x^2-y^2)$, $P_p^{\eta}(x)$, and $\bar{P}_p^{\eta}(x)$ as a function of temperature on 4×4 lattices at half filling. In Fig. 2, we show the effective vertex for the two channels. Γ is more strongly enhanced for the OPSP case than for the d wave [16]. The effective density of states in the OPSP pairing, which enters $\bar{P}_\alpha$, is, however, lower. In an RPA-like treatment, $\Gamma_\alpha\bar{P}_\alpha=1$ determines the transition temperature. At the lowest temperatures studied, $\Gamma_\alpha\bar{P}_\alpha$ is about 25% higher for the OPSP case than for the d wave. At half filling we do not expect superconducting order to develop. As one moves away from half filling, the two susceptibilities show similar behavior. The vertex enhancement appears maximal at half filling [14]. However, the low-temperature density of states will increase rapidly with doping. These two effects will give a maximum T_c at some finite doping.

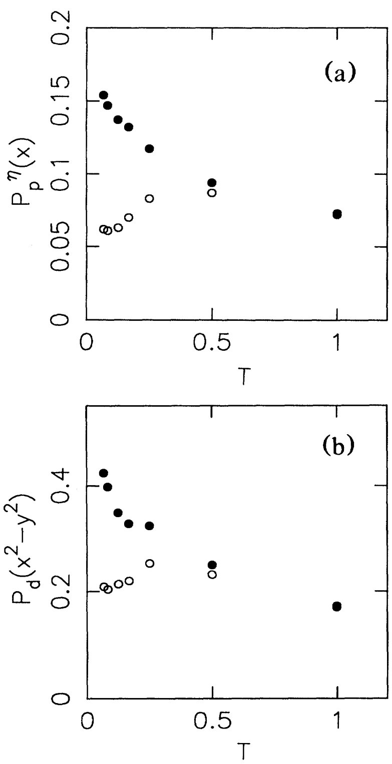

FIG. 1. Plots of the susceptibilities (a) $P_p^{\eta}(x)$ and (b) $P_d(x^2-y^2)$ as functions of temperature. The open circles include only the self-energy dressing of the individual quasiparticles, while the solid circles represent the fully correlated susceptibilities including the interaction vertex. All data are for the 4×4 system at half filling, with $U=4$ and $t=1$.

We shall address finite-size effects more fully in a subsequent paper. The vertex Γ remains large and increases slightly as the lattice size is increased to 6×6 and 8×8, but the equal-time structure factor decreases. It is generally believed that the susceptibilities, and hence Γ, are the more sensitive probe of pairing correlations. Thus the robustness of the vertex with increasing size might be the more fundamental feature. However, the equal-time measurements need to be carefully studied before the final interpretation of the finite-size effects is completed.

We now construct a BCS-like OPSP ground state and discuss its nature. Since Δ_x^{η} and Δ_y^{η} order are degenerate, the ground state will be an appropriate linear combination. We shall take the form $\Delta_x^{\eta}+i\Delta_y^{\eta}$ which leads to a full pairing gap over the Fermi surface and maximizes the gain in condensation energy. In the presence of such an order, the quasiparticles experience an anomalous scattering amplitude with the condensate, which is characterized by a gap function $\Delta(k_x,k_y)\propto\sin k_x+i\sin k_y$. To proceed further, we need to assume a form for the renormalized quasiparticle dispersion ε_k. The most natural description for momentum-π pairing arises in terms of the "pocket" Fermi surface [17] around $(\pm\pi/2,\pm\pi/2)$, as indicated in Fig. 3. OPSP corresponds to pairing the quasiparticle states in the same pocket but on opposite sides of the $U=0$ half-filled Fermi surface. Our analysis is unchanged for the case of a large Fermi surface if there exists a *ghost Fermi surface* of low-lying excitations composed of a bare particle near the Fermi surface and a low-lying magnon near (π,π) [18].

