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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1) 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$^1$.

![Diagram of Bogoliubov Angle](image)

FIG. 1: (Color online) Circle parametrizing Bogoliubov 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:

$$\Theta_k = \arctan \left( \frac{|u(k)|^2}{|v(k)|^2} \right)^{1/2},$$

with the conventional coherence factors, see Fig. 2.

Bogoliubov showed that natural excitations in the superconducting state are a linear combination of particle and hole excitations with the coherence factors $u_k$ and $v_k$. They describe the unitary transformation from particle and hole operators to quasiparticles that are:

$$\gamma_{k,\uparrow} = u_k c_{k,\uparrow} + v_k c_{-k,\downarrow}^\dagger,$$

with the constraint $|u_k|^2 + |v_k|^2 = 1$ for any $k$ (normalization)

Constraint is satisfied with the choice

$$|u_k|^2 = \sin^2 \Theta_k,$$

$$|v_k|^2 = \cos^2 \Theta_k,$$

and quantity

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

Thus defined Bogoliubov angle $\Theta_k$ is naturally related angle introduced by Anderson$^2$.

To make a connection to ARPES we use the identity$^2$:

$$A(k, \omega > 0) = |u(k)|^2 \delta(\omega - E_k),$$

$$A(k, \omega < 0) = |v(k)|^2 \delta(\omega + E_k)$$

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

$$\Theta_k = \arctan \left( \frac{A(k, \omega > 0)}{A(k, \omega < 0)} \right)^{1/2}.$$
(Color online) BCS coherence factors \( u^2(k), v^2(k) \) are shown as functions of energy. The function \( C(k) = |u^2(k) - v^2(k)| = |\cos 2\Theta(k)| \), shows substantial departures from unity only in the energy range on the scale of the gap \( \Delta \) near the Fermi energy, where there are substantial pairing correlations.

\[ \Theta_k \] 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 \( \Theta_k = \pi/4 = 45^\circ \).

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 (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 properties. 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. 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. 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
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.

To extract the peak intensity, we simply fit the FD-divided EDCs with two equal width Lorentzians in a narrow energy widow, ranging from -20 meV to 20 meV, in which the signal has not yet completely masked by the 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. 4(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 line. The normalized peak hight of the peak above $E_F$ is assigned a weight $|v_k|^2$, while that of the peak below $E_F$ 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.

The Bogoliubov angle $\Theta_k$ is displayed in Fig. 6 (b), which is calculated using Eq. 6. The $\Theta_k$ 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. 2). 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. 5 (b). Thus, $\Theta_k$ 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 $\Theta_k$ 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 5 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 away 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 $\phi = 15^\circ$, 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 though it is well defined at a temperature below $T_c$ (82 K). This may suggest a 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 $\Theta(k)$. 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 further 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 and D wave density wave (DDW).

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