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LETTER TO THE EDITOR

Pairing-fluctuation effect in d-wave superconductivity

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Abstract
On the basis of a ladder-diagram approximation, we study the pairing-fluctuation effect in d-wave superconductivity. The single particles and pairs are treated on an equal footing. In the superconducting state, the predominant pairing fluctuation is due to the excitation of pairs to the states of the Goldstone mode. These bosonic degrees of freedom are relevant to the pseudogap physics in high-T_c cuprates. The Green function of electrons is obtained as an analytic solution to a cubic equation. The superconducting order parameter and the transition temperature are substantially reduced from the values of the mean-field theory. The calculated phase boundary of the superconductivity can reasonably describe the experiment results for cuprates.

The pairing-fluctuation effect plays an important role in describing the superconductivity of a quasi-two-dimensional (quasi-2D) superconductor with low carrier density [1], as it prohibits off-diagonal long-range ordering in systems of dimensions $\leqslant 2$ [2]. The superconducting order parameter and thereby the transition temperature T_c can be considerably reduced from the values given by the mean-field theory (MFT). For underdoped high-T_c cuprates (HTC), Emery and Kivelson have argued that the long-range classical phase fluctuation can substantially suppress the transition temperature T_c [3]. Above T_c, pairing becomes local without long-range phase coherence. On the other hand, since there are preformed pairs above T_c, the superconductivity below T_c can be viewed as a consequence of Bose–Einstein condensation (BEC) [4–6]. Along with this approach, much effort has been devoted to investigation of the crossover from the weak-coupling BCS superconductivity to the BEC of bound pairs [7–18]. Most of the work has been performed for s-wave pairing because of its computational simplicity.

Here we note that according to the general theory of Goldstone *et al* [19] there exists a Goldstone mode in the broken-symmetry state of systems without long-range interaction. Since the states of this mode are the lowest excited states for the pairs, the excitations of pairs to these states are the most predominant fluctuations. For quasi-2D systems at finite temperature, the fluctuations can be equally significant as the mean-field ordering. Because the Goldstone mode coexists with the coherent pairing and may not be regarded as a perturbation in quasi-2D systems, treatment of the single particles and the collective modes on an equal footing is therefore desirable.

In this paper we intend to present a Green function approach to treat the pairing-fluctuation effect. In the present approach, the Green functions of the single particles and the pairs are self-consistently determined by a number of coupled integral equations. We find that BEC from single pairs begins to occur at T_c, but below T_c, with the condensation taking place, the single pairs begin to move collectively. Even at the ground state there remains zero-point motion. These bosonic degrees of freedom are relevant to the pseudogap physics in cuprates. For details of this work readers are referred to [20].

The Hamiltonian of the electron system is given by

$$H = \sum_{k\alpha} \xi_k c^\dagger_{k\alpha} c_{k\alpha} + \frac{1}{N} \sum_{kk'q} v_{kk'} p^\dagger(k, q) p(k', q) \tag{1}$$

where $c^\dagger_{k\alpha}$ ($c_{k\alpha}$) is the creation (annihilation) operator for electrons with momentum k and spin α, $\xi_k = -2t(\cos k_x + \cos k_y) - 2t_z \cos k_z - \mu$ with μ the chemical potential, N the total number of lattice sites, $v_{kk'} = -v\eta_k\eta_{k'}$ with $\eta_k = \cos k_x - \cos k_y$, and $p(k, q) = c_{-k+q/2\downarrow} c_{k+q/2\uparrow}$ is the pair operator. To take into account the constraint of no double occupation on the same site by the t–J model, the hopping integrals t and t_z are assumed to be proportional to the hole concentration δ, e.g. $t = t_0\delta$ with t_0 a constant [21]. For the quasi-2D system, $t_z/t \ll 1$ is supposed. This model has been adopted by a number investigators for studying d-wave superconductivity as well as the pseudogap phenomenon in cuprates [13–15, 22].

