Bogoliubov Angle, Particle-Hole Mixture and Angular Resolved Photoemission Spectroscopy in Superconductors.

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Superconducting excitations —Bogoliubov quasiparticles — are the quantum mechanical mixture of negatively charged electron (-e) and positively charged hole (+e). We propose a new observable for Angular Resolved Photoemission Spectroscopy (ARPES) studies that is the manifestation of the particle-hole entanglement of the superconducting quasiparticles. We call this observable a *Bogoliubov angle.* This angle measures the relative weight of particle and hole amplitude in the superconducting (Bogoliubov) quasiparticle. We show how this quantity can be measured by comparing the ratio of spectral intensities at positive and negative energies.

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i) *BA and particle-hole mixture in paired states.* The analog of the conduction electrons in the superconductors are the quasiparticles. Unlike electrons, the superconducting quasiparticles do not carry definite charge. The same quantum mechanical dualism that allows electron to be at the same in two states is at play when one considers the Bogoliubov quasiparticles in superconducting state: the quasiparticle is a coherent combination of an electron and its absence ("hole"). Particle-hole dualism of quasiparticles is responsible for a variety of profound phenomena in superconducting state such as Andreev reflection, the particle-hole conversion process that is only possible in superconductor.

In this paper we introduce a quantity that parametrizes the mixture in terms of an angle, we call this angle a *Bogoliubov angle* (BA), see Fig. 1. We discuss how ARPES measurements allow one to visualize the Bogoliubov angle and thus to reveal particle hole dualism. Here we introduce BA for ARPES in a similar way as it has been introduced in STM[1].
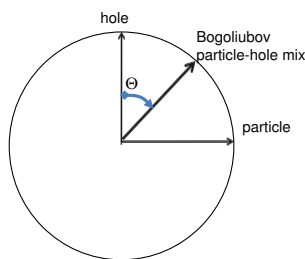

FIG. 1: (Color online) Circle parametrizing Bogoliubov admixture angle is shown. For $\Theta = 0, \pi/2$ the mixture reduces to purely hole-like and particle-like state. At arbitrary angle one deals with true Bogoliubov quasiparticles.

To illustrate the point about BA, we can look at the textbook BCS case first. We will show that convenient definition of BA is :

$$\Theta_k = \arctan[(\frac{|u(\mathbf{k})|^2}{|v(\mathbf{k})|^2})^{1/2}], \qquad (1)$$

with the conventional coherence factors, see Fig. 2.

Bogoliubov showed[2] that natural excitations in the superconducting state are a linear combination of particle and hole excitations with the coherence factors $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. They describe the unitary transformation from particle and hole operators to quasiparticles that are:

$$\gamma_{\mathbf{k},\uparrow} = u_{\mathbf{k}} c_{\mathbf{k},\uparrow} + v_{\mathbf{k}} c_{-\mathbf{k},\downarrow}^\dagger, \qquad (2)$$

with the constraint $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ for any $\mathbf{k}$ (normalization)

Constraint is satisfied with the choice

$$|u_k|^2 = \sin^2 \Theta_k,$$
$$|v_k|^2 = \cos^2 \Theta_k, \qquad (3)$$

and quantity

$$\Theta_k = \arctan((\frac{|u_k|^2}{|v_k|^2})^{1/2}) \qquad (4)$$

Thus defined Bogoliubov angle Θ_k is naturally related angle introduced by Anderson[3].

To make a connection to ARPES we use the identity[2]

$$A(k, \omega > 0) = |u(\mathbf{k})|^2 \delta(\omega - \mathbf{E_k}),$$
$$A(k, \omega < 0) = |v(\mathbf{k})|^2 \delta(\omega + \mathbf{E_k}) \qquad (5)$$

Thus we have finally the main result to be used in ARPES

$$\Theta_k = \arctan(\frac{A(\mathbf{k}, \omega > 0)}{A(\mathbf{k}, \omega < 0)})^{1/2}. \qquad (6)$$

