Unconventional particle-hole mixing in the systems with strong superconducting fluctuations

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Development of the STM and ARPES spectroscopies enabled to reach the resolution level sufficient for detecting the particle-hole entanglement in superconducting materials. On a quantitative level one can characterize such entanglement in terms of the, so called, Bogoliubov angle which determines to what extent the particles and holes constitute the spatially or momentum resolved excitation spectra. In classical superconductors, where the phase transition is related to formation of the Cooper pairs almost simultaneously accompanied by onset of their long-range phase coherence, the Bogoliubov angle is slanted all the way up to the critical temperature $T_c$. In the high temperature superconductors and in superfluid ultracold fermion atoms near the Feshbach resonance the situation is different because of the preformed pairs which exist above $T_c$ albeit loosing coherence due to the strong quantum fluctuations. We discuss a generic temperature dependence of the Bogoliubov angle in such pseudogap state indicating a novel, non-BCS behavior. For quantitative analysis we use a two-component model describing the pairs coexisting with single fermions and study their mutual feedback effects by the selfconsistent procedure originating from the renormalization group approach.

I. INTRODUCTION

Such vastly distinct systems as the classical and/or high $T_c$ cuprate superconductors, the ultracold superfluid fermion atoms as well as certain cosmological (superfluid neutron stars) and even subatomic objects (odd-odd nuclei) reveal signatures of ideally coherent pairs consisting of particles from a vicinity of the Fermi surface. Obviously, what differs one case from another is an underlying mechanism and energy scale engaged in the pairing. They all however share the universal feature related to the effective Bogoliubov quasiparticles representing a superposition of the fermion particles and their absence. This emerging particle-hole (p-h) mixing [1] has a purely quantum nature (imposed by the structure of the corpuscular-wave dualism. One of its spectacular manifestations is the mechanism of subgroup Andreev reflection where an incident fermion-particle can convert into the pair with a simultaneous reflection of the fermion-hole what is indeed observed experimentally in superconductors [2], for the relativistic-like particles [3] and in quantum dots attached to superconducting electrodes [4, 5].

In the recent papers A. Balatsky and coworkers have emphasized that p-h mixing can be quantitatively probed by the present-day STM [1] and ARPES spectroscopies [6]. These techniques are capable to determine either the spatially [7] or momentum resolved [8] single particle excitation spectra of superconductors. In principle also the simultaneous $k$- and $r$-space measurements are feasible by means of the Fourier transformed quasiparticle interference imaging [9]. Roughly speaking, the p-h mixing manifests itself in the single particle spectra by appearance of two peaks around the Fermi level separated by twice the (pseudo)gap and whose spectral weights yield the information on particle/hole contributions to the Bogoliubov quasiparticles.

Usually for conventional superconductors these contributions are given by the BCS coefficients $u^2_k$ and $v^2_k = 1 - u^2_k$, so it is convenient to define the Bogoliubov angle [10]

$$\theta_k = \frac{\pi}{2} - 2 \arctan \left( \frac{|u_k|}{|v_k|} \right)$$

as a measure of the particle-hole mixing. Its magnitude can vary between $-\pi/2$ and $\pi/2$ depending on a momentum and indirectly on temperature. $\theta_k$ has a particularly clear interpretation in the pseudospin representation $\hat{s}_{k,z} = \frac{1}{2} \left( 1 - \hat{c}_{k\uparrow} \hat{c}^\dagger_{-k\downarrow} - \hat{c}_{-k\downarrow} \hat{c}^\dagger_{k\uparrow} \right)$, $\hat{s}_{k,x(y)} = \frac{1}{\sqrt{2}(\hat{c}_{k\uparrow} \hat{c}_{-k\downarrow} + (-) \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow})}$ introduced by P.W. Anderson [11], where it denotes an azimuthal angle of the vector $\langle \hat{s}_k \rangle$. Restricting to the part of Hilbert space where $\langle \hat{c}_{k\uparrow} \hat{c}_{-k\downarrow} \rangle$ the pseudospin eventually points down (up) when effective quasiparticles are represented by particles (holes). The upper and bottom panels of figure 1 illustrate such behavior well known for the normal and superconducting states [11].

