Interplay of the superconducting state and orbital antiferromagnetic state of the high-temperature cuprate superconductors

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The phase diagram of the cuprates is studied in the vicinity of the tetracritical point arising due to the interplay of superconducting (SC) and orbital antiferromagnetic (OAF) ordered states. SC pairing from repulsion results in the two-component order parameter with relative phase associated with OAF order. There are two SC phases, with and without orbital currents, inside the SC dome. The weak pseudogap is associated with an OAF ordered state whereas the strong one exhibits developed fluctuations of the order parameter and enhanced diamagnetism inside this state.

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It is believed that a competition of the antiferromagnetic (AF) and superconducting (SC) pairing channels determines the typical phase diagram of quasi-two-dimensional (2D) doped cuprate compounds.[1–3] The SC dome arises in a region of doping, $x_* < x < x^*$, and the SC transition temperature T_C has its maximum value inside this region at $x = x_{opt}$. The weak pseudogap state in underdoped ($x \lesssim x_{opt}$) cuprates manifests itself at $T_C < T < T_w^*$ where T_w^* is a decreasing function of doping corresponding to a broad peak in the T-dependence of magnetic susceptibility. The strong pseudogap becomes apparent in the Nernst effect at $T_C < T < T_{str}^*$ where $T_{str}^* < T_w^*$ and can be associated with a rise of incoherent SC pairs[4] or unbound vortex-antivortex pairs.[5] The SC gap has some nodes on the Fermi surface and, just as the pseudogap, can be referred to as either d-wave or extended s-wave symmetry.[6]

We report a phase transition inside the SC dome resulting from SC pairing at large momentum under repulsive interaction. We argue that such a pairing leads naturally to a coexistence of SC and orbital AF ordered states and can qualitatively explain the principal features of the phase diagram of the cuprates.

Doping suppresses long-range spin AF ordering rapidly but, up to $x \approx x_{opt}$, there exists a short-range order as fluctuations of the spin-density wave (SDW).[3] Because of a lack of SDW nodal points there is an additional interruption of spin correlations due to electron-phonon interaction (EPI). On the contrary, orbital antiferromagnetic (OAF) order[7] results in an insulating gap with some nodal points and turns out to be more stable with respect to both doping and EPI.

Long-range OAF insulating order as a charge current density wave with $d_{x^2-y^2}$ symmetry (DDW) can compete with d-wave SC order in a rather wide doping region,[2] and the pseudogap state in the cuprates can be referred to as either long-range (*hidden*)[2] or short-range[8] DDW order. OAF state with a commensurate AF vector (the toroidal magnetic state[9] or the staggered flux state[10]) in 2D cuprates manifests itself as staggered current circulations inside a d-wave SC state.[11] There is a compatibility of the OAF and SC pairing with the same large incommensurate momentum being a remnant of the insulating spin AF state creating superconductivity under doping.

Singlet SC pairing with a large momentum turns out to be dominant under the condition that the Fermi surface shows the mirror nesting feature.[12] This pairing channel results in a periodic orbital structure of the order parameter defined inside a domain of kinematical constraint in the momentum space. Such a domain, in contrast to that arising in the case of Fulde-Ferrel-Larkin-Ovchinnikov nonuniform SC state,[13] maps the crystal symmetry and, due to mirror nesting, does not eliminate the logarithmic singularity from the self-consistency equation.

Repulsive pairing interaction results in the two-component SC order parameter with necessity.[14] Complex components $\Psi_s (s=1,2)$ of the order parameter minimize the free energy which, in the case of a spatially homogeneous system near the phase transition, can be expressed in the form of the Landau expansion in powers of the order parameter:[15]

$$F_1 = \sum_{ss'} A_{ss'} \Psi_s^* \Psi_{s'} + \frac{1}{2} \sum_{ss'tt'} B_{ss'tt'} \Psi_s^* \Psi_{s'}^* \Psi_t \Psi_{t'}. \qquad (1)$$

The matrix elements $A_{ss'}$ and $B_{ss'tt'}$ have three and five independent components, respectively, and depend on the temperature and doping. The free energy (1) is invariant under SU(2) transformations of the components Ψ_s. One can suppose that such a transformation is performed to diagonalize the first term in Eq. (1): $A_{ss'} = A_s \delta_{ss'}$.

