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Unconventional superconductivity in two-dimensional electron systems with long-range correlations

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Properties of superfluid states of two-dimensional electron systems with critical antiferromagnetic fluctuations are investigated. These correlations are found to result in the emergence of rapidly varying in the momentum space terms in all components of the mass operator, including the gap function $\Delta(\mathbf{p})$. It is shown that a domain, where these terms reside, shrinks with the temperature, leading to a significant difference between the temperature T_c, at which superconductivity is terminated, and the temperature T^*, where the gap in the single-particle spectrum vanishes.

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The problem of high-temperature superconductivity is known to defy solution within the Fermi liquid approach. Initially it looked like it had to do with only normal states of high-T_c superconductors. However, later it was acknowledged that the BCS theory fails in dealing with their superfluid states, as well [1, 2]. This is best demonstrated by the persistence of a gap Δ in the spectra of single-particle (sp) excitations of many high-T_c superconductors above the critical temperature T_c, at which superconductivity disappears (the so-called pseudogap phenomenon [1 – 4]).

Another salient feature of two-dimensional electron liquid of high-T_c superconductors is the universality of its phase diagram versus the doping x. At low $|x| \leq x_c \simeq 0.05$, corresponding to the filling, close to 1/2, two-dimensional compounds are antiferromagnetic insulators. At larger x, aniferromagnetic ordering is nil, but in the vicinity of the phase transition, long-range correlations with wave vectors $\mathbf{q}$, close to the antiferromagnetic vector $\mathbf{Q} = (\pi, \pi)$, turn out to be drastically enhanced, which results in the divergence of the electron-electron scattering amplitude $\Gamma = \Gamma_0 + \Gamma_a \sigma_1 \sigma_2$ with

$$\Gamma_a(\mathbf{q} \to \mathbf{Q}, \omega \to 0; x) \sim [(\mathbf{q} - \mathbf{Q})^2 + r_a^{-2}(x) + ic|\omega|]^{-1}, \quad (1)$$

the correlation radius $r_a(x)$ becoming infinite at $x = x_c$ [5, 6].

The impact of this singularity on sp properties is studied proceeding from the RPA formula $\Sigma_a = (\Gamma_a * G)$, which presents an associated with antiferromagnetic fluctuations part Σ_a of the mass operator Σ as a convolution of the amplitude Γ_a with the sp Green function G (see e.g. [5 – 9]). For a long time, attention was focused on the energy dependence of Σ, while its momentum dependent part $\Sigma(\mathbf{p}, \varepsilon = 0)$ was parameterized by the effective mass m^*. This is justified in systems with short-range correlations, where the mass operator $\Sigma(\mathbf{p}, \varepsilon = 0)$ is a smooth function of $\mathbf{p}$. But this is not the case. Straightforward calculations show that long-range correlations (1) trigger a rapidly varying with $\mathbf{p}$ component $\Sigma_a(\mathbf{p})$ of the function $\Sigma(\mathbf{p}, \varepsilon = 0) \equiv \Sigma_r(\mathbf{p}) + \Sigma_a(\mathbf{p})$, being a convolution of Γ_a and the pole part G^q of the Green function G. It should be emphasized that $\Sigma_a(\mathbf{p})$ has to be evaluated self-consistently, otherwise the flattening of the sp spectra $\xi(\mathbf{p})$ in normal states, found in Ref. [10] and observed in many high-T_c compounds, gets lost.

To get rid of the energy-dependent terms in Σ we calculate the derivative $\partial \mathrm{Re}\Sigma(\mathbf{p}, \varepsilon)/\partial \mathbf{p} \to (\mathrm{Re}\Gamma_a * \partial \mathrm{Im} G^q / \partial \mathbf{p})$. After simple algebra we obtain

$$\frac{\partial \mathrm{Re}\Sigma_a(\mathbf{p})}{\partial \mathbf{p}} = \frac{3}{2} z \int \Gamma_a(\mathbf{p} - \mathbf{p}_1, \omega = E(\mathbf{p})) \frac{\partial n(\mathbf{p}_1, T)}{\partial \mathbf{p}_1} d\tau_1. \quad (2)$$

