On the theory of pseudogap anisotropy in the cuprate superconductors

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Abstract

We show by means of the theory of the order parameter phase fluctuations that the temperature of the “closing” (or “opening”) of the gap (and pseudogap) in the electron spectra of superconductors with anisotropic order parameter actually takes place within a finite temperature range. Every Fourier-component of the order parameter has its own critical temperature.

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It is well known that the it is not easy to build a self-consistent theory of the copper oxide high-temperature superconductors (HTSCs) due to the necessity to take into account different properties of the cuprates, in particular strong electron correlations, low dimensionality of the electronic and magnetic properties, anisotropy of the order parameter, pseudogap presence, disorder etc. It is extremely difficult to include all these properties into the theory self-consistently. The choice of the properties is usually dictated by the aim of studies. Below we make an attempt to show that it is possible to explain such an unusual phenomenon as smooth disappearing (“closing”) of the pseudogap along the Fermi surface arcs from nodal points to M-points ((0, π) or (π, 0)) of the Brillouin zone in the momentum space.

It has been proved that the description of the superconductivity in the 2D metals with arbitrary carrier density requires not two, as usual, but three self-consistent equations (see review [1]). Two of them are well known. The first one is the gap equation, which defines the order parameter. It can be written in the following form in the case of a separable interaction [2]:

\[
\Delta_k = \frac{V}{N} \sum_q \gamma_l(q) \gamma_l(k) \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\varepsilon}{\exp(\varepsilon/T) + 1} \text{Im} \text{Tr} \left[ \hat{\tau}_1 \hat{G}_q(\varepsilon) \right],
\]

(1)

where

\[
\hat{G}_q(\omega_n) = \frac{1}{i\omega_n - \xi(k)\tau_1 - \Delta_k\tau_3},
\]

(2)

is the Matsubara fermion Green’s function in the Nambu representation, and

\[
\xi(k) = \frac{W}{2} - \frac{W}{4} \left( \cos(k_x a) + \cos(k_y a) \right) - \mu
\]

(3)

is a spectrum of one-particle fermi excitations on the square lattice with the constant \(a\) and with the bandwidth \(W\). The spectrum energy is measured with respect to the chemical potential \(\mu\). The order parameter in different pairing channels is \(\Delta(k) = \Delta_l(T)\gamma_l(k)\), where \(l\) stands for the symmetry of the order parameter. In the \(s\)-wave pairing channel we choose \(\gamma_s(k) = 1\), in the \(p\)-wave channel \(\gamma_p(k) = \sin(k_x a)\), and, finally, in the related to the HTSCs \(d\)-wave pairing channel \(\gamma_d(k) = \cos(ak_x) - \cos(ak_y)\). \(\omega_n = (2n + 1)\pi T\) are the Matsubara fermi-frequency, \(\hat{\tau}_i\) are the Pauli matrices, and \(V\) is the parameter which characterizes the fermion attraction (the separable pairing potential is chosen in the following form: \(V_l(k, q) = V\gamma_l(k)\gamma_l(q)\)).
The second equation can be written as:

\[
n_f = 1 - \frac{1}{N} \sum_k \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{d\varepsilon}{\exp(\varepsilon/T) + 1} \text{ImTr}[\hat{\tau}_3 \hat{G}_k(\varepsilon)]. \tag{4}
\]

This equation allows to connect the number of the mobile (doped) carriers in the conducting band with the dispersion law (3) and the chemical potential (usually, holes are the carriers in the copper oxide HTSCs). Generally, the value of the chemical potential is not equal to the value of the Fermi energy (see [1]).