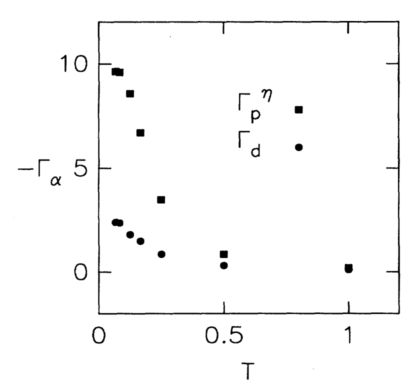

FIG. 2. The vertices Γ_p^{η} (squares) and Γ_d (circles) as functions of temperature.

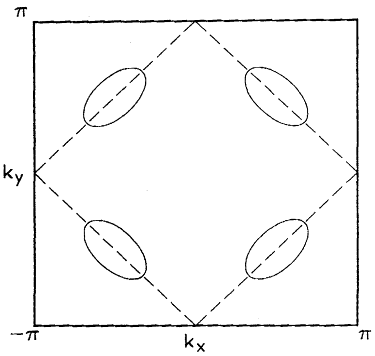

FIG. 3. Fermi surface with pockets around $(\pm\pi/2, \pm\pi/2)$. The dashed line shows the $U=0$ half-filled Fermi surface.

In both cases, one obtains $\varepsilon_{k+\pi} \approx \varepsilon_k$. The resulting equations of motion

$$-i\dot{c}_{k\uparrow} = -\varepsilon_k c_{k\uparrow} + \Delta_k c^\dagger_{\pi-k\downarrow}\,,$$
$$-i\dot{c}_{k\downarrow} = -\varepsilon_k c_{k\downarrow} - \Delta_k c^\dagger_{\pi-k\uparrow}\,, \tag{4}$$

can be diagonalized by the Bogliubov transformation

$$c_{k\uparrow} = u_k \gamma_{k\uparrow} + v_k \gamma^\dagger_{\pi-k\downarrow}\,,$$
$$c_{k\downarrow} = u_k \gamma_{k\downarrow} - v_k \gamma^\dagger_{\pi-k\uparrow}\,, \tag{5}$$

with *complex* coefficients u_k and v_k defined by

$$|u_k|^2 = \tfrac{1}{2}(1+\varepsilon_k/E_k),\quad |v_k|^2 = \tfrac{1}{2}(1-\varepsilon_k/E_k)\,,$$
$$E_k = (\varepsilon_k^2 + |\Delta_k|^2)^{1/2},\quad u_k v_k = \Delta_k/2E_k\,. \tag{6}$$

The OPSP ground state is annihilated by the operators $\gamma_{k\sigma}$. The squared modulus of the pairing gap is proportional to $\sin^2 k_x + \sin^2 k_y$, which is nonvanishing everywhere on the Fermi surface.

Both the single-particle and the two-particle correlations can now be calculated. The ground state $|\Omega\rangle$ does not have any nonvanishing charge, spin, or current density, i.e., $\langle\rho_{q\neq 0}\rangle = \langle\mathbf{S}_q\rangle = \langle\mathbf{J}_q\rangle = 0$, but it does have an anomalous pairing amplitude

$$b_k^* \equiv \langle c^\dagger_{\pi-k\uparrow} c^\dagger_{k\downarrow}\rangle = u_k^* v_k^* = \Delta_k^*/2E_k\,. \tag{7}$$

This pairing amplitude breaks U(1) phase symmetry, lattice translational symmetry, parity, and time-reversal symmetry. However, it conserves spin-rotation symmetry. Since $u_{\pi+k}v_{\pi+k} = -u_k v_k$, the Fourier transform of b_k gives a Cooper-pair wave function $\langle c_{r_1\uparrow} c_{r_2\downarrow}\rangle$ which vanishes identically when r_1 and r_2 belong to the same sublattice.