In general, pseudospins obey the non-trivial dynamics governed by the Bloch-type equations of motion [11]. This aspect has a particular importance in the context of ultracold atoms where traversing through the Feshbach resonance can lead to the soliton-like solutions [12]. On the other hand, in the highly inhomogeneous cuprate superconductors with pairing on a local (interactomic) distance both the excitation spectrum [7] and the Bogoliubov angle are strongly varying in space. Such issue has been already explored within the Bogoliubov de Gennes approach and results were confronted with the available STM data [1].

Since the Bogoliubov angle (1) is sensitive to existence of the paired fermions one may ask if any signatures of the p-h mixing would be able to appear above $T_c$. ARPES studies [13] confirm that the superconducting state of cuprates obeys roughly the usual BCS behavior but there
is still no firm agreement on the nature of pseudogap state and its relation to superconductivity [14]. Nevertheless, various experimental data [15, 16] seem to indicate that preformed fermions’ pairs are present already in the normal state (at least in the underdoped samples) at temperatures up to dozen Kelvin above $T_c$. Transition temperature might correspond to the onset of long-range phase coherence [17]. Another evidence of the preexisting pairs above $T_c$ is known for the ultracold atoms of Li$^6$ and K$^{40}$. Near the Feshbach resonance the weakly bound boson molecules are scattered into the Cooper-like pairs and such unitary limit is in a crossover between the BCS and BEC regimes being influenced by strong quantum fluctuations [18].

Our purpose here is to explore the impact of preformed pairs on the Bogoliubov angle in the pseudogap state. In particular, we address the question whether p-h mixing can at all show up above $T_c$ and if so, then how it would manifest itself. For the considerations we use a phenomenological two-component model [19] where itinerant fermions and their paired counterparts are introduced without referring to any specific microscopic mechanism. From the selfconsistent treatment of interactions between the paired and single fermions we find the evidence of particle-hole mixing signified by $|\theta_k| \neq \pi/2$. Furthermore, lack of the phase coherence above $T_c$ leads to a discontinuity of $\theta_k$ at $k_F$. We will show that in the pseudogap state the Bogoliubov angle behaves in a manner which partly resembles the normal and partly the superconducting phases (see figure 1).

In the next section we briefly introduce the model and discuss its main properties. Methodological details are presented in section III and the essential part on the p-h mixing for the pseudogap state is described in section IV. We finally summarize our results and point out some related unresolved problems.

II. PHENOMENOLOGICAL MODEL

For modelling the pseudogap state we use the following Hamiltonian [19]

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

(2)

where operators $\hat{c}_{\mathbf{k}\sigma}^\dagger$ refer to annihilation (creation) of single fermions with the energy $\varepsilon_k$ and $\hat{b}_{\mathbf{q}}^\dagger$ correspond to the local pairs of energy $E_{\mathbf{q}}$. Potential of the interac-
tion between the single and paired fermions is denoted by $g_{k,q}$. For simplicity, we shall assume that concentration of pairs per lattice site is small enough so that $\hat{\delta}^{(l)}_{q}$ obey the usual bosonic commutation relations (we neglect the hard-core effect).

This model (2) has been invented [19] and explored by J. Ranninger with coworkers [20] and independently by T.D. Lee et al [21] as well as some other groups. Starting from various microscopic models several authors [22] have also concluded that the relevant physics of strongly correlated cuprates is well captured by the fermion and boson degrees of freedom expressed by the Hamiltonian (2). Moreover, such model well describes the ultracold fermion atoms interacting with the Feshbach resonance [18, 23].

In the simplest mean-field approach one can linearize the interaction term so that the decoupled boson and fermion parts become exactly solvable [19]. The resulting spectrum of fermions has then BCS structure $A_{MF}(k,\omega) = v_{k}^{F} \delta(\omega - E_{k}) + v_{k}^{B} \delta(\omega + E_{k})$ with the usual quasiparticle energy $E_{k} = \sqrt{(\varepsilon_{k} - \mu)^{2} + \Delta_{k}^{2}}$ and coherence factors $v_{k}^{F}, v_{k}^{B} = \frac{1}{2}[1 \pm (\varepsilon_{k} - \mu)/E_{k}]$ which lead to the standard Bogoliubov angle. Energy gap of the single particle excitation spectrum is effectively given by $\Delta_{k} = g_{k,0} \sqrt{(v_{k}^{F})}$. This means that fermions undergo transition to the superconducting state if and only if the Bose-Einstein condensation of bosons takes place [19]. Actually, the latter property is valid exactly [24] without limitations to any approximation.