Experimentally $A(\mathbf{k}, \omega > 0), A(\mathbf{k}, \omega < 0)$ can be determined using ARPES intensity at positive (above E_F) and negative (below E_F) energy.
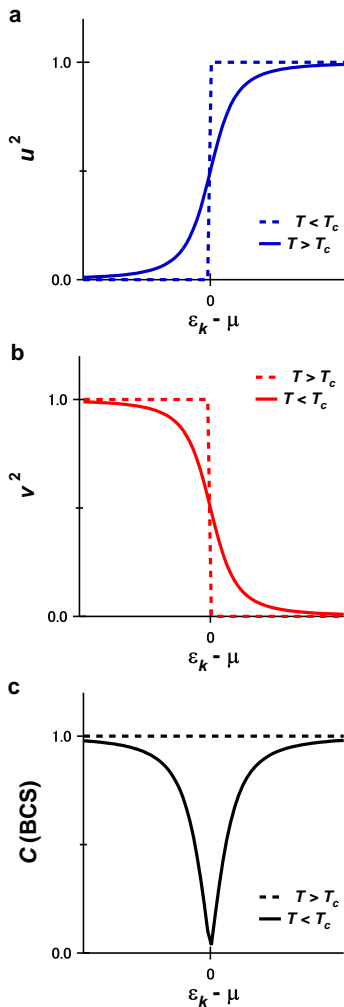
FIG. 2: (Color online) BCS coherence factors $u^2(\mathbf{k}), v^2(\mathbf{k})$ are shown as functions of energy. The function $C(\mathbf{k}) = |u^2(\mathbf{k}) - v^2(\mathbf{k})| = |\cos 2\Theta(\mathbf{k})|$, shows substantial departures from unity only in the energy range on the scale of the gap Δ near the Fermi energy, where there are substantial pairing correlations.
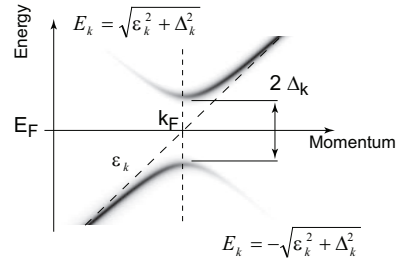

FIG. 3: Particle hole admixture in conventional BCS superconductor as a function of energy is shown. Experimental challenge is to find out BA as a function along the momentum on FS in real high T_c materials.

Θ_k is the central quantity we are interested in and we define it as a Bogoliubov angle. It represents a local mixture between particle and hole excitations for an eigenstate n (momentum k eigenstate in this context). For example, for $\Theta_k = 0$ the Bogoliubov excitation will be a hole. In the opposite case of $\Theta_k = \pi/2$ quasiparticle is essentially an electron. The angle that corresponds to the strongest admixture between particle and holes is $\Theta_k = \pi/4 = 45°$.

ii) *ARPES and BA analysis.* We will now demonstrate how one can extract BA from ARPES. Although ARPES probes mostly the occupied portion of the single-particle spectral function[4] (i.e. states below E_F, $\omega < 0$) due to the Fermi-Dirac function $f(\omega, T)$ cut-off near E_F, it is still possible to obtain some information about the states above E_F. Because of the high T_c of some superconducting cuprates, ARPES measurements could be performed in the superconducting state at a relatively high temperature; such that the upper branch of the Bogoliubov quasiparticle dispersion near the nodal region, where the gap is smaller, could lay within the energy range where the value of $f(\omega, T)$ still appreciably differs from zero. In this situation, the Bogoliubov band dispersion above E_F could be seen in the raw spectra allowing a further analysis of its property[5]. In a recent study of a high-T_c cuprate, Bi2212, the temperature dependence of the Bogoliubov dispersion were measured revealing a sudden onset of the superconducting gap at T_c near the nodal region[6]. In this section, the Bogoliubov angle analysis was applied near the nodal region to demonstrate the concepts aforementioned. The experimental details of the data presented here can be found in Ref.[6].