In Nambu's representation, the Green function $G(k, z_n)$ of the electrons is given by

$$G(k, z_n) = [z_n - \xi_k\sigma_3 - \Sigma(k, z_n)]^{-1} \tag{2}$$

where $z_n = \mathrm{i}(2n+1)\pi T$, n is an integer, T the temperature and σ the Pauli matrix. Throughout this paper we use the units in which $\hbar = k_B = 1$. To express the self-energy, we first note that the off-diagonal part comes from the averaged boson fields of momentum $q = 0$. In the superconducting state, $\langle p(k, 0)\rangle$ is a macroscopic quantity compared with all other pair fields elsewhere. Therefore, the predominant contributions are the static mean field

$$\Sigma_{12}(k, z_n) = \frac{1}{N} \sum_{k'} v_{kk'} \langle p(k', 0)\rangle \equiv \Delta_k. \tag{3}$$

For our uniform system, we suppose Δ_k is real. The quantity $\Delta_k \equiv \Delta\eta_k$ should be differentiated from that of the MFT since the fluctuation effect is under consideration in the present Green function. Secondly, we take into account the pair fluctuation terms $q \neq 0$ of the interaction in the diagonal part. By the ladder-diagram approximation, the diagonal part of the self-energy is given by

$$\Sigma_{\mu\mu}(k, z_n) = -\frac{T}{N} \sum_{qm} v^2 \eta^2_{k-q/2} G_{\bar{\mu}\bar{\mu}}(k - q, z_n - Z_m) \Pi_{\mu\mu}(q, Z_m) \tag{4}$$

where $Z_m = \mathrm{i}2m\pi T$, m is an integer, $\mu = 1, 2$ with $\bar{1} = 2$ and $\bar{2} = 1$, and the pair propagator $\Pi(q, Z_m)$ is given by

$$\Pi(q, Z_m) = [1 + v\chi(q, Z_m)]^{-1} \chi(q, Z_m) \tag{5}$$

where Π and χ are 2×2 matrices, with the elements of χ defined by

$$\chi_{\mu\nu}(q, Z_m) = \frac{T}{N} \sum_{kn} \eta^2_k G_{\mu\nu}(k + q/2, z_n + Z_m) G_{\bar{\nu}\bar{\mu}}(k - q/2, z_n). \tag{6}$$

The chemical potential μ is determined by

$$\frac{2T}{N}\sum_{kn} G_{11}(k, z_n)\mathrm{e}^{z_n\eta} = 1 - \delta \tag{7}$$

where η is an infinitesimal positive number. These equations (2)–(7) form the closed system that self-consistently determines the Green functions.

Two points about the present formalism need to be emphasized. First, the existence of the Goldstone mode in the superconducting state requires that the pair susceptibility $\chi(q, Z_m)$ should satisfy the condition [19]

$$\det|1 + v\chi(0, 0)| = 0. \tag{8}$$

This equation is exactly consistent with equation (3). Any improper treatment of off-diagonal self-energy leads to violation of this consistency. At T_c, equation (8) reduces to the Thouless criterion [23]. Secondly, because of equation (8), the pair propagator $\Pi_{\mu\mu}(q, Z_m)$ has a singularity at $q \to 0$ and $Z_m = 0$, and thereby the diagonal self-energy takes into account the predominant fluctuation effect.

It is a tremendous task to numerically solve equations (2)–(7) because many multi-dimensional integrals over the momentum and the summation over the Matsubara frequency need to be computed in each iteration. However, since $\Pi(q, Z_m)$ is strongly peaked with a divergence at $q \to 0$ and $Z_m = 0$, the diagonal self-energy can be approximately given by [14, 24]

$$\Sigma_{\mu\mu}(k, z_n) \approx \Gamma^2\eta_k^2 G_{\bar{\mu}\bar{\mu}}(k, z_n) \tag{9}$$

with

$$\Gamma^2 = -\frac{Tv^2}{N}\sum_{qm}{}' \Pi_{\mu\mu}(q, Z_m)\mathrm{e}^{\alpha_\mu Z_m\eta} \tag{10}$$