The mean-field treatment does not take into account the quantum fluctuations whose efficiency increases upon approaching $T_{c}$ and above of it. In the next section we present the method which enables a selfconsistent study of the boson-fermion feedback effects. In particular, we will analyze the remnants of superconducting correlations above $T_{c}$ and study their effect on the Bogoliubov angle.

III. THE PROCEDURE

For studying the model (2) we use the selfconsistent, non-perturbative procedure based on a canonical transformation $\hat{H} \longrightarrow e^{\hat{S}(l)} \hat{H} e^{-\hat{S}(l)}$ with a continuous formal parameter $l$ [25]. The main idea is to eliminate the interaction part $g_{k,q}$ through a sequence of infinitesimal steps $l \rightarrow l + \delta l$. Proceeding along the lines of the Renormalization Group (RG) technique one starts from renormalizing the high energy sector and subsequently turns to the low energy sector (by latter we mean the fermion states close to $\mu$ and boson states near $2\mu$). We briefly describe some technicalities in order to clarify how the particle and hole spectral contributions can be evaluated within this procedure.

Practically we start by setting $\hat{H}(l) \equiv e^{\hat{S}(l)} \hat{H} e^{-\hat{S}(l)}$, where $\hat{H}(0)$ corresponds to the initial Hamiltonian, and then construct the flow equation $\partial_{l}\hat{H}(l) = [\hat{\eta}(l), \hat{H}(l)]$ with the generating operator $\hat{\eta}(l) \equiv \partial_{l}\hat{S}(l)$. Following the original proposal of Wegner [25] we choose $\hat{\eta}(l) = [\hat{H}_{0}(l), \hat{H}_{int}(l)]$, where $\hat{H}_{0}(l)$ denotes the total kinetic energy of fermions and bosons whereas $\hat{H}_{int}(l)$ stands for their interaction. From a straightforward algebra we obtain $\hat{\eta}(l) = -\frac{1}{2\pi} \sum_{k,q} \alpha_{k,q}(l) \left(\hat{c}_{q}^{+} \hat{c}_{q - k}^{+} \hat{c}_{k} \hat{c}_{q} - \mathrm{h.c.}\right)$ with $\alpha_{k,q}(l) = (\varepsilon_{k}(l) + \varepsilon_{q - k}(l) - E_{q}(l)) g_{k,q}(l)$. One can prove analytically [26] that such antihermitean operator $\hat{\eta}(l)$ indeed guaranties an asymptotic disappearance of the boson-fermion coupling $\lim_{l \rightarrow \infty} g_{k,q}(l) = 0$.

Applying this scheme to the boson-fermion Hamiltonian (2) we obtain the following set of coupled flow equations [26]

$$\partial_{l} g_{k,q}(l) = -\alpha_{k,q}(l) g_{k,q}(l)$$
$$\partial_{l} \varepsilon_{k}(l) = \frac{2}{N} \sum_{q} \alpha_{k,q}(l) |g_{k,q}(l)|^{2} n_{q}^{(B)}$$
$$\partial_{l} E_{q}(l) = \frac{2}{N} \sum_{k} \alpha_{k-q,k}(l) |g_{k-q,k}(l)|^{2} \times \left(-1 + n_{k-q}^{(F)} + n_{k}^{(F)}\right)$$

We have solved them numerically considering fermions coupled with bosons on a lattice avoiding thus any need for the infrared cutoffs. The fixed point values

$$\lim_{l \rightarrow 0} \varepsilon_{k}(l) \equiv \tilde{\varepsilon}_{k}, \quad \lim_{l \rightarrow 0} E_{q}(l) \equiv \tilde{E}_{q}$$

turned out to reveal the following features:

(a) for $T < T_{c}$ the renormalized fermion dispersion $\tilde{\varepsilon}_{k}$ develops a true gap at $\mu$ which evolves into a pseudogap for $T_{c} < T < T_{p}$.
(b) the effective boson dispersion $\tilde{E}_q$ shows the long-wavelength Goldstone mode for $T < T_c$ and its remnants are preserved even in the pseudogap state \cite{27}.