Here $z = [1 - (\partial \Sigma(\varepsilon)/\partial \varepsilon)_0]^{-1}$ is the renormalization factor, $d\tau = d^2p/(2\pi)^2$, and

$$n(\mathbf{p}, T) = v^2(\mathbf{p})(1 - f(E)) + (1 - v^2(\mathbf{p}))f(E) = \\ = \frac{1}{2} - \frac{\xi(\mathbf{p})}{2E(\mathbf{p})} \tanh \frac{E(\mathbf{p})}{2T} \quad (3)$$

is the quasiparticle momentum distribution. In this formula, $f(E) = (1 + \exp(E/T))^{-1}$, while $v^2(\mathbf{p}) = (E(\mathbf{p}) - \xi(\mathbf{p}))/2E(\mathbf{p})$, where $E(\mathbf{p}) = \sqrt{\xi^2(\mathbf{p}) + \Delta^2(\mathbf{p})}$ and Δ is the gap function, while $\xi(\mathbf{p}) = z\left(\xi^0_{\mathbf{p}} + \Sigma_a(\mathbf{p}) + \Sigma_r(\mathbf{p})\right) \equiv \xi^0(\mathbf{p}) + z\Sigma_a(\mathbf{p})$ is the sp energy spectrum of the normal state measured

from the chemical potential μ. To a good approximation, the spectrum $\xi^0(\mathbf{p})$ and the LDA electron spectrum $\xi^0_{\mathbf{p}}$ are related by $\xi^0(\mathbf{p}) = \xi^0_{\mathbf{p}}/m^*$.

In what follows, the argument $\omega = E(\mathbf{p}_1)$ of the function $\Gamma_a(\mathbf{p}-\mathbf{p}_1,\omega)$ in Eq. (2) is replaced by 0, since both the functions $\partial n(\mathbf{p}_1,T)/\partial\mathbf{p}_1$ and $\Gamma_a(\mathbf{p}-\mathbf{p}_1)$, taken at $\xi(\mathbf{p}) = 0$, are peaked at $\xi(\mathbf{p}_1) = 0$. Upon inserting this result into Eq. (2) and integrating over momenta, one finds

$$\xi(\mathbf{p}) = \xi^0(\mathbf{p}) + \frac{3}{2}z^2\int \Gamma_a(\mathbf{p}-\mathbf{p}_1)n(\mathbf{p}_1,T)d\tau_1. \quad (4)$$

The gap $\Delta(\mathbf{p})$, obeying the BCS gap equation, is also decomposed into a sum $\Delta(\mathbf{p}) = \Delta_a(\mathbf{p}) + \Delta_r(\mathbf{p})$ of a regular $\Delta_r(\mathbf{p})$ and a rapidly varying with $\mathbf{p}$ component $\Delta_a(\mathbf{p})$. In the case of singlet pairing, the respective equation for $\Delta_a(\mathbf{p})$ reads [11]:

$$\Delta_a(\mathbf{p}) = -3z^2\int \Gamma_a(\mathbf{p}-\mathbf{p}_1)\frac{\tanh\dfrac{E(\mathbf{p}_1)}{2T}}{2E(\mathbf{p}_1)}\Delta(\mathbf{p}_1)\; d\tau_1. \quad (5)$$

The analysis of solutions of the above nonlinear equations is greatly facilitated, if the interaction (1), taken at $\omega = 0$, is approximated by a δ-function $\frac{3}{2}z^2\Gamma_a(\mathbf{q}) \to f_a\delta(\mathbf{q}-\mathbf{Q})$ [5], appropriate in a domain of the momentum space, where the functions $n(\mathbf{p})$ and $\Delta_a(\mathbf{p})$ change slower, than the amplitude $\Gamma_a(\mathbf{p}-\mathbf{p}_1)$. As a result, integrations cancel, and we are left with

$$\begin{aligned}\xi(\mathbf{p}) &= \xi^0(\mathbf{p}) + f_a n(\mathbf{p}-\mathbf{Q},T),\\ \xi(\mathbf{p}-\mathbf{Q}) &= \xi^0(\mathbf{p}-\mathbf{Q}) + f_a n(\mathbf{p},T),\end{aligned} \quad (6)$$

$$\begin{aligned}\Delta(\mathbf{p}) &= -f_a\Delta(\mathbf{p}-\mathbf{Q})\frac{\tanh(E(\mathbf{p}-\mathbf{Q})/2T)}{E(\mathbf{p}-\mathbf{Q})},\\ \Delta(\mathbf{p}-\mathbf{Q}) &= -f_a\Delta(\mathbf{p})\frac{\tanh(E(\mathbf{p})/2T)}{E(\mathbf{p})},\end{aligned} \quad (7)$$

where the constant $f_a > 0$, is small compared to the band width ω_0. In obtaining these equations we neglected the term $\Delta_r(\mathbf{p})$. Setting here $T = 0$, we arrive at a set of equations derived in Ref. [12] in a different way.