Fig. 4(a) demonstrates a false color plot of raw ARPES spectra along the cut position indicated in the inset of (d) at 87 K. In addition to the high intensity region below the Fermi energy (the occupied band dispersion), there is also a less-bright region above E_F, which is the thermally populated Bogoliubov band above E_F. The raw energy distribution curves (EDCs) in the region where the Bogoliubov dispersion is visible are displayed in Fig. 4 (c). A small peak above E_F representing the upper branch of Bogoliubov dispersion can be clearly seen near the Fermi crossing momentum k_F, where the gap is minimal. This small peak above E_F becomes less pronounced when moving away from k_F because the peak position of the Bogoliubov dispersion is moving away from E_F (see also Fig. 3) , thus it is no longer able to be thermally populated at this temperature.
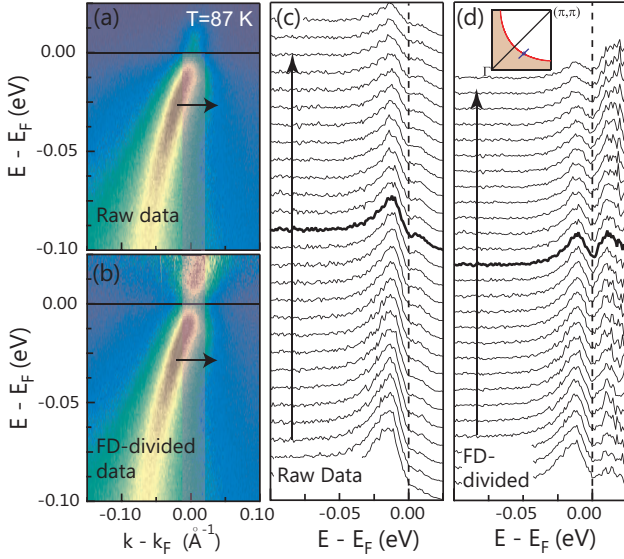
To illuminate these small features above E_F, the

FIG. 4: (Color online)(a) The false-color plot of raw ARPES spectra along the cut indicated in the inset of (d) in unit of the detector angle. The data were taken on a slightly underdoped Bi2212 single crystal with $T_C = 92$ K at a temperature of 87 K using 7 eV photons to excite the photoelectrons. The total energy resolution is set to 3.2 meV. (b) Fermi-Dirac function divided spectrum of (a). (c) EDCs stack plot of the raw spectra within the shaded area of (a). (d) EDC stack plot of the FD-divided spectra within the same shade area as also indicated in (b). The thick solid curve is the EDC where $|u_k|^2 \sim |v_k|^2$ and could be defined as the Fermi crossing point, k_F.

ARPES spectrum is divided by an effective Fermi-Dirac function, which is generated by convolving $f(\omega, T = 87K)$ with 3.2 meV instrument resolution via a Gaussian convolution. The FD-divided ARPES spectrum image is shown in Fig. 4 (b). The intensity break near the E_F vividly demonstrates the existence of a gap and two branches of dispersion centered at E_F, as expected for the Bogoliubov quasiparticle dispersion of a superconductor. The EDCs within the shaded area are plotted in Fig. 4(d). Two peaks in each EDC can now be clearly seen exhibiting a evolution of the relative peak height at different momentum positions due to the coherence factors. Before reaching k_F (EDCs below the thick solid curve), the peak below E_F has a higher intensity than that above E_F. After passing k_F (EDCs above the thick solid curves), the relation reverses; the peak above E_F now has a higher intensity than that below E_F. This cross over behavior near k_F is also known to be a characteristic of the Bogoliubov quasiparticle dispersion of a superconductor. Since the peak intensity are related to the coherence factors $|u_k|^2$ and $|v_k|^2$, they could be used for the Bogoliubov angle analysis[5].