The mean-field transition temperature $T_s(x)$ should be determined from the condition that $\det A_{ss'} = 0$. The coefficients A_s vanish when SC order disappears[15] and one can assume that $A_s \sim \tau_1$ where $\tau_1 = (T_s - T)/T_s$. The matrix $B_{ss'tt'}$ can be taken at $T_s(x)$ and is a function of doping only.

The components of the order parameter can be written in the form $\Psi_1 = \psi_1$, $\Psi_2 = \psi_2 e^{i\beta}$, where ψ_1 and ψ_2 are the absolute values of the components and β is their relative phase. At $T > T_s$, the trivial solution $\Psi_s = 0$ corresponds to the minimum value of the free energy whereas the nontrivial one arises in the opposite case. We restrict ourselves to a special case when $\psi_1 = \psi_2 \equiv \psi$. Such a simplification turns out to be sufficient to classify all principal peculiarities of the phase diagram.

One can rewrite Eq. (1) as

$$F_1 = a_1\psi^2 + (B + 2C\cos\beta + D\cos\beta^2)\psi^4/2, \qquad (2)$$

where $a_1 = A_1 + A_2 \equiv -\kappa_1\tau_1$, $\kappa_1 > 0$, and the coefficients B, C, and D can be expressed in terms of the elements $B_{ss'tt'}$. Here B and D are positive by definition. For the sake of simplicity, we assume that $C > 0$ as well.

At $T < T_s$, a nontrivial solution minimizing the free energy (2) corresponds to $\psi \neq 0$ and $\beta = \pi$ when $C \geqslant D$. In the opposite case $C \leqslant D$ the relative phase of the components of the order parameter is determined by the equality $\cos\beta = -C/D$. The equation $C(x) = D(x)$ determines a doping level $x = x_0$ corresponding to a qualitative change of SC order.

In a small vicinity of the point $x = x_0$, the ratio $C/D \equiv c(x)$ can be represented as $c(x) \approx 1 + c'(x_0)(x - x_0)$. We assume that, in the case when $c'(x_0) > 0$, doping region $x > x_0$ corresponds to the relative phase $\beta = \pi$. Then, at $x < x_0$, the relative phase $\beta < \pi$. One can define the order parameter which differentiates the phases with $\beta = \pi$ (π-phase) and $\beta \neq \pi$ (β-phase) as $\alpha = \pi - \beta$ ($\alpha = 0$ at $x > x_0$ and $0 < \alpha < \pi/2$ at $x < x_0$). Near the point $x = x_0$ of the phase transition, the order parameter α introduced in such a way is small and one can obtain an expansion of the free energy (2) in even powers of α. In thermal equilibrium, we have $\alpha^2 = 2c'(x_0)(x - x_0)$ when $x < x_0$. Thus, one can obtain the difference between the values of the free energy corresponding to the π and β phases, $F_\pi - F_\beta \sim \tau_1^2(x - x_0)^2$.

In the case of the π-phase, repulsive pairing interaction results in the real order parameter with the components of opposite sign.[14] The relative phase $\beta \neq \pi$ corresponds to the solution of the self-consistency equation with complex coherence factors and makes possible a rather obvious interpretation. Indeed, a change in the phase of the destruction operator of an electron with spin σ on a lattice site with radius-vector $\boldsymbol{n}$ can be associated with a magnetic field,

$$\hat{c}_{\boldsymbol{n}\sigma} \to \hat{c}_{\boldsymbol{n}\sigma} \exp[i(e/\hbar c)\boldsymbol{A}(\boldsymbol{n})\boldsymbol{n}], \qquad (3)$$

where $\boldsymbol{A}$ is the vector potential. Therefore the phase of the order parameter in the real space representation can be written as

$$\beta(\boldsymbol{n},\boldsymbol{n}') = \pi - (e/\hbar c)[\boldsymbol{A}(\boldsymbol{n})\boldsymbol{n} + \boldsymbol{A}(\boldsymbol{n}')\boldsymbol{n}']. \qquad (4)$$