where $\sum'$ means the summation over q runs over small q, and the convergent factor $\mathrm{e}^{\alpha_\mu Z_m\eta}$ with $\alpha_1 = 1$ and $\alpha_2 = -1$ has been introduced. This convergent factor comes from the fact that the Green function $G_{\bar{\mu}\bar{\mu}}(k - q, z_n - Z_m)$ in the summation in equation (4) is connected with the effective interaction $v^2\Pi_{\mu\mu}(q, Z_m)$. At small q and Z_m, the pair propagator can be approximated by the collective modes. At $T < T_c$, the collective modes are sound-like waves with energy $\Omega_q \propto q$, while at T_c, $\Omega_q \propto q^2$, the excitations are single pairs. The constant Γ^2 is essentially a measure of the density of these uncondensed pairs. Γ is called the pseudogap parameter since at T_c there remains a gap in the density of states (DOS) at the Fermi energy. The q-integral in equation (10) is over a cylindrical region in the momentum space. Since Ω_q depends weakly on the out-of-plane wavenumber q_z, the integral over q_z can be taken in the range $(-\pi, \pi)$. The cut-off q_c for the in-plane wavenumber is determined such that the largest in-plane energy $\Omega_{q_c} = 2\sqrt{\Delta^2 + \Gamma^2}$, since the collective mode is meaningful only within the gap.

Now, note that two equations from the diagonal parts of equation (2) with $\Sigma_{\mu\mu}$ given by equation (9) form the closed system for determining the diagonal Green functions. By eliminating one of them, we can obtain a cubic equation for G_0 or G_3. By introducing a function $y(k, z_n)$, the Green function is obtained as

$$G(k, z_n) = [z_n + 3\Delta_k\sigma_1/(1 + y) + \xi_k\sigma_3](2 - y)/3\Gamma_k^2 \tag{11}$$

where $\Gamma_k = \Gamma\eta_k$. The function $y(k, z_n)$ is a real root of the cubic equation

$$y^3 - 3Py - 2Q = 0 \tag{12}$$

where $P = 1 + 3(\Gamma_k^2 - \Delta_k^2)/(\xi_k^2 - z_n^2)$ and $Q = 1 + \frac{9}{2}(\Gamma_k^2 + 2\Delta_k^2)/(\xi_k^2 - z_n^2)$. The explicit form of $y(k, z_n)$ reads

$$y = \begin{cases} \sqrt[3]{Q + \sqrt{D}} + \sqrt[3]{Q - \sqrt{D}}, & D > 0 \\ 2\sqrt{P}\cos(\varphi/3), & D < 0 \end{cases} \tag{13}$$

where $D = Q^2 - P^3$ and $\varphi = \arccos(Q/\sqrt{P^3})$. The boundary condition $y \to 2+3\Gamma_k^2/(\xi_k^2 - z_n^2)$ at $|z_n| \to \infty$ is useful for analytic continuation to the real frequency $z_n \to \omega + \mathrm{i}\eta$.

To describe the cuprates, we take $v/2t_0 \simeq 0.1$ and $t_z/t \simeq 0.01$ [14]. For La_2CuO, $v \simeq 0.13$ eV has been determined by experiments [25]. Therefore, our choice of $v/2t_0$ corresponds to $t_0 \simeq 0.65$ eV, which is consistent with estimates from experimental data [14, 26]. The small quantity t_z/t describes the interlayer weak coupling and gives rise to a z-freedom energy in Ω_q. This weak coupling prevents the summation over q in equation (10) from a logarithm divergence at the $q = 0$ limit and ensures a finite transition temperature T_c.

The result for T_c as a function of hole concentration δ (solid curve) is plotted in figure 1. The MFT result (with the same scale as the present theory) and the experiment data [27] are also shown for comparison. The maximum transition temperature $T_{c,Max} \approx 0.015\,75 t_0 \approx 118$ K obtained by the present calculation appears at a certain δ between 0.125 and 0.15. In the optimally doped to overdoped region, the present theory fits the experimental data very well. In the underdoped region, the reduction of T_c from the MFT value is significant; in contrast to the MFT, the present T_c increases with δ. To see how the fluctuations occurring primarily in the diagonal part of the self-energy reduce T_c, we consider the gap equation

$$\frac{vT}{N}\sum_{kn}\frac{\eta_k^2}{(\xi_k + \Sigma_3)^2 - (z_n - \Sigma_0)^2} = 1 \tag{14}$$

where the Σ are the Pauli components of the self-energy. At small δ, $|\xi_k + \Sigma_3| \propto \delta$, the predominant contribution to the denominator in equation (14) comes from the term $-(z_n - \Sigma_0)^2$. Since $|z_n - \Sigma_0| = |z_n - G_0\Gamma_k^2| > |z_n| = (2n+1)\pi T$, T_c should be reduced to keep the equality of equation (14).

