Particle-hole mixing in the pseudogap state of preformed pairs

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Motivated by a novel ability of STM spectroscopy to measure the Bogolubov angle we propose to use this technique for identifying precursor effects above the transition temperature T_c of underdoped cuprate superconductors. Within phenomenological two-component model we show that *the Bogolubov angle can emerge already in the normal state* upon approaching T_c from above. Its measurements might clear up what part of the pseudogap region in the phase diagram corresponds to the Bogolubov-like quasiparticles and, ultimately whether T^* is related to superconducting fluctuations.

I. INTRODUCTION

In the recent paper Fujita et al [1] proposed to combine the STM tunneling conductance measured at positive and negative bias in order to determine the particle-hole mixing in superconductors. At sufficiently low temperatures the charge carriers (conduction electrons or holes) are bound into pairs and effectively the single-particle excitation spectrum (probed by STM) becomes gaped where the particle and hole contributions mix with one another. In conventional superconductors, they are expressed by the BCS coefficients $|u_{\mathbf{k}}^2|$ and correspondingly $|v_{\mathbf{k}}^2| = 1 - |u_{\mathbf{k}}|^2$. As a measure of the particle-hole mixing one defines the Bogolubov angle [2]

$$\theta_{\mathbf{k}} = \frac{\pi}{2} - 2\text{arctan}\left(\frac{u_{\mathbf{k}}}{v_{\mathbf{k}}}\right) \tag{1}$$

which varies between $-\pi/2$ and $\pi/2$ depending on the momentum $\mathbf{k}$ and indirectly on temperature. This angle (2) has a clear physical interpretation in terms of the pseudospin representation introduced for fermion pairs by Anderson [3]. In the Hilbert space restricted to $n_{\mathbf{k}\uparrow} - n_{-\mathbf{k}\downarrow} = 0$ such angle $\theta_{\mathbf{k}}$ points down (up) when true quasiparticles are represented by the particles (holes). The upper and bottom panels of figure 1 illustrate this behavior for the normal and superconducting states [3]. In general, $\theta_{\mathbf{k}}$ is a dynamical quantity governed by the Bloch type equations. Its dynamics is recently widely explored for the ultracold superfluid atoms where time-dependent magnetic field traversing the Feshbach resonance can lead to soliton-like solutions [4].

In the high temperature superconductors (HTSC) fermion pairs extend on a local (interactomic) distance therefore the energy gap [5] and the angle $\theta_{\mathbf{k}}$ [1] are both spatially dependent. In addition to electronic inhomogeneity, formation of the pairs (below some characteristic temperature T_p) is not accompanied by onset of superconductivity (which appears at $T_c \leq T_p$). Up to now there is no consensus whether T_p follows the transition temperature being close to T_c or perhaps the pairs exist in a whole pseudogap region up to T^* [6]. The new ability of STM spectroscopy [1] might finally resolve this intriguing issue.

In principle, the Bogolubov angle (1) is sensitive to existence of pairs at any temperature. From various experimental studies it is known that HTSC materials have roughly the BCS-type properties below T_c [7]. However, studying fermion pairing above T_c one usually encounters some difficulties because of the finite life-time effects, absence of the long range coherence, etc. On a theoretical level one must go there beyond the mean-field framework to account for these strong quantum fluctuations.

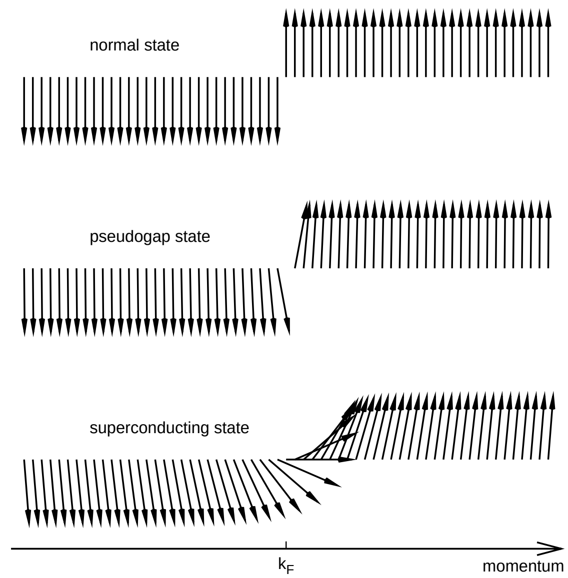

FIG. 1: Schematic view of the Bogolubov angle orientation. The upper and bottom plots correspond to the normal and superconducting phases [3] while the middle one illustrates the pseudogap state as deduced from the present analysis.