After the integration over the energy \(\varepsilon\) and by using (2) and (3), equations (1) and (4) can be transformed to a more familiar form:

\[
1 = V \int \frac{d^2k}{(2\pi)^2} \gamma_i(k)^2 \tanh\left[E(k)/(2T)\right]; \tag{5}
\]

\[
n_f = \int \frac{d^2k}{(2\pi)^2} \left[ 1 - \frac{\xi(k)}{E(k)} \tanh\left(\frac{E(k)}{2T}\right) \right], \tag{6}
\]

where \(E(k) = \sqrt{\xi^2(k) + |\Delta(k)|^2}\) is the excitation energy of the quasi-particles in the superconducting state. The function \(E(k)\) is equal to zero at so called nodal points (with \(|k_x| = |k_y| = |k_F|\), where \(k_F\) is the Fermi momentum).

The system (5) and (6) is the self-consistent system of equation of the BCS theory. Its solution in the 2D case describes the temperature dependence of the gap (amplitude of the order parameter) and of the chemical potential at given value of \(n_f\). It is impossible to estimate the correct value of the critical temperature from this system, since the critical temperature in the 2D case is equal to zero due to the long-wave fluctuations of the phase of the order parameter [3]. However, there is another phase transition in the 2D systems - the Berezinskii-Kosterlitz-Thouless (BKT) phase transition with the critical temperature \(T = T_{BKT}\) at which the correlation of the order parameter changes its space dependence from the exponential (at \(T > T_{BKT}\)) to the power law (at \(T < T_{BKT}\)). This transition was studied most completely in the case of the spin \(XY\)-model with the following Hamiltonian [4]:

\[
H_{XY} = \frac{J}{2} \sum_{n,\hat{n}} (\theta_n - \theta_{\hat{n}})^2, \quad \text{where} \quad J \text{ is the exchange coupling and} \quad \theta_n, \theta_{\hat{n}} \text{ are the phases of the spin vectors on the nearest sites} \ n \text{ and} \ \hat{n}. \quad \text{The critical temperature of the BKT transition is defined by the following equation:}
\]

\[
T_{BKT} = \frac{\pi J}{2} \tag{7}
\]
The order parameter of the superconducting metal is a complex (two-component) function, and usually it can be approximated as following (see, for example [5]): \( \Phi(r_1, r_2) \simeq \Delta(r)e^{i\theta(R)} \), where \( r = r_1 - r_2 \) and \( R = (r_1 + r_2) \) are the relative coordinate and the center of mass coordinate of the pair, correspondingly. In the case of the long-wave approximation the kinetic part of the thermodynamic potential has the form of \( H_{XY} \), but in this case the superconducting rigidity plays the role of the exchange parameter. This parameter is a function of \( T_c \equiv T_{BKT} \), \( \mu \) and \( \Delta_l(T_c) \).

Equation

\[ T_c = \frac{\pi}{2} J(T_c, \mu, \Delta_l(T_c)) \] (8)

makes the system of equations [5], [6] and [8] closed. This system of equations allows us to find the gap, the chemical potential and the critical temperature \( T_c \).

The expression for the function \( J(T_c, \mu, \Delta_l(T_c)) \) for the case with an anisotropic order parameter can be found in the complete analogy with the isotropic s-case [6] (see also [1]). It has the following form:

\[
J(T_c, \mu, \Delta_l(T_c)) = \frac{W}{16} T_c \sum_{n=-\infty}^{\infty} \frac{d^2k}{(2\pi)^2} Tr \left[ \hat{\tau}_3 G_k(i\omega_n)e^{i\delta\omega_n\hat{\tau}_3} + \frac{W}{8} k^2 G^2_k(i\omega_n) \right]
\]

\[ = \frac{W}{16} \left[ n_f - \frac{W}{16T_c} \int \frac{d^2k}{(2\pi)^2} k^2 \frac{1}{\cosh^2(E(k)/(2T_c))} \right] ; (\delta \to 0). \]

This expression together with [8] defines the equation for the critical temperature of the 2D superconducting metal with arbitrary carrier density:

\[
T_c = \frac{\pi}{32} W \left[ n_f - \frac{W}{16T_c} \int \frac{d^2k}{(2\pi)^2} k^2 \frac{1}{\cosh^2(E(k)/(2T_c))} \right]. \] (9)