There is still an obvious discrepancy between the present theory and the experiment at small δ. This may be a result of the crude treatment of the short-range pair correlations. Local pairing without long-range phase coherence is not fully taken into account in the present model. Besides this, the short-range antiferromagnetic coupling is not correctly accounted for. To describe the antiferromagnetism in cuprates at very small δ, one needs to restart with the t–J model. In addition, long-range Coulomb interaction may also take effect if there is no adequate screening.

The reduction of T_c from its MFT value stems from the fact that some of the pairs occupy low-lying excited states. As mentioned above, the density of these pairs is measured by Γ^2. In figure 2, the result for the pseudogap parameter Γ at T_c is compared with the MFT $\Delta_{MF}(T_c)$ as well as the pseudogap energy E_g determined by experiments [28]. The experimental observations indicate that E_g depends slightly on T above T_c [29]. We plot here the result for E_g to view the overall magnitudes only. The parameter Γ, similar to $\Delta_{MF}(T_c)$, decreases monotonically with δ. The larger ratio $\Gamma/\Delta_{MF}(T_c)$ at smaller δ implies a larger occupation of the uncondensed pairs. This is consistent with the more significant reduction of T_c in the underdoped region.

In figure 3 we show the numerical results for Δ and Γ as functions of T at $\delta = 0.1$. The superconducting gap opens below T_c and reaches its maximum at $T = 0$. The parameter Γ decreases with decreasing T and remains finite at $T = 0$. In the ground state, the fluctuation effect comes mainly from the zero-point motion (quantum fluctuation) of the pairs. Generally

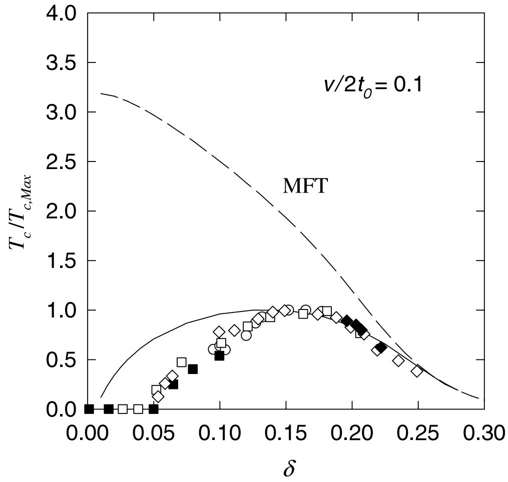

Figure 1. T_c as a function of δ. The solid and dashed curves represent the results of the present approach and the MFT respectively. The symbols indicate the experimental data for cuprates [27]: $Y_{1-x}Ca_xBa_2Cu_3O_6$ (solid squares), $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_{7-y}$ (open squares), $La_{2-x}Sr_xCuO_4$ (open diamonds), $Y_{1-x}Ca_xBa_2Cu_3O_{6.96}$ (solid diamonds) and $YBa_2Cu_3O_{7-y}$ (open circles).

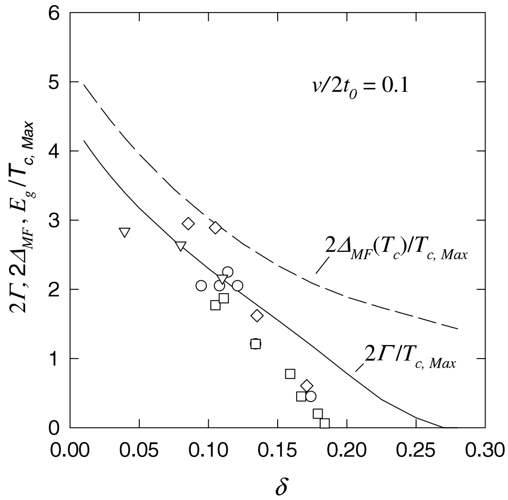

Figure 2. Pseudogap parameter Γ (solid curve) and order parameter Δ_{MF} (dashed curve, by the MFT) as functions of hole concentration δ at T_c. The symbols represent the pseudogap energy E_g for cuprates determined by experiments [28].

speaking, in a quasi-two-dimensional system, the order parameter of the broken-symmetry state can be considerably suppressed by the quantum fluctuation. This can also be confirmed by the perturbation calculations [30–33]. The Chicago group [13–15] has treated the bosonic degrees of freedom by a different ladder-diagram approach. By their theory, the uncondensed pairs are single pairs with energy $\Omega_q \propto q^2$, and complete condensation takes place at $T = 0$. This is the familiar BCS–BEC crossover picture. By the present treatment, the ladder diagrams for the self-energy are symmetric with all the Green functions renormalized. In contrast to the result of the Chicago group, the present approximation for the self-energy takes into account