To handle such problems we use here a phenomenological two-component model where fermion singles and the pairs are introduced right at the outset [8]. Our main objective is to show that the precursor pairing leads to a slanted Bogolubov angle $|\theta_{\mathbf{k}}| \neq \pi/2$ near the Fermi surface (see the middle panel in figure 1). We think that such behavior is generic for all situations with strong feedback effects between the single fermions and the pairs. In particular, similar results can be expected for the microscopic models of HTSC using the extended Hubbard, t-J or RVB scenarios.

II. MODEL

Superconductivity of the HTSC compounds is believed to originate from the strong electron correlations within CuO_2 planes. Various mechanisms have been explored so far but the discussion about microscopic physics is still going on [9]. We skip such a debate and focus simply on the effective model involving the coupled fermion and boson degrees of freedom. This scenario seems to be natural for the pseudogap state where single fermions coexist with the preexisting pairs and they both affect each other. There have been given some phenomenological [10] and microscopic arguments [11, 12, 13] supporting realization of this scenario in the HTSC materials as well as its usefulness for a description of the ultracold fermion atoms interacting with the Feshbach resonance [14].

We consider the Hamiltonian in the following form [8]

$$\hat{H} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}}-\mu)\, \hat{c}^{\dagger}_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} (E_{\mathbf{q}}-2\mu)\, \hat{b}^{\dagger}_{\mathbf{q}}\hat{b}_{\mathbf{q}} + \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} \left(g_{\mathbf{k},\mathbf{q}} \hat{b}^{\dagger}_{\mathbf{q}} \hat{c}_{\mathbf{q}-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} + g^{*}_{\mathbf{k},\mathbf{q}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{\mathbf{q}-\mathbf{k}\downarrow}\hat{b}_{\mathbf{q}} \right) , \quad (2)$$

where $\hat{c}^{\dagger}_{\mathbf{k}\sigma}$ ($\hat{c}_{\mathbf{k}\sigma}$) operators refer to creation (annihilation) of single fermions with the energy $\varepsilon_{\mathbf{k}}$ and $\hat{b}^{\dagger}_{\mathbf{q}}$ ($\hat{b}_{\mathbf{q}}$) correspond to the preformed fermion pairs. Interaction between the single fermions and the pairs is denoted by $g_{\mathbf{k},\mathbf{q}}$. For simplicity, we shall assume that concentration of pairs is small so that $\hat{b}^{(\dagger)}_{\mathbf{q}}$ operators obey the ordinary commutation relations (neglecting the hard-core effect).

In the simplest treatment the interaction part can be linearized and the decoupled boson and fermion parts become exactly solvable [8]. The resulting spectrum of fermions has then the BCS structure $A^{MF}(\mathbf{k},\omega) = u^2_{\mathbf{k}}\delta(\omega - E_{\mathbf{k}}) + v^2_{\mathbf{k}}\delta(\omega + E_{\mathbf{k}})$ with the quasiparticle energy $E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}}-\mu)^2 + \Delta^2_{\mathbf{k}}}$ and the usual coherence factors $u^2_{\mathbf{k}}, v^2_{\mathbf{k}} = \frac{1}{2}[1 \pm (\varepsilon_{\mathbf{k}}-\mu)/E_{\mathbf{k}}]$. The energy gap of single particle excitation is effectively given by $\Delta_{\mathbf{k}} = g_{\mathbf{k},\mathbf{0}}\sqrt{\langle n^B_{\mathbf{0}}\rangle}$ which means that fermions undergo the transition to superconducting state simultaneously with appearance of the Bose-Einstein condensate of (preformed) pairs [8].

