Superconductivity in a two-dimensional hole-doped spin-orbital system

Bo Song[1,2,3] and Yupeng Wang[1]
[1]*Institute of Physics, Chinese Academy of Sciences, Beijing 100080, People's Republic of China*
[2]*Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100080, People's Republic of China*
[3]*Graduate School of the Chinese Academy of Sciences, Beijing 100039, People's Republic of China*
(Received 12 May 2003; published 17 September 2003)

A two-dimensional electron system with both spin and orbital degrees of freedom is investigated with the slave-boson mean-field approaches. By introducing the resonating-valence-bond order parameters, we show that the system may exhibit superconductivity after the slave bosons "condensation." It is found that the electron pairs are spin singlets and orbital singlets but the system shows *p*-wave superconductivity with the symmetry of $k_x \pm i k_y$.

DOI: 10.1103/PhysRevB.68.104512 PACS number(s): 74.72.−h, 74.20.−z, 74.20.Rp

After the discovery of the BCS superconductivity (SC), looking for new types of superconductors, namely, the "unconventional" superconductors, has become an important issue in condensed-matter physics. The first example found is the superfluid ^{3}He, in which the pairing symmetry of the atoms has been demonstrated to be *p* wave. Subsequently, a variety of heavy fermion superconductors were discovered and most of them exhibit nodes in their gap functions, and therefore belong to the class of unconventional superconductors. One of the most exciting discoveries in the last two decades is the high-T_c superconductors. It is generally believed that the hole-doped high-T_c superconductors are *d*-wave paired. Recently, *p*-wave SC has also been found in several materials. One of such materials is Sr_2RuO_4,[1] in which *p*-wave SC exists[2] with strong ferromagnetic (FM) fluctuation.[3] This material has a layered structure with the total spin of Cooper pairs lying in the basal plane.[4] Its SC properties have been widely studied[5–7] and the pairing symmetry was predicted to be $k_x \pm i k_y$. The heavy fermion material UGe_2 also shows the *p*-wave SC on the border of itinerant-electron ferromagnetism.[8] A more interesting material is $ZrZn_2$,[9] in which *p*-wave SC and long-range FM carried by the same electrons coexist. A few theories have been raised to explain the mechanism of this kind of SC.

However, most of the heavy fermion superconductors possess strong antiferromagnetic (AF) fluctuation above T_c and shows odd pairing behavior in the gap functions. This strongly suggests that the orbital degrees of freedom of the electrons may play important roles in their SC. On the other hand, orbital degeneracy in the transition-metal oxides may also affect their superconductivity under hole doping, if the Hund's coupling and the crystal fields are weak enough. The insulating spin-orbital systems have been studied for a long time.[10] The minimum model to describe a twofold orbital degenerate spin-1/2 system is the so-called SU(4) model.[11] As is well known, the high-T_c superconductors are in fact the hole-doped Mott insulators without orbit degeneracy. It is therefore interesting to study the hole-doped spin-orbital systems. The key issue in such hole-doped systems is whether there is any superconductivity, and if yes, what is the symmetry of the paring state? For some insulating materials with orbital degeneracy, Santoro *et al.* proposed and studied a spin-orbital coupling superexchange Hamiltonian,[12–15]

$$H=-\sum_{\langle i,j\rangle}\left(2\vec{S}_i\cdot\vec{S}_j-\frac{1}{2}\right)\left(2\vec{T}_i\cdot\vec{T}_j-\frac{1}{2}\right). \tag{1}$$

This Hamiltonian was shown to describe the spin-orbital interaction in many compounds of C_{60},[16] compounds of layered fullerides, and some two-dimensional (2D) copolymers.[17] They also showed[14,15] that the ground state of the model (1) is spin-Peierls-like dimerized in one dimension. Zhang and Shen[18] investigated the ground state of this model in two dimensions using interesting approaches. They simplified the spin-orbital interaction to a reduced form in an SU(4) Schwinger boson representation.[19] By introducing a symmetric resonating valence bonds (RVB) (Ref. 20) ordering parameter and applying mean-field theory, they found a different spin-orbital FM ordered state corresponding to a short-ranged RVB crystal state, while both the spin and orbital degrees of freedom form AF ordering.