The phase (4) contains a contribution into the phase of SC condensate, $\Phi = (2e/\hbar c)\boldsymbol{A}(\boldsymbol{R})\boldsymbol{R}$, $\boldsymbol{R} = (\boldsymbol{n} + \boldsymbol{n}')/2$. It is quite natural to assume that $\boldsymbol{A}$ is due to orbital currents circulating inside a unit cell as a result of the relative motion of the pair. When $x \approx x_0$, that is near the phase transition, the change in the relative phase is small and one can represent it as

$$\alpha \approx \frac{e}{2\hbar c}\frac{\partial A_i}{\partial x_k}x_i x_k, \qquad (5)$$

where summation over repeated $i,k = 1,2$ is understood.

Within the framework of Ginzburg-Landau (GL) phenomenology, the SC order parameter should be implied as averaged over the relative motion of the pair. In the case of pairing with large momentum $\boldsymbol{K}$, the order parameter periodicity in the real space is $2\pi/K$. Therefore a mean square value of the relative phase of the components Ψ_s can be estimated as $2\alpha^2 \approx (\pi eH/2\hbar cK)^2$ where H is the strength of the *internal* magnetic field of circulating orbital currents. Thus the deviation of the relative phase from π leads to a rise of an additional contribution into the GL functional which has meaning of the energy of the magnetic field of circulating currents.

The magnetic field resulting in the change in the relative phase of the components of SC order parameter can be related to staggered orbital currents that arise in the SC state[11] and survive as long-range[2] or short-range[8] OAF order above T_C in the pseudogap region. In a sense, this internal field $A \sim H/K \sim \alpha$ can be considered as a gauge field linking together the SC (charge) and OAF (current) degrees of freedom similar to the fields introduced in GL functional, for example, in the bosonic version of the spin-charge separation scheme.[16] Thus in a spatially homogeneous system in the absence of an *external* magnetic field, a rise of the relative phase change α results in an additional contribution into the free energy following from the gradient term of the GL functional.[15] One can represent this contribution as $F_{12} = b_{12}\psi^2\alpha^2$ considering $b_{12}(x) > 0$ phenomenologically.

One can consider α as an order parameter associated with the OAF insulating state. Therefore, another contribution being Landau free energy of this state,

$$F_2 = a_2\alpha^2 + b_2\alpha^4/2, \qquad (6)$$

should be added into the free energy of the system. Here, b_2 is a positive function of doping and the coefficient a_2 vanishing at the mean-field OAF transition temperature $T_d(x)$, under the condition that $|\tau_2| \ll 1$, can be written as $a_2 = -\kappa_2\tau_2$ where $\kappa_2 > 0$, $\tau_2 = (T_d - T)/T_d$. The magnetic field energy of circulating currents, being also proportional to α^2, can be included into the term $a_2\alpha^2$. In the absence of OAF ordering, a rise of the thermally stable SC β-phase turns out to be impossible and, in such a case, the condition $C(x) = D(x)$ should be understood as the equation which determines the lower boundary x_* of the SC dome with only one possible π-phase.

The free energy, up to the terms of the fourth order, can be written as

$$F = a_1\psi^2 + a_2\alpha^2 + \frac{1}{2}b_1\psi^4 + b_{12}\psi^2\alpha^2 + \frac{1}{2}b_2\alpha^4. \qquad (7)$$

The condition that $a_1(T,x) = 0$ determines the mean-field temperature $T_s(x)$. Therefore taking into account that $a_1 = -\kappa_1\tau_1$ one can assume that the expansion (7) is valid at $|\tau_1| \ll 1$. Both κ_1 and b_1 are positive functions of doping. At small x, OAF order dominates decreasing rapidly when x increases. Therefore one can assume that there is an intersection of the functions $T_d(x)$ and $T_s(x)$ at a point corresponding to the doping level $x = x_0$ as it is shown in Fig. 1. It should be emphasized that the expression (7) represents the free energy inside the relatively small region of the phase diagram where both $|\tau_1| \ll 1$ and $|\tau_2| \ll 1$. Therefore the extension of the lines shown in Fig. 1 outside this region must be considered as reasonably simulated.

