Bogoliubov angle and visualization of particle-hole mixture in superconductors.

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Recent Scanning Tunneling Microscope (STM) experiments offer a unique insight into the inner workings of the superconducting state of superconductors. We propose a new observable quantity for STM studies that is the manifestation of the particle-hole dualism of the quasiparticles. We call it a Bogoliubov angle. This angle measures the relative weight of particle and hole amplitude in the superconducting (Bogoliubov) quasiparticle. We argue that this quantity can be measured locally by comparing the ratio of tunneling currents at positive and negative biases. This Bogoliubov angle allows one to measure directly the energy and position dependent particle-hole admixture and therefore visualize robustness of superconducting state locally. It may also allow one to measure the particle-hole admixture of excitations in normal state above critical temperature and thus may be used to measure superconducting correlations in pseudogap state.

I. INTRODUCTION

The dual particle-wave character of microscopic objects is one of the most striking phenomena in nature. This dualism is ubiquitous in the microworld. Most notably, the two-slit experiments of Stern and Gerlach revealed the interference and, hence, the wave nature of electrons. In the condensed matter systems, such explicit visualization of the wave nature of the constituent electrons was missing until just recently. The breakthrough came when the researchers from the IBM labs realized that the best way to elucidate the electrons inside a material is to place an impurity in an otherwise perfect crystal structure. By building corrals of the impurities on the clean surface, and observing the generated patterns through the scanning tunneling microscope (STM), the experimenters were able to demonstrate the laws of the wave optics using the conduction electron waves.

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 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 propose a technique to reveal this coherent particle-hole mixture locally. In order to discuss the particle-hole mixture 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 argue that STM measurements allow one to visualize the Bogoliubov angle maps and thus to reveal particle hole dualism. Bogoliubov angle maps as a function of position and energy offer a tool to investigate strength of superconducting state locally.

Bogoliubov showed that in order to obtain natural excitations in the superconducting state one needs to use a linear combination of particle in hole excitations with the coherence factors $u_n(r_i)$ and $v_n(r_i)$. They describe the unitary transformation from particle and hole operators to quasiparticles that are:

$$\gamma_{n,\uparrow}(r_i) = u_n(r_i)c_{n,\uparrow} + v_n(r_i)c_{n,\downarrow}^\dagger, \hspace{1cm} (1)$$

with the constraints that $\int d^3r |u_n(r_i)|^2 + |v_n(r_i)|^2 = 1$ for any $n$ (normalization) and $\sum_n (|u_n(r_i)|^2 + |v_n(r_i)|^2) = 1$ for any $i$ (orthonormality), $i$ being the site index on our lattice.

In the normal state, either $u_n(r_i)$ or $v_n(r_i)$ are identically zero and there is no mixing between the particle- and hole-component of Bogoliubov quasiparticle. Once superconductivity sets in, the mixing between these components develops. This mixing strength can be repre-
sented by
\[ \Theta_n(r_i) = \arctan\left( \frac{|u_n(r_i)|^2}{|v_n(r_i)|^2} \right)^{1/2}, \tag{2} \]
which is a central quantity we are interested in. We define this quantity as a Bogoliubov angle. The high resolution STM allows us to study the spatial dependence of the BA for the states whose energy can be selected by tuning STM bias.

\[ \Theta_\kappa = \arctan\left( \frac{|u(\kappa)|^2}{|v(\kappa)|^2} \right)^{1/2}, \tag{3} \]

The plan of the paper is as follows. We first present a general theoretical background and define BA from the local tunneling conductance measurements \(dI/dV(r, V)\) at different bias values \(V\). Then we describe the numerical results for the calculation of BA.

II. THEORETICAL DISCUSSION

To illustrate the point about BA, we can look at the uniform BCS case first. Using Bogoliubov quasiparticles one can introduce BA as:

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

We suggest a way to visualize the BA maps that allow us to develop a more detailed understanding of the superconducting state. To illustrate this approach we will use the local STM data obtained on high-\(T_c\) superconductor, namely on \(Bi_2Sr_2CuCu_2O_{8+\delta}\) material.

Note, we intentionally do not simplify the expression in Eq. [2] for the reasons that will be clear in the next section. It represents a local mixture between particle and hole excitations for an eigenstate \(n\) at a given site \(i\). For example, for \(\Theta_n(r_i) = 0\) the Bogoliubov excitation will be a hole. In the opposite case of \(\Theta_n(r_i) = \pi/2\) quasiparticle is essentially an electron. The angle that corresponds to the strongest admixture between particle and hole is \(\Theta_n(r_i) = \pi/4 = 45^\circ\). Obviously, in case of inhomogeneous state the BA is a function of a position where it is measured and also is a function of energy \(E\).