The mean-field approximation is not able to take into account any quantum fluctuations therefore for $T > T_c$ the fermion spectrum reduces to a single peak at $\omega = \varepsilon_{\mathbf{k}} - \mu$. This would imply that in the normal state $|\theta_{\mathbf{k}}| = \pi/2$ and only in the superconducting state the Bogolubov would mix the particle and hole excitations [3]. In the next section we use a method capable to track the mutual boson-fermion feedback effects and show that due to the precursor of the superconducting correlations the Bogolubov angle gets tilted above T_c. Moreover, at the Fermi surface it shows a novel behavior which is distinct from that of the BCS superconductor and from the usual normal state.

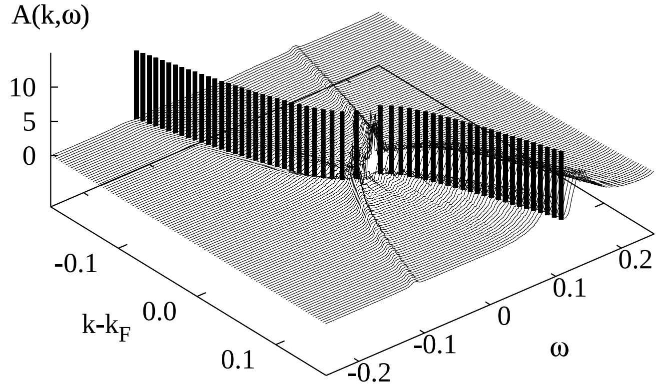

FIG. 2: The single particle excitation spectrum of fermions in the pseudogap regime. Besides the long-lived quasiparticle at $\omega = \tilde{\varepsilon}_{\mathbf{k}} - \mu$ there emerges its mirror reflection corresponding to the damped Bogolubov shadow branch. Both branches develop a pseudogap feature in the dispersion curves at k_F.

III. METHOD

For a selfconsistent study of the model (2) we use nonperturbative procedure based on a continuous canonical transformation $\hat{H} \longrightarrow e^{\hat{S}(l)}\hat{H}e^{-\hat{S}(l)} \longrightarrow \hat{\tilde{H}}$ [15]. The main idea is to eliminate the interaction part $g_{\mathbf{k},\mathbf{q}}$ through a sequence of infinitesimal steps. Proceeding along the lines of the Renormalization Group (RG) techniques one starts from the high energy sector and progressively goes down renormalizing the low energy states (by which we mean fermion states close to μ and boson states near 2μ).

In practice this is done by setting $\hat{H}(l) = e^{\hat{S}(l)}\hat{H}e^{-\hat{S}(l)}$ (where $\hat{H}(0)$ corresponds to the initial Hamiltonian) and analyzing the flow equation $\partial_l \hat{H}(l)$ using an appropriate choice of $\hat{S}(l)$ operator. For constructing the generating operator $S(l)$ we have followed the initial proposal of Wegner which guaranties that $\lim_{l\to\infty} g_{\mathbf{k},\mathbf{q}}(l) = 0$. Some necessary technical details have been given in our previous paper [16].

The model Hamiltonian (2) evolves continuously according to the set of flow equations $\partial_l \varepsilon_{\mathbf{k}}(l)$, $\partial_l E_{\mathbf{q}}(l)$ and $\partial_l g_{\mathbf{k},\mathbf{q}}(l)$ [16]. Since they are convoluted with one another one must solve them simultaneously step by step. We managed to do it by numerical means considering the fermion and boson particles on a lattice (when no infrared cutoffs are needed). Eventually for $l \to \infty$, we obtained the fixed point values

$$\varepsilon_{\mathbf{k}} \longrightarrow \tilde{\varepsilon}_{\mathbf{k}}, \qquad E_{\mathbf{q}} \longrightarrow \tilde{E}_{\mathbf{q}}, \qquad \tilde{g}_{\mathbf{k},\mathbf{q}} \longrightarrow 0. \quad (3)$$

In particular, we found the fermion dispersion $\tilde{\varepsilon}_{\mathbf{k}}$ to have a true gap for $T < T_c$ or a pseudogap for $T_p > T > T_c$

[16]. Simultaneously $\tilde{E}_{\mathbf{q}}$ develops the collective sound-wave (Goldstone) mode at $T<T_c$ which survives even in the normal state but at finite momenta [18].