The solution of the system of self-consistent equations [5], [6], and [8] can be found analytically in the s-wave case with quadratic dispersion of the quasi-particles, \( \xi(k) \sim k^2 \). In this case \( \Delta_l(0) \sim \sqrt{n_f}T_c \sim n_f \) and \( \mu \) is always negative when the fermion density \( n_f \to 0 \). In the case case of more general dispersion (see, for example [3]), and, moreover, in the case of the anisotropic order parameter, the solution can be found only numerically. This solution gives us the dependencies of \( T_c, \mu \) and \( \Delta_l(T_c) \) on \( n_f \). On the other hand, it is possible to find the amplitude \( \Delta_l(T) \) as a function of \( T \) from [3] and [4]. The solution of these equations at \( \Delta_l(T) = 0 \) gives us the carrier density dependence of the critical mean-field temperature \( T^{MF}_c \) in the \( l \)-pairing channel. This temperature does not correspond to any observable phase transition, since there are no phase transitions in the 2D systems, except \( BKT \)-transition.
as it was mentioned above \[7\]. This transition is a superconducting phase transition in the metal with inter-fermion attraction, despite there is no general spontaneous symmetry breaking in all the system \[6\] (for details, see \[1\]).

The solution of the system of equations \[8\], \[9\], and \[10\] in the \(s\)-wave pairing channel is presented in Figs.1 and 2. It is important to note that the system of equations can be analyzed analytically in this case. It is easy to see the complete symmetry of the solutions with respect to the point \(n_f = 1\) (the case of half-filling), what was already mentioned in \[8, 9\]. The two-particle (local) bound states exist at any value of \(V/W\) at small values of \(n_f\) (or \(2 - n_f\), when we consider the hole pairing). In other words, there is no threshold value of the coupling for the bound state formation in the \(s\)-wave pairing channel in the 2D case. In this case the chemical potential is negative at any value of \(V/W\) and small enough \(n_f\), what indicates the crossover from Bose-Einstein condensation regime to BCS superconductivity with carrier density increasing (or coupling decreasing)\[10, 11\]. As it follows also from these Figures, the following inequality is always correct \(T_c << T_c^{MF}\), and the carrier density dependencies are close to those found analytically in the case of the quadratic dispersion: \(T_c^{MF} \sim \sqrt{n_f}, T_c \sim n_f\) in the low carrier density limit. The canonical BCS relation \(2\Delta_s(0)/T_c^{MF} = 3.52\) holds at any carrier density except very low values of \(n_f\) (see Fig.3), but the relation \(2\Delta_s(0)/T_c\) is increasing with carrier density decreasing, since it is easy to see that \(\Delta_s(0)/T_c \sim \sqrt{n_f}\) at small \(n_f\).

In the cases of the anisotropic \(p\)-wave and \(d\)-wave pairing (Figs.4-6 and 7-9, correspondingly) the behavior of the superconducting parameters with doping is qualitatively the same. The only difference is that the crossover to superfluidity takes place only above some critical values of \(V\). The local pairs with non-zero orbital momentum can be formed only when the attraction is strong enough \[12, 13\]. In the cases of the moderate or low attraction the chemical potential of the system is positive at any value of \(n_f\), therefore only Cooper \(p\)- and \(d\)-wave pairs can exist in this case. The chemical potential in this case practically coincides with the Fermi energy. As it follows from Figures 5 and 8, the relation \(T_c << T_c^{MF}\) holds also in these cases, and the ratios \(2\Delta_p(0)/T_c^{MF}\) and \(2\Delta_d(0)/T_c^{MF}\) are even higher in comparison with the \(s\)-wave case, what shows that the isotropic condensate is more stable with respect to the thermal fluctuations. The region between \(T_c\) and \(T_c^{MF}\), where the superconducting fluctuations are incoherent and rapidly decay and the order parameter modulus is finite, should be interpreted as the pseudogap region. Above \(T_c^{MF}\) (which in some papers
(for example, in \([14, 15]\)) is called the temperature of the decay of superconducting fluctuations \(T_{scf}\) the gap in the superconducting spectrum disappears, while there is no any phase transition at the point \(T_c^{MF}\) or around it.