In the present paper, we investigate a toy model of a hole-doped 2D spin-orbital system based on the model (1). By introducing the SU(4) fermion representation, the interaction part of the model Hamiltonian can be reduced to bond-charge interaction, which has the same form as that of the Schwinger boson representation.[18] Upon this reduction, the slave-boson mean-field phase diagram has been derived. It is shown that the pairing symmetry is *p* wave though the electron pairs are both spin and orbit singlet. With the slave boson condensation, superconductivity may exist in some doping region. The Hamiltonian we shall study reads

$$\begin{aligned}H=&-t\sum_{\langle i,j\rangle,\sigma,\tau}\mathcal{P}(C^\dagger_{i,\sigma,\tau}C_{j,\sigma,\tau}+C^\dagger_{j,\sigma,\tau}C_{i,\sigma,\tau})\mathcal{P}\\&-J\sum_{\langle i,j\rangle}\left(2\vec{S}_i\cdot\vec{S}_j-\frac{1}{2}n_in_j\right)\left(2\vec{T}_i\cdot\vec{T}_j-\frac{1}{2}n_in_j\right)\\&-\mu_0\sum_{i,\sigma,\tau}C^\dagger_{i,\sigma,\tau}C_{i,\sigma,\tau},\end{aligned} \tag{2}$$

where t is the hopping constant, and $J>0$ is the superexchange constant; μ_0 is the chemical potential; $C^\dagger_{i,\sigma,\tau}(C_{i,\sigma,\tau})$ is the creation (annihilation) operator of electrons on site i with spin and orbit components σ,τ; $\mathcal{P}\cdots\mathcal{P}$ indicates the single occupation $n_i=\Sigma_{\tau\sigma}C^\dagger_{i,\sigma,\tau}C_{i,\sigma,\tau}\leqslant 1$; $\vec{S}_i$

$=\Sigma_{\sigma,\sigma',\tau}C^{\dagger}_{i,\sigma,\tau}\vec{\sigma}_{\sigma,\sigma'}C_{i,\sigma',\tau}$ and $\vec{T}_i=\Sigma_{\sigma,\tau,\tau'}C^{\dagger}_{i,\sigma,\tau}\vec{\tau}_{\tau,\tau'}C_{i,\sigma,\tau'}$ denote the spin-1/2 and orbital-1/2 operators, respectively, at a lattice site i; $\sigma=\pm\frac{1}{2}$, $\tau=\pm\frac{1}{2}$ represent the spin and orbital indices, respectively; $\langle i,j\rangle$ denotes the summation over the nearest neighbors. The model is constructed in a 2D square lattice. We note that though the second term of Eq. (2) contains more than four fermion product, it is indeed a two-body interaction term because of the hard-core nature of the fermions.

For convenience, we introduce the notations $|\sigma,\tau\rangle$:

$$|1\rangle=\left|+\frac{1}{2};+\frac{1}{2}\right\rangle,|2\rangle=\left|-\frac{1}{2};+\frac{1}{2}\right\rangle,$$

$$|3\rangle=\left|+\frac{1}{2};-\frac{1}{2}\right\rangle,|4\rangle=\left|-\frac{1}{2};-\frac{1}{2}\right\rangle, \tag{3}$$

and creation (annihilation) operators $d^{\dagger}_{i,\nu}(d_{i,\nu})$ creating (annihilating) the four states, where ν takes 1, 2, 3, 4. By a projection procedure on the spin-spin and orbital-orbital quardratic superexchange interactions,[18] the Hamiltonian can be written as

$$H=-t\sum_{\langle i,j\rangle,\nu}\mathcal{P}(d^{\dagger}_{i,\nu}d_{j,\nu}+d^{\dagger}_{j,\nu}d_{i,\nu})\mathcal{P}$$
$$-J\sum_{\langle i,j\rangle}B^{\dagger}_{ij}B_{ij}-\mu_0\sum_{i,\nu}d^{\dagger}_{i,\nu}d_{i,\nu}, \tag{4}$$

with

$$B^{\dagger}_{ij}=d^{\dagger}_{i,1}d^{\dagger}_{j,4}+d^{\dagger}_{i,4}d^{\dagger}_{j,1}-d^{\dagger}_{i,2}d^{\dagger}_{j,3}-d^{\dagger}_{i,3}d^{\dagger}_{j,2}.$$