For a complete information about the effective fermion spectrum one needs besides $\tilde{\varepsilon}_{\mathbf{k}}$ also the transformed operators $\hat{c}^{(\dagger)}_{\mathbf{k}\sigma}(l\rightarrow\infty)$ [19]. Such flow equations $\partial_l \hat{c}^{(\dagger)}_{\mathbf{k}\sigma}(l)$ have been explored by us for arbitrary temperatures [17, 18]. Here it would be sufficient to focus on the normal state when the flow equations of fermion operators simplify to

$$c_{\mathbf{k}\uparrow}(l) \;=\; \mathcal{P}_{\mathbf{k}}(l)\; c_{\mathbf{k}\uparrow} + \frac{1}{\sqrt{N}}\sum_{\mathbf{q}}{}' \, r_{\mathbf{k},\mathbf{q}}(l)\; b_{\mathbf{q}} c^{\dagger}_{\mathbf{q}-\mathbf{k}\downarrow} \quad (4)$$

$$c^{\dagger}_{-\mathbf{k}\downarrow}(l) \;=\; -\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}{}' \, r^{*}_{\mathbf{k},\mathbf{q}}(l)\; b^{\dagger}_{\mathbf{q}} c_{\mathbf{q}+\mathbf{k}\uparrow} + \mathcal{P}^{*}_{\mathbf{k}}(l)\; c^{\dagger}_{-\mathbf{k}\downarrow} \quad (5)$$

with the initial condition $\mathcal{P}_{\mathbf{k}}(0)=1$ and $r_{\mathbf{k},\mathbf{q}}(0)=0$. Equations (4,5) describe the process in which c-fermion scatters into b-boson with an involvement of the opposite spin fermion. The equations (4,5) remind the Bogolubov-Valatin transformation but here, for the normal state, they differ because a damping of cooperons.

The effective single particle spectral function of $\sigma=\uparrow$ fermions is finally given by the following form

$$\begin{aligned} A(\mathbf{k},\omega) &= |\tilde{\mathcal{P}}_{\mathbf{k}}|^2 \delta\left(\omega+\mu-\tilde{\varepsilon}_{\mathbf{k}}\right) \qquad (6)\\ &+ \frac{1}{N}\sum_{\mathbf{q}}{}' \left(n^B_{\mathbf{q}} + n^F_{\mathbf{q}-\mathbf{k}\downarrow}\right) |\tilde{r}_{\mathbf{k},\mathbf{q}}|^2 \delta(\omega+\mu-\tilde{E}_{\mathbf{q}}+\tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}) \end{aligned}$$

where the coefficients $\tilde{\mathcal{P}}_{\mathbf{k}}$ and $\tilde{r}_{\mathbf{k},\mathbf{q}}$ refer to $l=\infty$ fixed values, $n^B_{\mathbf{q}}$ is the occupancy of $\mathbf{q}$-momentum bosons and $n^F_{\mathbf{k}\sigma}$ denotes the filling of $(\mathbf{k},\sigma)$ fermion state. The flow equations for l-dependent coefficients $\mathcal{P}_{\mathbf{k}}(l)$ and $r_{\mathbf{k},\mathbf{q}}(l)$ have been derived in our previous work [17]. They have been solved numerically together with a set of interdependent equations for $\varepsilon_{\mathbf{k}}(l)$, $E_{\mathbf{q}}(l)$ and $g_{\mathbf{k},\mathbf{q}}(l)$.