The ideas presented here are quite general and are applicable to a variety of superconductors, including conventional superconductors. Imaging of BA can be performed in any inhomogeneous state. One can investigate BA in a variety of states, including vortex state and normal state with superconducting correlations, e.g. so called pseudogap (PG) state. To illustrate this approach we will use the local STM data obtained on high-\(T_c\) superconductor, namely on \(Bi_2Sr_2CuCu_2O_{8+\delta}\) material.
smooth function of energy and at small energies $E \sim 10 - 100 m eV$ it is a constant. $f(E)$ is Fermi distribution function. At very low temperatures $f'(E)$ becomes a nearly $\delta(E)$ function, a fact that we will use often. We can simplify the formulas if we introduce the density of states (DOS) for quasiparticles: $\rho(E) = \sum_{n,s} \delta(E - E_n)$. For simplicity we will assume particle-hole symmetry in the normal state.

Then, for a given eigenspectrum and eigenfunctions $u_n(r_i - r_j), v_n(r_i - r_j)$ we can rewrite Eq. (6) as:

$$dI/dV_+(r_i, |eV|) = - \int dE \rho(E) |u_{E,s}|^2(r_i)f'(|eV| - E),$$

$$E \geq 0,$$

$$dI/dV_-(r_i, |eV|) = - \int dE \rho(E) |v_{E,s}|^2(r_i)f'(|eV| + E),$$

$$E \leq 0.$$  

(7)

Hence the ratio of $dI/dV$, taken at the same $|E|$, that we label as $Z(r_i, |eV|)$, will be

$$Z(r_i, |eV| = E) = \frac{dI/dV_+(r_i, |eV|)}{dI/dV_-(r_i, |eV|)} = \frac{|u_{E,s}|^2(r_i)}{|v_{E,s}|^2(r_i)} = \tan^2 \Theta(r_i, E),$$

(8)

where the last step is taken assuming that there are few, often one state, that contributes to the summation in Eqs. (6) a energy $E = |eV|$. Then Eq.(8) can be inverted as:

$$\Theta(r_i, E) = \arctan\left[\frac{dI/dV_+(r_i, |eV|)}{dI/dV_-(r_i, |eV|)}\right]^{1/2}$$

(9)

this result along with Eq. (2) is the main result of this section. It allows a direct determination of Bogoliubov angle $\Theta(r_i, E)$ from the experimentally measured tunneling conductances at positive and negative bias.

BA as a measure of particle-hole admixture appears naturally in the Anderson mapping\(^\text{10}\) of BCS model on the effective spin model. We briefly recall the mapping in Appendix A.

To visualize the local quasiparticle states we employ the Scanning Tunneling Microscopy (STM) technique. Crucial aspect of the electron tunneling into the superconducting state that makes it qualitatively different from the tunneling in conventional metals is that the STM tip contains only the regular electrons which carry a unit of charge ($-e$). We can inject either electrons or holes in superconductor. On the other hand as was pointed out early on starting with Bogoliubov, quasiparticles that live inside the superconductor do not possess a well-defined charge. Upon entering the superconductor, an electron/ hole that arrived from the normal STM tip must undergo a transformation into the Bogoliubov quasiparticles native to the superconductor\(^\text{11,12}\). Hence electrons that are injected or extracted form superconductor would need to be “assembled” from Bogoliubov excitations. At any site and at specific bias this conversion into particles and holes will depend on relative weights $u_n(r_i), v_n(r_i)$. Hence the intensity of a tunneling signal will depend on these coherence factors.

Qualitatively, the spatial distribution of tunneling intensity can be understood as follows. Respective amplitudes of particle and hole parts of the Bogoliubov quasiparticle, are $u_n(r_i)$ and $v_n(r_i)$ for site $i$ and for particular eigenstate $n$. Consider now a site where, say, $u_n(r_i)$ is large and close to 1. It follows therefore that for the same site the $v_n(r_i)$ would have to be small, since the normalization condition is almost fulfilled by $u_n(r_i)$ term alone. Similarly, for the sites where $v_n(r_i)$ has large magnitude, $u_n(r_i)$ would have to be small. Recall now that large $u_n(r_i)$ component would mean that quasiparticle has a large electron component on this site. Hence the electron will have large probability to tunnel into superconductor on this site and the tunneling intensity for electrons (positive bias) will be large. Conversely, for those sites the hole amplitude is small $v_n(r_i) \ll |u_n(r_i)|$ and the hole intensity (negative bias) will be small. Similarly, for sites with large hole amplitudes $|v_n(r_i)| \gg |u_n(r_i)|$ the electron amplitude will be suppressed and this site will be bright on the hole bias. We observe alternation of the form:

$$|v_n(r_i)|^2 \approx 1, |u_n(r_i)|^2 \ll 1,$$

$$|v_n(r_i)|^2 \ll 1, |u_n(r_i)|^2 \approx 1.$$  

(10)

Therefore if there is a particular pattern for the large particle amplitude (sampled on positive bias) on certain sites $i$, the complimentary pattern of bright sites for hole tunneling (on negative bias) will develop as a consequence of the inherent particle-hole mixture in superconductor. This antiphase behavior is a clear indication of the “natural quasiparticles” having both particle and hole character. It is the main effect that can be visualized by considering $\Theta(r_i, E)$ maps. Antiphase shift in positive and negative bias intensity is ubiquitously seen in tunneling spectra. The “antiphase” behavior of the components $|u_{E}(r_i)|^2, |v_{E}(r_i)|^2$ is explained here as a case of BA changing from particle to hole-like configuration on alternating sites. We see that this is the case in our numerical simulations, (see Numerical Simulations below), without any need to assume that only one state dominates the sum over states in Eq.(7). So the phenomenon is more general. We find it easiest to explain assuming only one term dominating. But given numerical results it holds for broader cases.