To extract the peak intensity, we simply fit the FD-divided EDCs with two equal width Lorentizans in a narrow energy widow, ranging from -20 meV to 20 meV, in which the signal has not yet completely masked by the
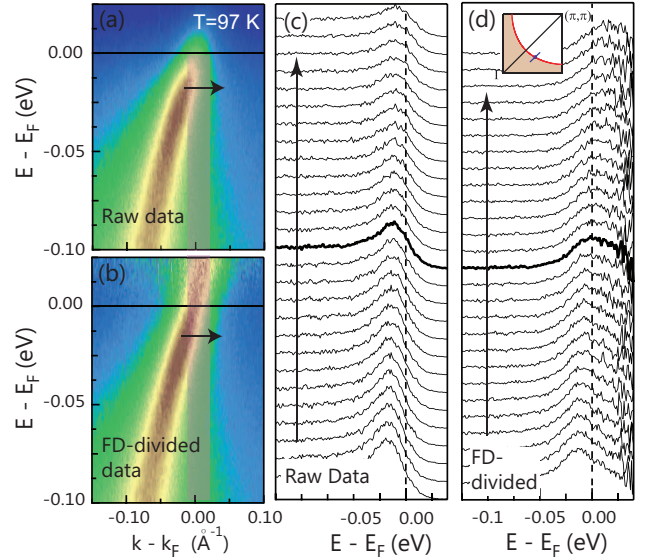
FIG. 5: (Color online) Spectra taken at a temperature of T =97 K (above T_c) at the same momentum position as that shown in Fig. 4.
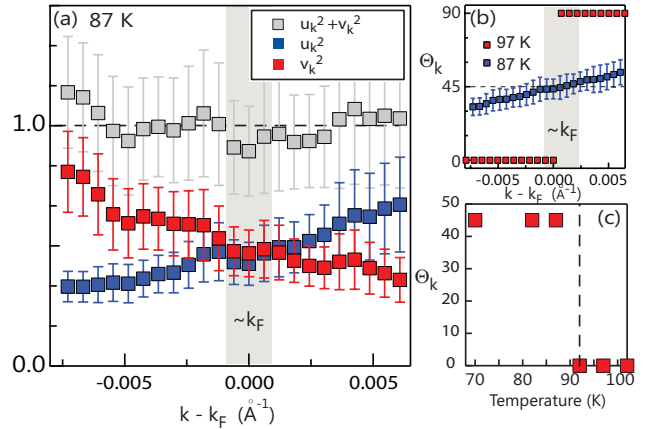

FIG. 6: (Color online) (a) The extracted $|u_k|^2$ and $|v_k|^2$ at 87 K. (b) The Bogoliubov angle Θ_k near the Fermi crossing point at 87 K. (c) The temperature dependence of Θ_k at k_F. The error bars are estimated by the 99.7% confidence interval of the fitting parameters.

amplified noise due to the Fermi function division. This noise amplification at higher energy above E_F is also the main reason why we use the peak intensity for the BA analysis, instead of using peak area. We also note that this Lorentizan fitting is primarily used for obtaining the peak height, not for achieving a good fit to the spectrum line shape. Fig. 6 (a) shows the extracted peak heights, which are normalized by the average sum of the two peaks in each FD-divided EDC within this momentum region. The normalized peak hight of the peak below E_F is assigned a weight $|v_k|^2$, while that of the peak above E_F is assigned a weight $|u_k|^2$. Compared to Fig. 2(a) and (b), the $|u_k|^2$ and $|v_k|^2$ extracted form the data

are qualitatively consistent with what is expected in the conventional BCS superconductor. We also note that the sum of the extracted $|u_k|^2$ and $|v_k|^2$ is a constant within the experimental error bars. This suggests that the normalization condition of $|u_k|^2 + |v_k|^2 = 1$ is satisfied in this momentum region, as a conventional BCS superconductor does. We also note that this analysis is fully consistent with an earlier work on a different cuprate[5].

The Bogoliubov angle Θ_k is displayed in Fig. 6 (b), which is calculated using Eq. 6. The Θ_k increase monotonically across the Fermi crossing point k_F suggesting a continuously evolution of the particle and hole mixing within this momentum window. Furthermore, $\Theta_k = \pi/4$ at k_F within the error bar of our experimental data. This confirms that the particle and hole mix equally at k_F as expected for a superconductor.