For a complete information about the fermion and boson spectra we need to proceed with transformations for the individual operators $c_{\kappa \sigma}^{(t)}(l) \equiv e^{S(t)} c_{\kappa \sigma} e^{-S(t)}$ and $\hat{b}_q^{(t)}(l) \equiv e^{S(t)} \hat{b}^+_q e^{-S(t)}$ which is a rather difficult task because $\hat{S}(t)$ is not known explicitly. Since our primary interest is in estimating the particle-hole mixing for the single particle fermion excitations we focus on the flow equation $\partial_t \hat{c}_{\kappa \sigma}^{(t)}(l) = [\hat{n}, \hat{c}_{\kappa \sigma}^{(t)}(l)]$. The generating operator $\hat{n}$ chosen according to Wegner's prescription \cite{25} yields the following ansatz for fermion operators \cite{27}

$$
\begin{align*}
\partial_t u_k(l) &= v_k(l) c_k(l) + v_k(l) c^+_{-k}
\end{align*}
$$

We explored them numerically along with the equations $\partial_t \hat{c}_{\kappa \sigma}(l)$, $\partial_t E_q(l)$, $\partial_t g_{k q}(l)$ on the 2-dimensional square lattice with the initial $l = 0$ tight-binding dispersion $\varepsilon_k(0) = -2t \cos(k_x a) + \cos(k_y a)$ and the localized boson energy $E_q(0) = E_0$. Moreover, we imposed $g_{k q}(0) = g \left( \cos(k_x a) - \cos(k_y a) \right)$ to obtain the d-wave symmetry of energy gap (pseudogap) below (above) $T_c$. We solved the coupled flow equations iteratively by the Runge-Kutta method for $E_0(0) = 0.2t$ keeping a fixed charge concentration $n_{tot} = 2$ when the concentration of fermions $n^F = 1 + x$ yield the realistic value $x \sim 0.1$. In figures 2-4 we present the results obtained along the antinodal direction (0, 0) $\leftrightarrow (\pi, 0)$ i.e. for $k_y = 0$.

Our ansatz (7,8) generalizes the standard Bogoliubov-Valatin transformation by including the effect of scattering on finite momentum preformed pairs. Influence of such scattering shows up in the effective single particle spectral function which takes the following form

$$
\begin{align*}
A(k, \omega) &= |\tilde{u}_k|^2 \delta (\omega + \mu - \tilde{\varepsilon}_k) + \frac{1}{N} \sum_{q \neq 0} (n^B_q + n^F_{q + k}) |\tilde{u}_{k, q}|^2 \delta (\omega + \mu - \tilde{\varepsilon}_{q + k} + \tilde{E}_q) \\
+ |\tilde{v}_k|^2 \delta (\omega - \mu + \tilde{\varepsilon}_k) + \frac{1}{N} \sum_{q \neq 0} (n^B_q + n^F_{q - k}) |\tilde{v}_{k, q}|^2 \delta (\omega - \mu + \tilde{\varepsilon}_{q - k} - \tilde{E}_q),
\end{align*}
$$

where $\tilde{u}_k$, $\tilde{v}_k$ and $\tilde{u}_{k, q}$, $\tilde{v}_{k, q}$ denote the asymptotic $l \to \infty$ values. We have determined them numerically solving the flow equations (9-12) for the fixed total charge concentration $n_{tot} = 2 \sum_q n^B_q + \sum_k (n^F_k + n^F_{-k})$.