IV. BOGOLUBOV ANGLE

The first term of the spectral function (6) represents the long-lived quasiparticles whose renormalized energies are denoted by $\omega=\tilde{\varepsilon}_{\mathbf{k}}-\mu$. The coefficients $|\tilde{\mathcal{P}}_{\mathbf{k}}|^2$ can thus be interpreted as

$$|\tilde{\mathcal{P}}_{\mathbf{k}}|^2 \equiv \begin{cases} u^2_{\mathbf{k}} & \text{for} \;\; |\mathbf{k}|<k_F \\ v^2_{\mathbf{k}} & \text{for} \;\; |\mathbf{k}|>k_F . \end{cases} \qquad (7)$$

The remaining part of (6) describes damped fermion states which are spread over a wide energy region. Most of them constitute an incoherent background almost insensitive to temperature. Among them there is however a certain fraction (very important for us) of a different character – these are the quasiparticle states emerging near the Fermi energy upon approaching T_c from above. They are located around $\omega=-(\tilde{\varepsilon}_{\mathbf{k}}-\mu)$ as can be seen in figure 2. This particular excitation branch, which is sort of a mirror reflection to the quasiparticle dispersion $\tilde{\varepsilon}_{\mathbf{k}}-\mu$, yields a missing information about the hole (particle) contribution $v^2_{\mathbf{k}}$ ($u^2_{\mathbf{k}}$) for momenta below (above) k_F. With these ingredients we can now estimate the Bogolubov angle (1) in the pseudogap regime.

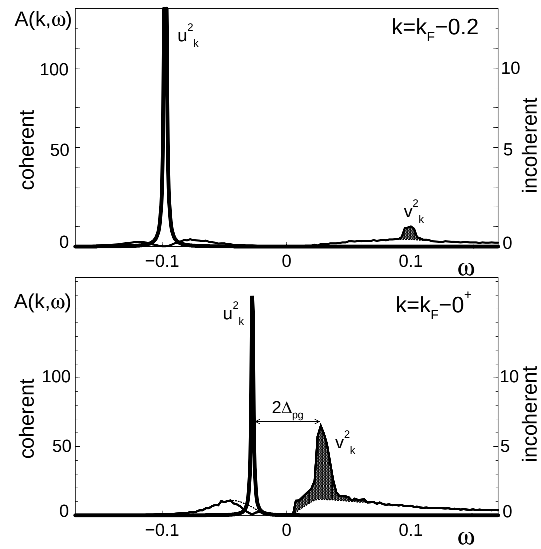

FIG. 3: Spectral function of the coherent (labels on the left axis) and the damped fermion states (labels on the right axis) for the momentum distant (upper panel) and close (lowe panel) to the Fermi surface. The weight of quasiparticle peak $|u_{\mathbf{k}}|^2$ and the weight of the hole contribution $|v_{\mathbf{k}}|^2$ were determined for the pseudogap regime at $T=0.004D$ (where D denotes the bandwidth).

We investigated numerically the spectral function (6) for several temperatures keeping a fixed total concentration of charge $n^F_{\uparrow}+n^F_{\uparrow}+2n^B$. The shadow branch appeared below T_p and we observed that a broadening of this branch gradually narrowed upon decreasing temperature. Ultimately, at $T\rightarrow T_c$, the shadow branch evolved into the delta function [17], signaling that cooperons became the long-lived quasiparticles.

One can give a simple analytical argument explaining appearance of the Bogolubov shadow branch upon approaching T_c from above. With a decreasing temperature bosons start gathering at lower and lower energies. Since their distribution $n^B_{\mathbf{q}}$ shrinks practically only to the smallest available energies (just above $E_{\mathbf{q}=\mathbf{0}}$) this produces a broadened peak of almost the Lorentzian shape

$$\frac{1}{N}\sum_{\mathbf{q}}{}' |\tilde{r}_{\mathbf{k},\mathbf{q}}|^2 n^B_{\mathbf{q}} \delta(\omega-\mu+\tilde{\varepsilon}_{\mathbf{q}-\mathbf{k}}) \simeq \frac{\Gamma_{\mathbf{k}}}{(\omega-\mu+\tilde{\varepsilon}_{\mathbf{k}})^2+\Gamma^2_{\mathbf{k}}} \quad (8)$$

because $E_{\mathbf{q}\sim\mathbf{0}} \sim 2\mu+0^{+}$. The other term in (6) containing $n^F_{\mathbf{q}-\mathbf{k}\downarrow}$ is responsible solely for the structureless incoherent background.