In the slave-boson approach,[21] the single-occupation condition can be treated self-consistently with the following operator transformation:

$$d^{\dagger}_{i,\nu}\to a^{\dagger}_{i,\nu}b_i, \tag{5}$$

where $a^{\dagger}_{i,\nu}$ is creation operator of fermion and b_i is the annihilation operator of the hole boson. With this transformation, the constraint can be expressed as

$$\sum_{\nu}a^{\dagger}_{i,\nu}a_{i,\nu}+b^{\dagger}_ib_i=1. \tag{6}$$

Then the Hamiltonian can be written as

$$H=-t\sum_{\langle i,j\rangle,\nu}(a^{\dagger}_{i,\nu}b_ib^{\dagger}_ja_{j,\nu}+\text{H.c.})-\mu_0\sum_{i,\nu}a^{\dagger}_{i,\nu}a_{i,\nu}$$
$$-J\sum_{\langle i,j\rangle}B^{\dagger}_{a,ij}B_{a,ij}+\sum_i\lambda_i\left(\sum_{\nu}a^{\dagger}_{i,\nu}a_{i,\nu}+b^{\dagger}_ib_i-1\right), \tag{7}$$

where $B_{a,ij}$ is B_{ij} with d replaced by a. With mean-field approximation, we replace λ_i by its static value λ, and assume $b^{\dagger}_ib_i=|b_i|^2=\delta$. Introducing a unique short-ranged RVB pairing order parameter,

$$\Delta_{ij}=\langle B_{a,ij}\rangle, \tag{8}$$

we obtain

$$H=-t\delta\sum_{\langle i,j\rangle,\nu}(a^{\dagger}_{i,\nu}a_{j,\nu}+\text{H.c.})-\mu\sum_{i,\nu}a^{\dagger}_{i,\nu}a_{i,\nu}$$
$$-J\sum_{\langle i,j\rangle}[B^{\dagger}_{a,ij}\Delta_{ij}+\Delta^{*}_{ij}B_{a,ij}-|\Delta_{ij}|^2]-N(1-\delta)\lambda, \tag{9}$$

with $\mu=\mu_0-\lambda$. The Green's functions of the mean-field Hamiltonian read

$$\langle\langle a_{k,\nu};a^{\dagger}_{k,\nu}\rangle\rangle=\frac{\omega+\epsilon_k}{(\omega+E_k)(\omega-E_k)}, \tag{10}$$

$$\langle\langle a^{\dagger}_{\overline{k},\overline{\nu}};a^{\dagger}_{k,\nu}\rangle\rangle=\frac{\pm i\Delta^{*}_k}{(\omega+E_k)(\omega-E_k)}, \tag{11}$$

where $a_{k,\nu}$ is the Fourier transformation of $a_{i,\nu}$; $\pm$ takes $+$for $\nu=1,4$ and $-$ for $\nu=2,3$; $\overline{k}=-k$ and $\overline{\nu}=1,4$ if $\nu=4,1$ and $\overline{\nu}=2,3$ if $\nu=3,2$. The excitation spectrum is

$$E_k=\sqrt{\epsilon_k^2+|\Delta_k|^2}, \tag{12}$$

with $\epsilon_k=-2t\delta[\cos(k_xa)+\cos(k_ya)]-\mu$ and $\Delta_k=2J[\Delta_x\sin(k_xa)+\Delta_y\sin(k_ya)]$, where Δ_x and Δ_y are Δ_{ij} along the x and y axis, respectively. From Eqs. (10) and (11) we obtain[21]

$$\langle a^{\dagger}_{k,\nu}a_{k,\nu}\rangle=\frac{1}{2}-\frac{\epsilon_k}{2E_k}\tan h\frac{1}{2}\beta E_k, \tag{13}$$