The structure of spectral function (13) indicates that besides the narrow peaks (long-lived states) there also forms a background of the damped (finite lifetime) states. If we neglected $u_{k, q}$ and $v_{k, q}$ then the flow equations (9,10) would simplify to $\partial_t u_k(l) = \sqrt{n^B_0} \alpha_{-k, 0}(l) v_k(l)$ and $\partial_t v_k(l) = -\sqrt{n^B_0} \alpha_{k, 0}(l) u_k(l)$ yielding the invariance $|v_k(l)|^2 + |u_k(l)|^2 = 1$. By rewriting the first equation as $\int_{u_k(l)=0}^\infty \frac{du_k(l)}{\sqrt{1 - |u_k(l)|^2}} = \sqrt{n^B_0} \int_0^\infty \alpha_{-k, 0}(l) dl$ we then right away reproduce the mean-field solution $\tilde{u}_k, \tilde{v}_k = \frac{1}{2} \left( 1 \pm \frac{\tilde{\varepsilon}_k - \mu}{\sqrt{\tilde{\varepsilon}_k^2 - n^F_q |\tilde{u}_{k, 0}|^2}} \right)$.

In order to go beyond this BCS solution we need to take into account the effect of scattering on the finite momentum pairs affecting the spectral function (13) through the coefficients $\tilde{u}_{k, q}$ and $\tilde{v}_{k, q}$. We shall do it for $T > T_c$.

IV. PARTICLE-HOLE MIXING ABOVE $T_c$

Preformed pairs occupy in the normal phase only the finite momenta states (in other words $\langle \tilde{b}_{q=0} \rangle = 0$) therefore the equations (10, 11) imply $\nu_k(l) = 0$ and $u_{k, q}(l) = 0$. 


These states emerge around fraction (very important to us) of a different character – most insensitive to temperature and can be regarded as among the damped fermion states. Most of them are aliasing temperature the preformed pairs start populating the lower and lower energies so that \( u_\text{q}^2 \) is dominated by the states located just above \( E_{\text{Q=0}} \). The resulting spectral function (16) reduces then to

\[
A(k,\omega) \simeq |\tilde{u}_k|^2 \delta (\omega + \mu - \tilde{\varepsilon}_k) + |v_k|^2 \frac{\Gamma_k}{\pi} \left( \omega - \mu - \tilde{\varepsilon}_k \right)^2 T_k^2
\]

where the last term describes solely the structureless incoherent background. We obtained \(|v_k|^2\) by integrating the spectral function with respect to \( \omega \) for a given \( T \) and subtracting from it the integrated spectral function for high temperatures.

We notice that near \( k_F \) the long-lived state and its mirror reflection (a shadow) do not merge because of a finite value of the pseudogap \( \Delta_{pg} \). Figure 4 shows the calculated Bogoliubov angle as a function of momentum measured with respect to the Fermi surface. In the pseudogap region the shadow branch has a substantial effect on the Bogoliubov angle leading to the p-h mixing near \( k_F \). Yet, exactly at the Fermi surface the Bogoliubov angle is discontinuous. The BCS-type behavior is finally recovered at temperatures \( T \lesssim T_c \) as marked by the open circles in figure 4. Since the magnitude of superconducting gap does not much change \([28]\) the Bogoliubov angle is below \( T_c \) practically frozen (temperature-independent).

**V. CONCLUDING REMARKS**

We have analyzed the effect of strong superconducting fluctuations above the transition temperature \([29]\) where the single fermions coexist and interact with the preformed pairs. Influence of pairs on the single particle excitation spectrum has been studied within the selfconsistent RG-like method \([25]\). We have found that near \( k_F \) the renormalized dispersion \( \tilde{\varepsilon}_k \) is depleted above \( T_c \) and additionally there appears a shadow branch in the fermion spectrum responsible for the particle-hole mixing. We have estimated the particle and hole spectral weights thereby determining the Bogoliubov angle for the normal state with preformed pairs.
We have found that momentum dependence of the Bogoliubov angle in the pseudogap regime differs qualitatively from its behavior for the normal and superconducting states. In the normal state (where particle-hole mixing is absent) $\theta_k$ changes abruptly at $k_F$ from $-\pi/2$ to $\pi/2$ whereas in the superconducting state (below $T_c$) the Bogoliubov angle continuously evolves between these extreme values over an energy regime $\sim \Delta_{sc}$, so that particle and hole excitations are mixed with one another. In the pseudogap regime we find that $|\theta_k| \neq \pi/2$ but still at the Fermi surface the Bogoliubov angle is discontinuous. We hope that STM and ARPES techniques would be able to detect such unconventional relation between the particle and hole weights predicted for the systems with strong pairing fluctuations.

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