There is another principal difference between \(T_c\) and \(T_c^{MF}\) due to the anisotropy of the electron spectra in the superconducting phase. The temperature \(T_c\) is critical temperature of the phase transition, and therefore it is unique for all the system and for all its excitations. This temperature can be measured as the temperature below which the resistivity goes to zero, or by the Meissner effect, for example. On the other hand, this statement can not be used with respect to \(T_c^{MF}\). This temperature is not the critical temperature of any phase transition in the 2D system, similarly to the case with the \(s\)-wave pairing. The important question is whether the critical temperature of the formation of different Fourier-components or the order parameter is unique. Even the temperature \(T_c\) can have such values that the following rations are true at different directions of the momentum \(k\): \(T_c \leq \Delta(k)\), or \(T_c \geq \Delta(k)\), including \(T_c \gg \Delta(k)\). More important question is whether the order parameter modulus forms at any value of \(k\). A simple (and, in some sense qualitative) answer to this question can be given by using the canonical BCS ratio rewritten in the following form:

\[
\frac{2\Delta_l(T = 0)}{T_c^{MF}} \rightarrow \frac{2\Delta_l(T = 0)|\gamma_l(k)|}{T_c^{MF}(k)},
\]

which shows that every Fourier-component of the anisotropic order parameter has its own “closing” critical temperature. It should be emphasized that this temperature does not correspond to any phase transition.

The relation \((10)\) is an estimation which actually defines the temperature \(T_c^{MF}(k) = T_c^{MF} |\gamma_l(k)|\) (or \(T_{scf}(k)\)). As it follows from this relation, the gaped quasi-particle spectra of the 2D superconductor with anisotropic order parameter shows its momentum dependence also when the temperature changes. It is important that the gap disappears continuously from the nodal point, where \(\gamma_l(k) = 0\) at any \(T\), to the \(M\)-points, where the gap and the corresponding temperature \(T_c^{MF}\) are maximal, with temperature increasing. The gapless (or, actually “pseudogapless”) character of the spectra will cover larger parts of the Fermi surface with temperature increasing at any values of \(k\), at which \(T = T_c^{MF}(k)\). This behavior was observed in the ARPES experiments (see recent review \([16, 17]\) and references therein).

Thus, it is shown that the self-consistent study of the phase fluctuations of the superconducting order parameter allows one to describe qualitatively the anisotropy of the pseudogap
and its disappearance within a rather wide range of temperatures.

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FIG. 1: The carrier density dependence of a) $\Delta_s$ and b) $\mu$ at $T = 0$ and different values of $V$ in the $s$-wave pairing channel.

FIG. 2: The carrier density dependence of a) $T_{c}^{MF}$ and b) $T_c$ at different values of $V$ in the $s$-wave pairing channel.

FIG. 3: The carrier density dependence of the ratios a) $2\Delta_s(T = 0)/T_{c}^{MF}$ (a)) b) $2\Delta_s(T = 0)/T_c$ at different values of $V$ in the $s$-wave pairing channel.
FIG. 4: The same as in Fig.1 for the $p$-wave pairing case.

FIG. 5: The same as in Fig.2 for the $p$-wave pairing case.

FIG. 6: The same as in Fig.3 for the $p$-wave pairing case.
FIG. 7: The same as in Fig.1 for the $d$-wave pairing case.

FIG. 8: The same as in Fig.2 for the $d$-wave pairing case.

FIG. 9: The carrier density dependence of the ratios a) $4\Delta_d(T = 0)/T_c^{MF}$ and b) $4\Delta_d(T = 0)/T_c$ at different values of $V$ in the $d$-wave pairing channel (The maximal value of the gap in the $d$-wave pairing case is $2\Delta_d(T = 0)$, not $\Delta_d(T = 0)$ like in the $s$- and $p$-wave cases.)