$$\langle a^{\dagger}_{\overline{k},\overline{\nu}}a^{\dagger}_{k,\nu}\rangle=\frac{\pm i\Delta^{*}_k}{2E_k}\tan h\frac{1}{2}\beta E_k, \tag{14}$$

where the $\pm$ takes $-$ for $\nu=1,4$ and$+$for $\nu=2,3$. Applying Fourier transformation to Hamiltonian (9), and with Eqs. (13) and (14), we obtain the free energy

$$F=\frac{1}{\beta}\int_0^{\beta}\langle H\rangle d\beta$$
$$=-\frac{4}{\beta}\sum_k\ln\cos h\frac{1}{2}\beta E_k-2\mu N+H_0, \tag{15}$$

where $H_0=N[\lambda(\delta-1)+J(|\Delta_x|^2+|\Delta_y|^2)]$, and $\beta=T^{-1}$.

The relative phase factor between Δ_x and Δ_y is introduced as

$$\Delta_y=\Delta_x\exp i\theta. \tag{16}$$

By minimizing the free energy, we can determine $\theta=\pm\pi/2$. Therefore the RVB order parameter can be rewritten as

$$\Delta_k=2J\Delta_x[\sin(k_xa)\pm i\sin(k_ya)]. \tag{17}$$

Obviously, the above gap function has a $k_x\pm ik_yp$-wave symmetry.

With Eqs. (13) and (14), we obtain the self-consistent equations of the mean-field order parameters $\Delta(=\Delta_x)$ and the chemical potential satisfies the following equations:

$$\delta=\frac{2}{N}\sum_k \frac{\epsilon_k}{E_k}\tanh\frac{1}{2}\beta E_k-1, \tag{18}$$

$$1=\frac{2J}{N}\sum_k \frac{(\sin^2 k_x a+\sin^2 k_y a)}{E_k}\tan h\frac{1}{2}\beta E_k. \tag{19}$$

Solving the above equations in the limit $\Delta\to 0$, the pre-pair temperature T_{RVB} below which $\Delta\neq 0$ can be derived numerically.

In order to determining the superconductivity transition temperature T_{SC}, we need to know when the phase coherence among the RVB pairs occurs. The physical electrons are represented by the operator $d^\dagger_{i,\nu}=a^\dagger_{i,\nu}b_i$, and superconducting order parameter is given by

$$\langle B^\dagger_{ij}\rangle\approx\langle b_i b_j\rangle\cdot\Delta^*. \tag{20}$$

Thus the superconducting state is a state with both $\langle b_i b_j\rangle\neq 0$ and $\Delta^*\neq 0$. With a simple mean-field approximation, the slave-boson degrees of freedom can be described in our case as

$$H=-t\sum_{\langle i,j\rangle\nu}(\langle a^\dagger_{i,\nu}a_{j,\nu}\rangle b_i b^\dagger_j+\text{H.c.})-\mu\sum_i b^\dagger_i b_i$$

$$=\sum_k b^\dagger_k b_k[\epsilon_b(k)-\mu], \tag{21}$$

with

$$\epsilon_b(k)=-t\gamma_k\sum_\nu \langle a^\dagger_{i+a,\nu}a_{i,\nu}\rangle. \tag{22}$$

Then the Bose-Einstein condensation (BEC) temperature T_{BEC} is determined by

$$\delta=\frac{1}{N}\sum_{k\neq 0}\frac{1}{\exp\{[\epsilon_b(k)-\epsilon_b(0)]\beta_{BEC}\}-1}, \tag{23}$$

with $\beta_{BEC}=T^{-1}_{BEC}$. Below T_{BEC} the slave bosons undergo Bose-Einstein condensation and $\langle b_i\rangle\neq 0$.