Minimization of the free energy (7) leads to some essential conclusions relating to the phase diagram. When $T > \max(T_d, T_s)$, the free energy exhibits a minimum at $\psi = 0$,

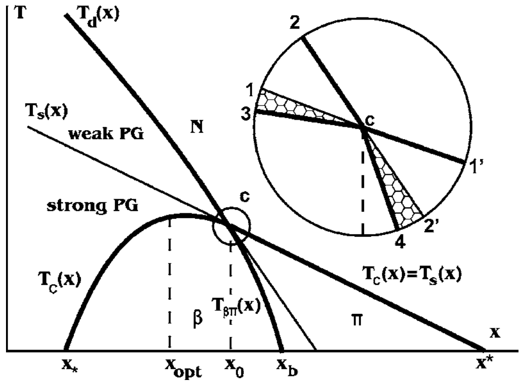

FIG. 1. Schematic phase diagram of doped cuprate compound. Inset shows the phase diagram in the vicinity of the tetracritical point *c*.

$\alpha=0$ (the sector $2c1'$ in the inset in Fig. 1) corresponding to the normal (N) phase. A piece of the boundary of this sector, $2c$, is a line of the phase transition from the N to OAF phase ($\psi=0$, $\alpha=-a_2/b_2$) existing inside the sector $2c3$. The lower boundary of this sector, $c3$, determined by the equation $b_2a_1=b_{12}a_2$, is situated below $T_s(x)$. This is a line of the phase transition from OAF to SC β-phase thus $c3$ can be attributed to the temperature of the SC transition, $T_C(x)$, when $x<x_0$. The line $c1'$ in Fig. 1 corresponds to the SC phase transition from N to SC π-phase and, in the case when $x>x_0$, $T_C(x)$ coincides with the mean-field temperature $T_s(x)$. The boundary separating two SC (β and π) phases corresponds to the phase transition temperature $T_{\beta\pi}$ which turns out to be below $T_d(x)$ in the doping region $x>x_0$. Thus the domains of the phase diagram in which the SC β- and SC π-phases exist are the sectors $3c4$ and $4c1'$ (Fig. 1), respectively. We consider the SC β-phase as a phase in which OAF order coexists with SC π order. Each of four stable phases discussed here corresponds to a minimum of the free energy (7). The intersection point c of the functions $T_d(x)$ and $T_s(x)$, being also a convergent point of four lines of the phase transitions, can be referred to as a *tetracritical* point.[17]

In Fig. 2, we present schematically a picture of free energy isolines $F(\psi,\alpha)=\text{const}$ for each of the above-mentioned sectors. It should be noted especially that both in OAF and SC π states (the sectors $2c3$ and $4c1'$, respectively) of the phase diagram there exist the domains in which, together with a minimum, the free energy (7) exhibits a *saddle point*. Inside the sector $1c3$ belonging to the OAF ordered state the free energy has a minimum with respect to α at $\psi=0$ whereas a saddle point arises at $\alpha=0$ and the value of ψ corresponding to the equilibrium order in π-phase, $\psi^2=-a_1/b_1$. In a small vicinity of the tetracritical point, the values of the free energy corresponding to the minimum and the saddle point are close to each other. Therefore one can expect an increase in the probability of fluctuations giving rise to incoherent long-living quasistationary states (QSS) of SC pairs with the relative phase π in the OAF state.[18] One can imagine the decay of such QSS as a creation of unbound pairs of opposite-sign orbital current circulations which can be also treated as unbound vortex-antivortex pairs.[5] Thus, inside the sector $1c3$, the pairs with a relative phase β can be considered as intermediate states arising during π-pair decay.