The amount of spectral weight contained in the shadow branch can be determined by integrating the spectral function describing the damped fermion states for a given T and subtracting from it the integrated spectral function at high temperatures. We illustrate this procedure

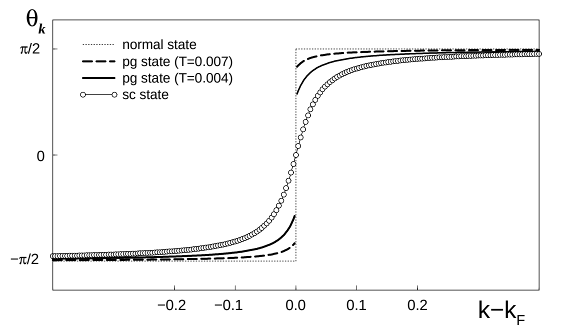

FIG. 4: Momentum dependence of the Bogolubov angle (1) for the superconducting, pseudogap and normal states.

in figure 3 for two representative momenta $k<k_F$ when the hole coefficient $v_{\mathbf{k}}^2$ is given by the shaded area. In the upper panel (corresponding to k located fairly below k_F) we obtain a residual (but still finite) hole contribution, hence the Bogolubov angle (1) is close to $-\pi/2$. In the bottom panel we show the situation corresponding to the fermion state located infinitesimally below k_F. One can notice that the quasiparticle peak and its mirror reflection (shadow) do not merge because of the finite pseudogap Δ_{pg}. The hole coefficient $v_{\mathbf{k}}^2$ increases for $k \rightarrow k_F - 0^+$ but still the particle weight (7) is dominant.

In figure 4 we show the calculated Bogolubov angle as a function of momentum measured from the Fermi surface. The thin line refers to the usual normal state with an abrupt change of $\theta_{\mathbf{k}}$ by π at k_F. For the pseudogap region we notice that appearance of the shadow branch has a substantial effect on the Bogolubov angle which becomes tilted near k_F. Yet, exactly at the Fermi surface the Bogolubov angle is discontinuous. The continuous BCS-type behavior is finally revived for temperatures $T \leq T_c$. Since the energy gap is almost fixed below T_c therefore the Bogolubov angle is practically frozen.

V. CONCLUDING REMARKS

We studied the effect of strong superconducting fluctuations above the transition temperature where the single fermions coexist and interact with the preformed pairs. To account for the influence of preformed pairs on the single particle excitation spectrum we used the selfconsistent RG-like method [15]. We found that in the pseudogap regime the long-lived quasiparticles (whose renormalized dispersion $\tilde{\varepsilon}_{\mathbf{k}}$ is depleted near k_F) are accompanied by the additional (shadow) branch responsible for the particle-hole mixing. We estimated the amount of particle and hole spectral weights and thus determined the Bogolubov angle above T_c which to our knowledge has not been done so far in any microscopic model.

Momentum dependence of the Bogolubov angle in the pseudogap regime was found to be distinct from the behavior of the normal and superconducting states. In the normal state (where no particle-hole mixing exists) $\theta_{\mathbf{k}}$ changes abruptly at k_F from $-\pi/2$ to $\pi/2$ while in the superconducting state (below T_c) it evolves continuously between these limiting values over the energy regime of several Δ_{sc} (where effectively the particle and hole excitations are mixed with one another). In the pseudogap regime the particle-hole mixing does show up leading to $|\theta_{\mathbf{k}}| \neq \pi/2$ but the Bogolubov angle is still discontinuous at the Fermi surface. If the novel STM technique could resolve the particle-hole mixing above T_c one may hope to obtain here discussed results for the underdoped HTSC cuprates. In this way, experimental measurements of the Bogolubov angle might explain what part of the phase diagram corresponds to the superconducting fluctuations.

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