The numerically calculated phase diagram from Eqs. (18), (19), and (23) for $t=6J$ is shown in Fig. 1. T_{RVB} decreases to zero with increasing δ, while T_{BEC} decreases to zero with decreasing δ. Curves T_{RVB} and T_{BEC} intersect each other. In the area above T_{RVB}, the electrons do not form RVB pairs, the system should behave as a normal Fermi liquid. While in the area under the envelop formed by the two curves, the fermions form RVB pairs with p-wave symmetry and the slave bosons condense. Therefore p-wave SC, a quantum ordered liquid state, occurs in this region. In the region under T_{RVB} but above T_{BEC} (to the left of the curves' intersection), RVB pairs without phase coherence exist in the sense that the slave bosons do not condense. This phase may corresponds some kind of anomaly Fermi liquid state, similar to that of the high-T_c superconductors.

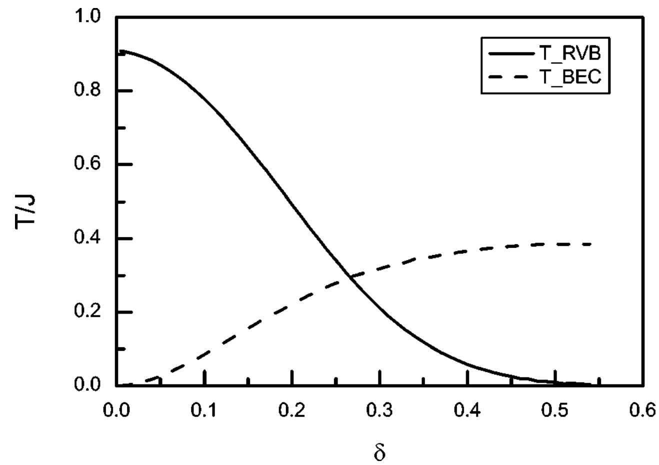

FIG. 1. The mean-field phase diagram for $t=6J$. The solid line represents pre-pair temperature T_{RVB}, below which the p-wave RVB pairs appear. The dotted line is BEC temperature T_{BEC}, below which the slave bosons undergo BEC. δ is the density of doping holes.

To show the symmetry of the pairing clearly, we study the mean-field ground state

$$|GS\rangle=\prod_k (u_k+v_k a^\dagger_{k,1}a^\dagger_{k,4})(u_k-v_k a^\dagger_{k,2}a^\dagger_{k,3})|0\rangle, \tag{24}$$

with

$$u_k^2=\frac{1}{2}\left(1+\frac{\epsilon_k}{E_k}\right),$$

$$v_k^2=\frac{1}{2}\left(1-\frac{\epsilon_k}{E_k}\right). \tag{25}$$

One can notice that the total spin, orbital, and combined spin-orbital operators,

$$S^\alpha=\sum_i S^\alpha_i, \tag{26}$$

$$T^\alpha=\sum_i T^\alpha_i, \tag{27}$$

$$L^{\alpha\beta}=2\sum_i e^{iQ\cdot R_i}S^\alpha_i T^\beta_i, \tag{28}$$

generate an SU(4) Lie algebra, where α,β denote x,y,z; Q is the commensurate anti-ferromagnetic wave vector, and R_i is the coordinate of site i on the square lattice. Our Hamiltonian commutes with the 15 operators. It is easy to show that $S^z|GS\rangle=T^z|GS\rangle=L^{zz}|GS\rangle=0$. Further, the Casmir of this algebra can be constructed as

$$\hat{C}=S_z^2+T_z^2+L_{zz}^2+E_{+S}E_{-S}+E_{-S}E_{+S}+E_{+T}E_{-T}+E_{-T}E_{+T}$$
$$+E_{+L}E_{-L}+E_{-L}E_{+L}+E_{+S+T}E_{-S-T}+E_{-S-T}E_{+S+T}$$
$$+E_{+S+L}E_{-S-L}+E_{-S-L}E_{+S+L}+E_{+T+L}E_{-T-L}$$
$$+E_{-T-L}E_{+T+L}, \tag{29}$$

where

$$E_{\pm S} = \mp \frac{1}{\sqrt{2}}(S_x \pm i S_y),$$

$$E_{\pm T} = \mp \frac{1}{\sqrt{2}}(T_x \pm i T_y),$$

$$E_{\pm L} = \mp \frac{1}{\sqrt{2}}(L_{xx} \pm i L_{yy}),$$

$$E_{\pm S \pm T} = [E_{\pm S}, E_{\pm T}]. \tag{30}$$

Acting the Casmir onto the ground state we readily have $\hat{C}|GS\rangle = 0$. Therefore the ground state is an SU(4) singlet with zero spin, orbital, and combined spin-orbital eigenvalues. This result is also correct for a single pair state $B^{\dagger}_{ij}|0\rangle$. However, due to the existence of the additional internal degrees of freedom, i.e., the local orbits, the parity of the electron pairs must be odd, which in our case possesses the $k_x \pm i k_y p$-wave symmetry.