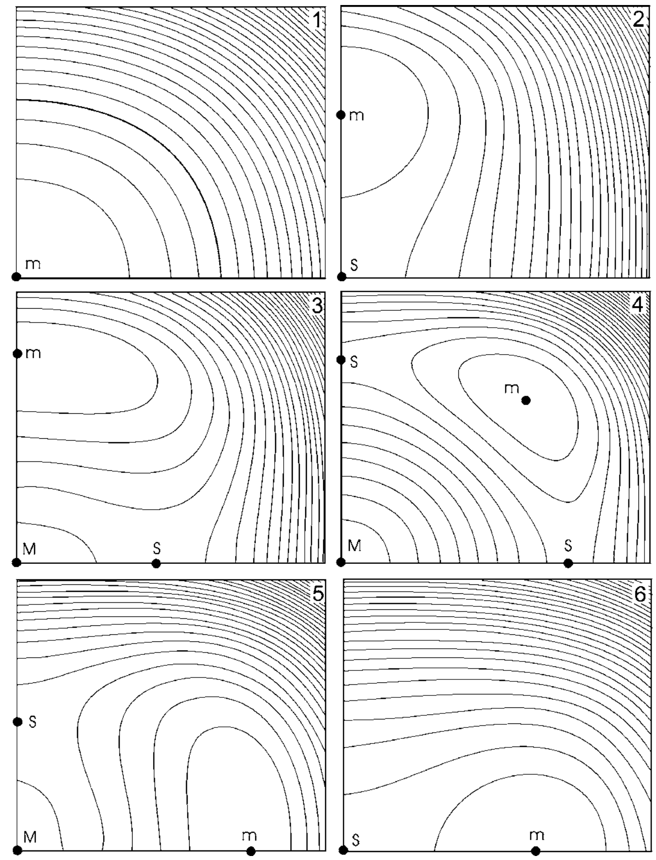

FIG. 2. Outline of ψ (horizontal axis)-α (vertical axis) topology of the free energy. Numbers from 1 to 6 correspond to the sectors $1'c2$, $2c1$, $1c3$, $3c4$, $4c2'$, and $2'c1'$ in the inset in Fig. 1.

The temperature $T_s(x)$ at $x<x_0$ ($1c$ in Fig. 1) has meaning of an upper boundary of the region with developed fluctuations of the absolute value of the SC order parameter and should not be associated with a phase transition. One can expect a significant enhancement of the Nernst effect[19] in this region therefore the line $1c$ can be identified with the upper (crossover) boundary of the strong pseudogap region, $T_s(x)\approx T^*_{str}$ when $x<x_0$. It should be noted that this pseudogap, perhaps, can penetrate into an extremely low-doping region, $x<x_*$.

Inside the sector $4c2'$, the free energy exhibits a minimum at $\psi^2=-a_1/b_1$, $\alpha=0$ and a saddle point at $\psi=0$, $\alpha^2=-a_2/b_2$ (Fig. 2) with the values close to each other. Thus, in the stable SC π-phase, one can expect an enhancement of fluctuations in the form of QSS of circulating orbital currents. The decay of such QSS is realized via intermediate states of the SC β-phase.

At $x_0<x<x^*$ (generally speaking, x_0 is greater than the optimal doping, $x_0>x_{opt}$), the mean-field temperature $T_s(x)$ is the temperature of the phase transition from N into SC π-phase, $T_s(x)=T_C(x)$. In the case of doping level close enough to x_0 ($x_0<x<x_b$, Fig. 1), after the BCS-like phase transition $N\rightarrow\text{SC}\pi$, the system, at first, goes through the region of developed OAF fluctuations (the sector $4c2'$) and next experiences the second phase transition (the line $4c$) from SC π into SC β phase. This *second order* phase tran-

sition might be detected in an appropriate heat capacity experiment.

The phenomenological scheme of competing SC and OAF ordered states allows us to consider the existence of an enhanced diamagnetism recently observed in the pseudogap state on the cuprate compound Bi2212.[20]

Since the equilibrium absolute value ψ of the order parameter equals zero in the α-phase, to consider a magnetic response the free energy must be supplemented by the term F_m taking into account the coupling between the OAF order and the external magnetic field. Such a term includes the invariants, L^2B^2 and $(\boldsymbol{LB})^2$, where $\boldsymbol{L}$ has meaning of the difference between the magnetizations of AF sublattices,[17] $\boldsymbol{B}$ is the magnetic induction. In a 2D system of cuprate layers, $\boldsymbol{L}$ is always normal to a layer, therefore, the OAF order parameter turns out to be a scalar, $L\sim\alpha$ and one can obtain $F_m=\nu\alpha^2B^2$. Here, $\nu=\nu_1+\nu_2\cos^2\vartheta$, ν_1 and ν_2 are phenomenological parameters, and ϑ is the angle between $\boldsymbol{B}$ and the normal to a cuprate layer. The magnetic susceptibility of the α-phase is given by $\chi^{(\alpha)}\approx\chi+(2\nu/b_2)a_2$, where χ is the paramagnetic susceptibility of the normal phase. One can see that diamagnetic response arises at $T<T_d(1-b_2\chi/2\nu\alpha')$.