If pairing correlations are somehow suppressed, Eqs. (7) are knocked out. Upon solving the two remaining Eqs. (6) we find that in case the van Hove points $(\pm\pi, 0)$ and $(0, \pm\pi)$ are situated quite close to the Fermi line (FL), a portion of the sp spectrum, adjacent to the van Hove points (vHP), turns out to be flat [12]. We shall see later that the flattening holds, if pairing correlations come into play.

As seen from Eq.(7), the gap $\Delta(\mathbf{p})$ changes its sign going over to a neighbor vHP, as in the conventional D-pairing model, in which the gap $\Delta_D(\mathbf{p}) \sim (\cos p_x - \cos p_y) \neq 0$ anywhere in the momentum space but the zone diagonals. However, in contrast to this model, nontrivial solutions of Eqs.(7) exist only in a domain C, boundaries of which are found by combining two Eqs.(7), which yields

$$f_a^2\frac{\tanh(E(\mathbf{p})/2T)}{E(\mathbf{p})}\frac{\tanh(E(\mathbf{p}-\mathbf{Q})/2T)}{E(\mathbf{p}-\mathbf{Q})} = 1, \quad \mathbf{p}\in C. \quad (8)$$

Otherwise $\Delta_a \equiv 0$, and $E(\mathbf{p}) = |\xi(\mathbf{p})|$, as in the Nozieres model [13–15] with the effective long-range interaction $\Gamma(\mathbf{q}) \sim \delta(\mathbf{q})$.

In overdoped compounds, the domain C is made up of two quite narrow stripes. The first, denoted further C_F and described by equation $\xi^0(\mathbf{p}) = 0$, is adjacent to the FL. The second, associated with the conjugate line (CL), is determined by equation $\xi^0(\mathbf{p}-\mathbf{Q}) = 0$. In these compounds, the FL and CL are well separated, and when dealing with $\mathbf{p}\in C_F$ the energy $E(\mathbf{p}-\mathbf{Q})$ can be replaced by $|\xi^0(\mathbf{p}-\mathbf{Q})|$, so that Eq. (8) is recast to

$$E(\mathbf{p}) = g(\mathbf{p})\tanh(E(\mathbf{p})/2T), \quad \mathbf{p}\in C_F, \quad (9)$$

with the coupling constant $g(\mathbf{p}) = f_a^2/|\xi^0(\mathbf{p}-\mathbf{Q})|$.

As x drops, the FL and the CL approach to meet each other at a critical doping x_m. In most of high-T_c compounds, such as Bi2212, Bi2201 etc., the FL is concave, while the CL, respectively, convex, and the first meeting between these lines occurs at the vHPs. Close to the vHPs, boundaries of the C domain are calculated combining Eq. (8) with relations $E(\mathbf{p}) = |\xi^0(\mathbf{p})|$ and $E(\mathbf{p}) = |\xi^0(\mathbf{p}) + f_a|$, respectively, which yields restrictions $-2f < \xi^0(\mathbf{p}) < f$. In this case, Eq.(8) is easily solved, and close to the vHPs, the sp spectrum turns out to be quite flat: $E(\mathbf{p}, T = 0) \simeq f_a$. We see that this value is significantly in excess of those obtained, if the FL and the CL have no points of intersection. When the gap landscape is drawn in the doping region $x \sim x_m$, it comprises four "twin towers", each one being associated with its own vHP. Each tower, whose height $\Delta_{vHP}(T = 0, x_m)$, according to Eq.(8), equals f_a, is connected with its neighbors by narrow "walls". According to Eq. (9), their height drops towards the zone diagonals, where the gap Δ vanishes. Thus, we infer that the gap function $\Delta(p_x, p_y)$ attains its maximum $\Delta_{\max}(T = 0) = f_a$ at the vHPs. This picture, confirmed by numerical calculations of Ref. [12], is in agreement with the available experimental data [2].