The static structure factor in the OPSP state is given by

$$S_{+-}(q) = \sum_k (|u_k|^2 |v_{q+k}|^2 - u_k v_k u^*_{q+k} v^*_{q+k})\,. \tag{8}$$

At $q=0$, the two terms cancel each other, showing that the ground state is a total spin singlet, while at $q=(\pi,\pi)$ they add constructively as $\Delta_{\pi+k} = -\Delta_k$. This leads to a peak of $S_{+-}(q)$ near $q=(\pi,\pi)$. $S_{+-}(q)$ decays as one moves away from the (π,π) point, giving rise to an antiferromagnetic correlation length of order the superconducting coherence length. Within the single-mode approximation, a peak in $S_{+-}(q)$ implies the presence of a low-energy magnetic excitation near (π,π). Coupling these soft magnons to the quasiparticles naturally leads to the pocket band structure [18].

The breaking of parity and time-reversal symmetry by b_k may be related to anyon superconductivity [5]. Here, we compare it to superfluid ^{3}He. Since the pair wave function $b(r) \equiv \sum_k e^{ikr} b_k$ is intrinsically complex, there is an associated current $b^*(r)\nabla b(r) - b(r)\nabla b^*(r)$. However, this does not give rise to a macroscopic current but only to a density-current correlation function $\langle\rho(0)\mathbf{J}(r)\rangle$, similar to the Anderson-Morel phase of ^{3}He. Such a *P*-*T*-breaking correlation function might give a "chiral sense" to the system if it leads to a net orbital angular momentum. It has been argued by Leggett [19] that such an effect is only microscopic, i.e., of the order of 1 rather than *N*. For this reason, we believe that this *T*-breaking effect is not macroscopically observable.

Since the gap in the OPSP state is nonvanishing everywhere on the Fermi surface, experiments which are only sensitive to its magnitude, such as the temperature dependence of the London penetration depth $\lambda(T)$, the lower critical field $H_{c1}(T)$, and the Knight shift $K_s(T)$, should yield results similar to the conventional BCS superconductors. This is consistent with most of the experimental data on high-T_c superconductors. On the other hand, an NMR experiment below T_c is sensitive to the coherence factors which, with standard hyperfine coupling, enter in the form $|u_k u^*_{k'} + v_k v^*_{k'}|^2$ for a scattering from k to k'. For the conventional case, u_k and v_k are uniform, leading to a constructive interference and the Hebel-Slichter peak. For the OPSP state, $u_{\pi+k}v_{\pi+k} = -u_k v_k$, leading to destructive interference if the susceptibility is dominated by $\mathbf{q}=\boldsymbol{\pi}$. This could explain the suppression of the Hebel-Slichter peak in high-T_c superconductors [20,21]. Another striking feature of the OPSP state is the coexistence of superconductivity with short-ranged antiferromagnetic correlations and low-energy magnons near (π,π). These features are also observed in recent neutron-scattering experiments on 1-2-3 materials [22].

We now discuss an experiment which is unique to OPSP order. Zhang has shown [23] that any form of superconductivity in the Hubbard model leads to well-defined collective modes whose existence is dictated by the pseudospin SU(2) symmetry. In the present case, Δ_x^η (and similarly Δ_y^η), its Hermitian conjugate, and the current operator $j_x = \sum_{r\sigma}(c^\dagger_{r\sigma} c_{r+\hat{x}\sigma} c_{r\sigma})$ form a triplet representation of the pseudospin SU(2) group. Below T_c this leads [23] to an extra absorption peak in the optical conductivity $\sigma(\omega)$ at energy $U-2\mu$, with intensity proportional to $|\langle\Delta_x^\eta\rangle|^2$. Hence, as long as the system is well described by the Hubbard model, the OPSP order can be directly observed in the optical conductivity.

To conclude, in this paper we have considered a new symmetry for the superconducting gap function, namely, an odd-parity singlet pairing state, and argued that it is most favored by antiferromagnetic correlations. Quantum Monte Carlo simulations show that such a pairing vertex is more strongly enhanced in a nearly half-filled repulsive-U Hubbard model than are other channels considered earlier. A BCS-type theory has been constructed for the OPSP state where the gap is shown to be nonvanishing over the entire Fermi surface. This state breaks P and T symmetries, and has short-ranged antiferromagnetic correlations. We have argued that it may lead to a suppression of the Hebel-Slichter peak in NMR, and have made predictions for a collective mode which may be observable in optical-absorption experiments.