The interplay of the OAF and SC ordered states leads quite naturally to the principal observable features of the phase diagram of the cuprates including, in particular, the shape of the SC dome, weak and strong pseudogap states, developed fluctuations of the order parameter, and enhanced diamagnetism in the strong pseudogap regime. Apparently, there is no strong evidence of the OAF order in the cuprates because it is difficult to detect a very weak magnetic field associated with orbital currents. We believe that, if the transition between two SC phases predicted here were detected, it might be one more indirect evidence in favor of the concept[2] of hidden OAF order and, also, an argument in behalf of the SC pairing with large momentum under repulsion.

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[1] M. Vojta, Y. Zhang, and S. Sachdev, Phys. Rev. B **62**, 6721 (2000).
[2] S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B **63**, 094503 (2001).
[3] P. A. Lee, N. Nagaosa, and X-G. Wen, cond-mat/0410445 (unpublished).
[4] V. J. Emery and S. A. Kivelson, Nature (London) **374**, 434 (1995).
[5] M. Franz, Z. Tešanović, and O. Vafek, Phys. Rev. B **66**, 054535 (2002).
[6] G. M. Zhao, Phys. Rev. B **64**, 024503 (2001); B. H. Brandow, *ibid.* **65**, 054503 (2002).
[7] B. I. Halperin and T. M. Rice, Solid State Phys. **21**, 115 (1968).
[8] X-G. Wen and P. A. Lee, Phys. Rev. Lett. **76**, 503 (1996).
[9] V. L. Ginzburg, A. A. Gobatsevich, Yu. V. Kopaev, and B. A. Volkov, Solid State Commun. **50**, 339 (1984).
[10] J. B. Marston and I. Affleck, Phys. Rev. B **39**, 11538 (1989).
[11] D. A. Ivanov, P. A. Lee, and X-G. Wen, Phys. Rev. Lett. **84**, 3958 (2000).
[12] V. I. Belyavsky and Yu. V. Kopaev, Phys. Rev. B **67**, 024513 (2003); Phys. Lett. A **322**, 244 (2004).
[13] P. Fulde and R. A. Ferrel, Phys. Rev. **135**, A550 (1964); A. I. Larkin and Yu. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **47**, 1136 (1964) [Sov. Phys. JETP **20**, 762 (1964)].
[14] V. I. Belyavsky, Yu. V. Kopaev, and S. V. Shevtsov, J. Supercond. Novel Magn. **17**, 297 (2004).
[15] V. I. Belyavsky and Yu. V. Kopaev, Zh. Eksp. Teor. Fiz. **127**, 45 (2005) [JETP **100**, 39 (2005)].
[16] V. N. Muthukumar and Z. Y. Weng, Phys. Rev. B **65**, 174511 (2002).
[17] L. D. Landau and E. M. Lifshitz, *Course of Theoretical Physics, Vol. 5: Statistical Physics*, 4th ed. (Butterworth, London, 1999).
[18] V. I. Belyavsky, Yu. V. Kopaev, Yu. V. Togushova, and S. V. Shevtsov, Zh. Eksp. Teor. Fiz. **126**, 672 (2004); [JETP **99**, 585 (2004)].
[19] Y. Wang, S. Ono, Y. Onose, G. Gu, Y. Ando, Y. Tokura, S. Uchida, and N. P. Ong, Science **299**, 86 (2003).
[20] Y. Wang, L. Li, M. J. Naughton, G. D. Gu, S. Uchida, and N. P. Ong, cond-mat/0503190 (unpublished).