As T rises, the region C, where $\Delta_a(\mathbf{p}) \neq 0$ shrinks, the effect, found first in Ref. [15] under investigation of

the Nozieres model [13]. Indeed, for points, fairly far away from the vHPs, Eq.(9) can be employed. Its nontrivial solutions exist only if $g(\mathbf{p}) > 2T$. Since the function $|\xi^0(\mathbf{p}-\mathbf{Q})|$, identifying the energy splitting between the FL and the CL, rises, while the magnitude of the function $g(\mathbf{p})$ drops, respectively, as the vector $\mathbf{p}$ moves along the FL towards the zone diagonal, the shrinkage begins in the diagonal region at $T_i(x) \simeq f_a^2/2|\xi_{\max}(x)|$, where $\xi_{\max}(x)$ is the bare sp energy, corresponding to the point of intersection between the CL and the zone diagonal. With further T increase, the shrinkage region is augmented, approaching the vHPs, where the gap Δ has its maximum value. Eventually, the whole C domain shrinks into several symmetric points at the FL, closest to the vHPs. Recently, such a behavior of the gap landscape, the so-called arc phenomenon [2] was experimentally observed. The final shrinkage temperature $T^*(x \sim x_m)$ is easily evaluated from Eq. (8). It is $T^*(x \sim x_m) \simeq f_a/2$, so that the gap $\Delta_{\max}(T=0)$ and T^* are connected with each other by

$$\Delta_{\max}(T=0) \simeq 2T^*, \quad x \sim x_m, \tag{10}$$

being in accord with the available experimental data [1, 2].

It is worth noting that inside the C region, the behavior of Δ remains the same as that in the BCS theory, since by retaining in Eq. (9) the leading terms, one obtains

$$\Delta^2(\mathbf{p}; T \to T^*) \simeq 12T^*(T^* - T), \quad \mathbf{p} \in C. \tag{11}$$

Let us now turn to a rather rare case of the convex FL. Here the first intersection between the FL and the CL occurs at the zone diagonals, and if one rotates all the zone picture by the angle $\phi = \pi/4$, these points will coincide with the intersection points between the FL and the CL in the case of the concave FL. The analysis shows that this feature seems to hold in dealing with all the solutions, including the gap landscape. We shall revisit this prediction of our model in a future paper.

So far we have neglected all the electron-electron interactions but the longe-range one given by Eq. (1). By involving an electron-phonon exchange, the most pronounced out of the remaining ones, we trigger, on one hand, a regular component $\Delta_r(\mathbf{p}) \neq 0$ anywhere in the momentum space. As a result, the Landau criterion for superconductivity, violated in the above model at $T > T_i$, is now satisfied. Presumably, the magnitude of $\Delta_r(\mathbf{p})$ slowly varies with x, allowing us to estimate it from highly overdoped compounds. Since in this case, T_c is small, we infer that the impact of Δ_r on properties of the superfluid state is insignificant. On the other hand, the electron-phonon exchange, specified by the phonon propagator $D(\omega, k) = k^2/(\omega^2 - c^2k^2)$, gives rise to a renormalization of the constant f_a, as well. The respective contribution $\delta\Delta(\mathbf{p})$ to the gap Δ is given by the integral

$$\delta\Delta(\mathbf{p}) \sim \int D(\mathbf{p}-\mathbf{p}_1, \omega_1) \frac{\Delta_a(\mathbf{p}_1)}{\omega_1^2 - E^2(\mathbf{p}_1)} d\tau_1 \frac{d\omega_1}{2\pi i}. \tag{12}$$

Employing in the integral (12) the "tower" structure of the function $\Delta_a(\mathbf{p}, x \sim x_m)$, one can decompose ovewhelming contributions into two: one from the same "tower" and the other, from the neighboring one. The first contribution, proportional to the "tower" range, is small. When calculating the second one, where the momentum transfer $\mathbf{p}-\mathbf{p}_1$ is comparable to p_F, the propagator D can be replaced by -1, yielding a number, which suppresses the initial f_a value. This interference may be significant.