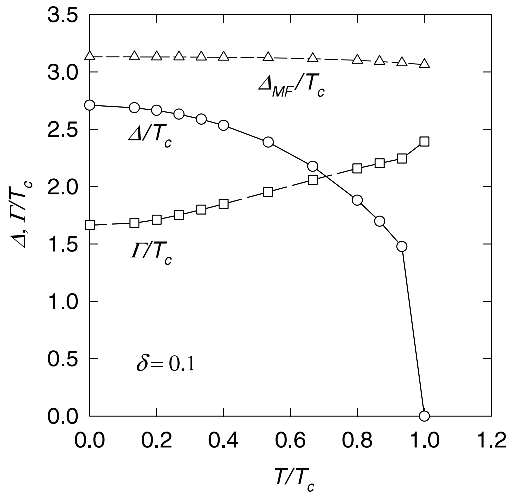

Figure 3. Superconducting order parameter Δ and pseudogap parameter Γ as functions of temperature T at $\delta = 0.1$. The order parameter Δ_{MF} given by the MFT is also plotted for comparison.

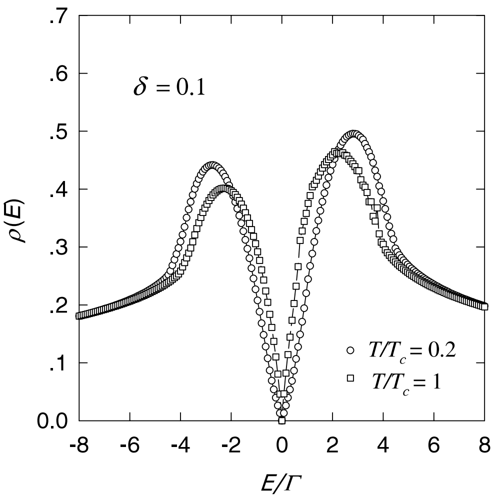

Figure 4. DOS $\rho(E)$ at $T/T_c = 0.2$ and 1. The hole concentration is $\delta = 0.1$.

the contribution from the Goldstone modes. In the ground state, especially, there are zero-point motions of these collective modes. Because the pairs occupying these modes do not contribute to the condensation, the superconducting order parameter is reduced even at the ground state.

Shown in figure 4 are the results for the dimensionless DOS of electrons,

$$\rho(E) = -2t \sum_k \mathrm{Im}\, G_{11}(k, E + \mathrm{i}\eta)/\pi N$$

at $\delta = 0.1$ and $T/T_c = 0.2$ and 1. $\rho(E)$ depends on E linearly at small E. This is in the character of the d-wave gap. In contrast to the well-known MFT, the peaks in the DOS are broadened even at $T < T_c$ due to the fluctuation effect. The reason is that the pairing fluctuation introduces a certain lifetime to the single quasiparticles. The width scales with

Γ. At T_c, $\rho(E)$ still shows the existence of the d-wave gap with a magnitude of about 2Γ. That is the pseudogap. To understand the pseudogap better, we consider the spectral function at T_c, $A(k, E) = \sqrt{(\xi_k^2 + 4\Gamma_k^2 - E^2)/(E^2 - \xi_k^2)}(E + \xi_k)/2\pi\Gamma_k^2$ which is non-zero only for $E^2 - 4\Gamma_k^2 < \xi_k^2 < E^2$, with the non-interacting delta-function peak becoming a square root singularity. Near the Fermi energy, the k-space is constrained so that the volume decreases at $E \to 0$, resulting in a suppression of DOS at the Fermi energy. This leads to the formation of a pseudogap in the DOS.

In summary, we have investigated the superconductivity in the tight-binding model with d-wave attraction. The analytic Green function is given by equation (13). The low-lying collective modes are treated as the predominant long-range pairing fluctuation in the self-energy. The pairing fluctuation results in a lifetime effect for single particles below T_c and a pseudogap in the DOS at T_c. The transition temperature is substantially suppressed from its mean-field value. The phase boundary of superconductivity given by the present theory is close to the experimental results for the cuprates.

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