Situation is very different, however, at $T > T_c$. No Bogoliubov quasiparticle dispersion, nor a spectral gap at E_F can be resolved in this momentum region, as demonstrated in Fig. 5 (see also Ref.[6]). There is only one peak can be identified in the Fermi function divided EDCs, which disperses across E_F (Fig. 5 (b) and (d)) suggesting there is no gap in the spectral. To generalize Bogoliubov angle to this situation, we define $(u_k, v_k) = (1,0)$ when the quasiparticle peak in the FD-divided EDC is below or at E_F, and $(u_k, v_k) = (0,1)$ when the peak of the FD-divided EDC is above E_F. This will induce an angle jump from 0 to 90 deg near the k_F as shown in Fig. 6 (b). Thus, Θ_k equals to zero at k_F and a sudden jump across the K_F suggests an absence of the particle and hole mixing above T_c at this momentum position. The Θ_k at k_F at several different temperatures is shown in Fig. 6(c). Here we used notations that the Bogoliubov angle is zero by taking its value for filled states. The behavior of the electron at this momentum position (near nodal region) appears to be very conventional, despite the existence of a pseudogap near the antinodal region, see also[6] and the reference therein.

The BA at several different positions near the nodal region on the Fermi surface at a temperature of 82 K is shown in Fig. 7(a). The BA is found to be $\pi/4$ suggesting again that the particle and hole mix equally on the Fermi surface at least near the nodal region. For the region in the shaded area indicated in Fig. 7(a), the upper branches of the Bogoliubov band disperses too far way from the E_F and become less accessible by the thermal energy at this temperature. We note that although the feature of Bogoliubov peak above E_F can still be identified in the raw EDCs near k_F up to $\phi = 15°$, the Bogoliubov peak above E_F in the FD-divided spectrum is too noisy to be useful for the BA analysis. Therefore, we can't obtain any conclusive information about the BA for the momentum positions within this shaded area of Fig. 7. We also remark that at a temperature above T_c, Fig. 7 (b), the Bogoliubov quasiparticle peak above E_F has not yet been resolved in the pseudogap state at

this momentum region, even through it is well defined at a temperature below T_c (82 K). This may suggest a
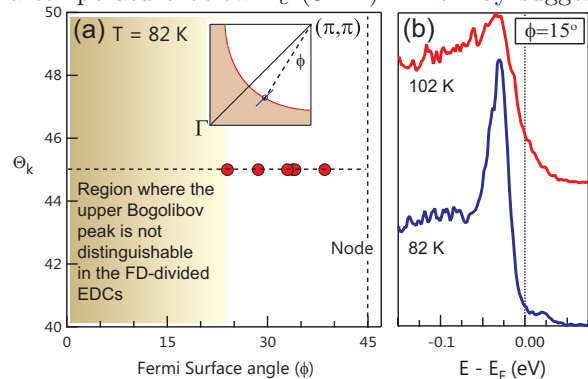

FIG. 7: (Color online) (a) The Bogoliubov angle at a temperature 82 K along the Fermi surface where the Bogoliubov peak can be unambiguously distinguished from the noise level in the FD-divided spectrum. (b) Raw EDC at $\phi = 15°$ at temperatures above (102 K, red curve) and below T_c (82K, blue curve). At this momentum position, a gap (pseudogap) still exists in the spectrum of 102 K.

qualitative difference of the particle-hole mixing in the pseudogap state from that of the superconducting state. However, we could not rule out the possibility that the absence of a Bogoliubov quasiparticle dispersion feature above T_C at this momentum region region is due to the significant broadening of the peak in the spectrum. Further study is needed to clarify this issue.

In conclusion, we have introduced a new spectroscopic measure, Bogoliubov angle $\Theta(\mathbf{k})$. BA can be extracted from existing ARPES data. This measure allows one to image particle-hole admixture in the superconducting state.

The ideas presented here are quite general and are applicable to a variety of superconductors, including conventional superconductors. One can investigate Bogoliubov angle in a variety of states, including vortex state and normal state with superconducting correlations, e.g. so called pseudogap (PG) state. As a future application of these ideas we suggest using Bogoliubov angle to identify how robust the particle-hole mixture is in the normal state of cuprates. At present stage we do not have enough resolution to perform this analysis. Another interesting question is the BA behavior with temperature. Answers to these questions will shed light on the nature of PG state and would allow us to differentiate between different scenarios of PG state, e.g. flux phases[7] and D wave density wave (DDW)[8].

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