Now we proceed to evaluation of the superfluid density $\rho_s(T)$, expressed in terms of a correlator of the velocities $\partial\xi^0(\mathbf{p})/\partial\mathbf{p}$. Evaluation of this correlator in crystals with the help of the Larkin-Migdal method [16, 17] yields:

$$\rho_s(T) = -\frac{1}{2}\int \frac{\partial\xi^0(\mathbf{p})}{\partial p_i}\left[\frac{\partial n(\mathbf{p},T)}{\partial p_i} - \frac{\partial f(E)}{\partial E}\frac{\partial\xi(\mathbf{p})}{\partial p_i}\right] d\tau, \tag{13}$$

the function $n(\mathbf{p}, T)$ being given by Eq. (3). In ideal homogeneous Fermi gas, where $\xi(p) = p^2/2M - \mu$, Eq. (13) is converted into the ordinary textbook formula. Obviously, no contributions to ρ_s are made from regions in momentum space, where the ratio $\Delta(\mathbf{p})/T$ is negligible. Indeed, if $\Delta(\mathbf{p}) = 0$, the distribution $n(\mathbf{p}, T)$ is converted to $n_F(\mathbf{p}, T) = (1 + \exp(\xi(\mathbf{p})/T))^{-1}$, while the product $(\partial f(E)/\partial E)(\partial\xi(\mathbf{p})/\partial p_i) \to \partial n_F(\mathbf{p}, T)/\partial p_i$, and both the terms in Eq. (13) cancel each other. As a result, at $T > \Delta_r$, contributions from regions, other than the C domain, may be neglected.

A full examination of the formula (13) will be done elsewhere. Here we restrict ourselves to the region of the dopings $x \simeq x_m$ and temperatures $T \to T^* \simeq f_a/2$. In this case, the ratio $E(\mathbf{p} \in C)/T$ is small, and expansion of the terms in the integrand of Eq. (13) yields $\partial n(\mathbf{p}, T)/\partial p_i \simeq -(\partial\xi(\mathbf{p})/\partial p_i)/4T + \xi^2(\mathbf{p})(\partial\xi(\mathbf{p})/\partial p_i)/16T^3 + \Delta^2(\mathbf{p})(\partial\xi(\mathbf{p})/\partial p_i)/48T^3$ and $\partial f(E)/\partial E \simeq -1/4T + E^2(\mathbf{p})/16T^3$. After cancelling similar terms and employing relation (11), we are left with

$$\rho_s(T \to T^*) \simeq \frac{1}{48}\int_C \frac{\partial\xi^0_{\mathbf{p}}}{\partial p_i}\Delta^2(\mathbf{p})\frac{\partial\xi(\mathbf{p})}{\partial p_i} d\tau \simeq$$
$$\simeq \alpha n(T^* - T)^2/T^{*2}, \tag{14}$$

where the numerical factor α is of the order of 10^{-2}. As we shall see, such a suppression of $\rho_s(T \to T^*)$, results in a marked distinction between the critical temperature T_c for termination of superconductivity and the temperature T^* for vanishing of the gap Δ. The reason for that is a great diversity in the gap values, which, as we have seen, results in the temperature shrinkage of the domain of integration over momentum space in Eq. (13).

Strictly speaking, in two-dimensional systems, the temperatures T^* and T_c never coincide because of the Berezinskii-Kosterlitz-Thouless (BKT) phase transition [18–20], terminating superconductivity due to a spontaneous generation of an infinite number of vortices. This transition always occurs before vanishing of the gap Δ. The BKT temperature, being, in fact, the critical temperature T_c, is given by the equation [18]

$$\pi T_c = 2\rho_s(T_c). \tag{15}$$

In conventional superconductors, where $\rho_s(T \to T^*) \sim n(T^* - T)/T_c$, and, hence, $(T^* - T_c) \sim T_c^2/\epsilon_F^0$, the ratio T_c/ϵ_F^0 does not exceed 0.2%. However, in two-dimensional electron compounds with the doping $x \sim x_m$, the situation is different. Indeed, upon inserting the result (14) into Eq.(15), one obtains

$$T_c = \alpha_m \epsilon_F^0 (T^* - T_c)/T^*, \tag{16}$$

where the factor $\alpha_m \simeq 10^{-2}$. In high-T_c superconductors, the ratio T_c/ϵ_F^0 is of order of 10^{-2}, and, hence, the ratio $\tau = (T^* - T_c)/T^*$ may attain values comparable to unity.

In conclusion, we have evaluated the effect of critical antiferromagnetic fluctuations on electron spectra and superfluid densities of superfluid states of overdoped and optimally doped high-T_c compounds. In underdoped electron systems, the situation is more complicated due to the emergence of a branch of low-lying collective excitations, whose contribution to properties is significant [21]. The interplay between these oscillations and critical fluctuations in underdoped compounds will be studied a separate paper.

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