We would like to thank Professor D. J. Scalapino and Professor J. R. Schrieffer for discussions. This work is supported in part by the NSF under grant No. DMR-9017361.

Note added.—After completion of this paper, we became aware of a preprint by G. Fano, F. Ortolani, and A. Parola, who show that the ground state of the 4×4 Hubbard model with two holes has p-wave symmetry with momentum (π,π) for $U<3$. For larger U this state stays very close to the ground state. This is further evidence that the OPSP state is a candidate for superconductivity in the repulsive Hubbard model. We also learned of unpublished work by A. Moreo, where finite-momentum pairing is studied and a similar conclusion is reached.

[1] For a review of the experiments, see *High Temperature Superconductivity, Proceedings of the Los Alamos Symposium, 1989,* edited by K. S. Bedell *et al.*

[2] P. W. Anderson, Science **235**, 1196 (1987); S. A. Kivelson, D. Rokhsar, and J. Sethna, Phys. Rev. B **35**, 8865 (1987).

[3] J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. B **39**, 11 663 (1989); A. Kampf and J. R. Schrieffer, Phys. Rev. B **41**, 6399 (1990).

[4] D. J. Scalapino, J. E. Hirsch, and E. Y. Loh, Phys. Rev. B **34**, 8190 (1986).

[5] R. G. Laughlin, Science **242**, 525 (1988).

[6] C. N. Yang, Phys. Rev. Lett. **63**, 2144 (1989).

[7] C. N. Yang and S. C. Zhang, Mod. Phys. Lett. B **4**, 759 (1990); S. C. Zhang, Int. J. Mod. Phys. B **5**, 153 (1991).

[8] R. R. P. Singh and R. T. Scalettar, Phys. Rev. Lett. **66**, 3203 (1991).

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

[10] S. C. Zhang, Phys. Rev. B **42**, 1012 (1990).

[11] We thank J. R. Schrieffer for a discussion clarifying this point.

[12] The connection of this work to the theory of Kampf and Schrieffer is discussed in a forthcoming paper by E. Dagotto, A. Kampf, and J. R. Schrieffer.

[13] S. R. White *et al.*, Phys. Rev. B **39**, 839 (1989).

[14] The actual filling is a slightly subtle issue since the susceptibility in Eq. (2) measures the propagation of two *additional* holes injected into the lattice. For small systems this can correspond to significant doping. We will discuss the doping dependence further: R. R. P. Singh, R. T. Scalettar, and S. C. Zhang (to be published).

[15] R. T. Scalettar *et al.*, Phys. Rev. B **44**, 770 (1991).

[16] The vertex for momentum-π p-wave pairing of second-neighbor spins is also strongly enhanced. This is in contrast to the d-wave second-neighbor pairing which is strongly suppressed. This is another indication that the antiferromagnetic correlations favor the former.

[17] B. I. Shraiman and E. D. Siggia, Phys. Rev. B **40**, 9162 (1989); S. Trugman, Phys. Rev. B **37**, 1597 (1988).

[18] A. Kampf and J. R. Schrieffer, Phys. Rev. B **42**, 7967 (1990); B. I. Shraiman (to be published); see also P. A. Lee, in *High Temperature Superconductivity, Proceedings of the Los Alamos Symposium, 1989* (Ref. 1).

[19] A. J. Leggett, Rev. Mod. Phys. **47**, 332 (1975).

[20] N. Bulut, D. J. Scalapino, and N. E. Bickers have developed similar arguments for the absence of the Hebel-Slichter peak for the d-wave case.

[21] If the hyperfine coupling is of the form $I^\mu c_{i\alpha}^\dagger \sigma_{\alpha\beta}^\mu c_{j\beta}$, where I is the nuclear spin and i and j are on opposite sublattices, then momentum-π pairing reverses the conditions for constructive interference. This may be responsible for the absence of the Hebel-Slichter peak in the oxygen NMR.

[22] H. Chou *et al.* (to be published).

[23] S. C. Zhang, Phys. Rev. Lett. **65**, 120 (1990).