In summary, a strongly correlated electron model with orbital degeneracy defined in a square lattice is studied. By introducing the short-ranged RVB order parameter, the mean-field phase diagram of the system is obtained. It is shown that the RVB electron pairs are spin-singlet, orbital-singlet, and combined SU(4) singlet objects. However, the gap function of the electron pairs in the momentum space possess a $k_x \pm i k_y$-type p-wave symmetry. Therefore our model provides a simple example which shows p-wave SC without ferromagnetic fluctuation.

ACKNOWLEDGMENTS

One of the authors (Y.W.) acknowledges F. C. Zhang for stimulating discussions. This work was supported by NSFC under Grant No. 90103024.

[1] Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J. G. Bednorz, and F. Lichtenberg, Nature (London) **372**, 532 (1994).
[2] K. Ishida, H. Mukuda, Y. Kitaoka, K. Asayama, Z. Q. Mao, Y. Mori, and Y. Maeno, Nature (London) **396**, 658 (1998).
[3] M. Mukuda, K. Ishida, Y. Kitaoka, K. Asayama, R. Kanno, and M. Takano, Phys. Rev. B **60**, 12 279 (1999).
[4] J. A. Duffy, S. M. Hayden, Y. Maeno, Z. Mao, J. Kulda, and G. J. Mcintyre, Phys. Rev. Lett. **85**, 5412 (2000).
[5] M. Sigrist and M. E. Zhitomirsky, J. Phys. Soc. Jpn. **65**, 3452 (1996).
[6] G. Baskaran, Physica B **223**, 490 (1996).
[7] K. Machida, M. Ozaki, and T. Ohmi, J. Phys. Soc. Jpn. **65**, 3720 (1996).
[8] S. S. Saxena, P. Agarwal, K. Ahilan, F. M. Grosche, R. K. W. Haselwimmer, M. J. Steiner, E. Pugh, I. R. Walker, S. R. Julian, P. Monthoux, G. G. Lonzarich, A. Huxley, I. Sheikin, D. Braithwaite, and J. Flouquet, Nature (London) **406**, 587 (2000).
[9] C. Pfleiderer, M. Uhlarz, S. M. Hayden, R. Vollmer, H. v. Löhneysen, N. R. Bernhoeft, and G. G. Lonzarich, Nature (London) **412**, 58 (2001).
[10] K. I. Kugel and D. I. Khomskii, Usp. Fiz. Nauk. **136**, 621 (1982) [Sov. Phys. Usp. **25**, 231 (1982)].
[11] Y. Q. Li, D. N. Shi, M. Ma, and F. C. Zhang, Phys. Rev. Lett. **81**, 3527 (1998).
[12] G. Santoro *et al.*, Phys. Rev. B **55**, 16 168 (1997).
[13] G. Santoro *et al.*, Phys. Rev. Lett. **83**, 3065 (1999).
[14] G. Santoro *et al.*, Phys. Rev. B **53**, 828 (1996).
[15] G. Santoro *et al.*, Phys. Rev. Lett. **55**, 4039 (1995).
[16] P. Paul *et al.*, J. Am. Chem. Soc. **116**, 4145 (1994).
[17] J. Choi *et al.*, Phys. Rev. Lett. **80**, 1328 (1998).
[18] G. M. Zhang and S. Q. Shen, Phys. Rev. Lett. **87**, 157201 (2001).
[19] D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).
[20] P. W. Anderson *et al.*, Phys. Rev. Lett. **58**, 2790 (1987).
[21] G. Kotliar and J. Liu, Phys. Rev. B **38**, 5142 (1988).