We discuss it in more details below when we turn to $\Theta(r_i, E)$ maps.

A. Particle-Hole asymmetry of normal state

The question of the underlying band particle-hole asymmetry often comes up in these materials at low doping. One way to “factor out” this asymmetry that is extrinsic to the particle-hole mixture measure, is to factor...
out the normal state conductances; namely one can take a ratio of $dI/dV_{\pm}(r_i, V, T)$ to their proper normal state values at high temperatures $T > T_c$:

$$dI/dV_{\pm}(r_i, V, T) \rightarrow \frac{dI/dV_{\pm}(r_i, E, T)}{dI/dV_{\pm}(r_i, E, T > T_c)}. \quad (11)$$

This procedure will factor out the particle hole asymmetry for the underlying band and will allow more direct measure of particle-hole asymmetry.

### III. IMAGING BOGOLIUBOV ANGLE IN NORMAL AND PSEUDOGAP STATE

The BA, as defined, is not sensitive to the SC quantum phase fluctuations. Indeed BA is defined as a function of ratio of the $|u_E(r_i)|^2/|v_E(r_i)|^2$. Therefore $\Theta(r_i, E)$ can be defined even in the presence of such phase fluctuations. Thus we propose that the discussion about BA may be extended to the normal state.

Imagine we are approaching a normal state of superconductor by warming it up. We can see that there will be temperature dependence of the BA. There is no reason to expect an abrupt termination of SC correlations as one crosses $T_c$. Remnant superconducting correlations are present above $T_c$ and hence one can still have excitations that will have a particle-hole admixture. The difference will be that we are no longer in the state with well defined superconducting Josephson phase.

To illustrate this point consider Bogoliubov-Valatin transformation in the presence of phase fluctuations:

$$\gamma_{n,1}(r_i) = u_n(r_i)c_{n,1} + \exp(i\phi(r_i))v_n(r_i)c^\dagger_{n,1}. \quad (12)$$

We then can use the same definition for BA, Eq. 2 in this case even in the presence of random Josephson phase $\phi$. Since one uses amplitudes of $u$, $v$, spatial phase disorder does not enter into $\Theta(r_i, E)$. So far the frozen and presumably for the slowly varying in time phase fluctuations once can use the BA as defined and image the local particle-hole admixture in the normal state.

One would need to take care of thermal broadening of the tunneling characteristics at higher temperatures. Namely one could divide the tunneling characteristics by derivatives of the Fermi thermal distribution function:

$$\Theta_{PG}(r_i, V) = \arctan\left[\frac{dI/dV_+(r_i, V,f(E + |eV|))^{1/2}}{dI/dV_-(r_i, V,f(E - |eV|))^{1/2}}\right]. \quad (13)$$

The problem of dynamic phase fluctuations in the state with superconducting fluctuations is complicated. More detailed analysis would require a specific model for the dynamics of the superconducting phase. An approach to phase fluctuations in PG state using localized Cooper pairs state with no long range phase coherence was advocated in, using STM data.

One can also study the behavior BA for other states, such as flux phase state and density wave state. Consider density wave states, e.g. d- density wave state (DDW). DDW is often mentioned as a possible state that can explain PG. In any density wave state, including DDW, particle-hole symmetry is violated and the poles of single particle excitations are not appearing in pairs symmetrically around chemical potential. Therefore single electron tunneling DOS does not have the components that appear symmetrically at positive and negative bias. If there is a particle hole symmetric spectrum for DDW state it can occur only as a special case at one doping level.

Absence of particle-hole symmetry will be easily detected by BA as it will tend to pure hole or particle angle, $\Theta \rightarrow 0, \pi/2$. Thus we think BA can be used as a spectroscopy tool to detect presence/absence of superconducting correlations in normal state. Another interesting question to address is how BA behaves upon rising temperature. At low energy it will be close to $\pi/2$ but then it can quickly move away to indicate purely particle or hole states at $T > T_c$ for non-pairing PG state.

These questions go beyond the scope of this paper and will be addressed in separate publication.

### IV. EXPERIMENT

In order to visualize the BA, we have performed an experimental investigation of the Spectroscopic Imaging Scanning Tunneling Microscopy (SI-STM) measurement on high temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. A single crystal of Bi-2212 grown by floating zone method, is hole-doped by introducing non-stoichiometric oxygen atoms per unit cell, and its hole concentration is adjusted for slightly overdoping ($T_c = 89K$). The crystal is cleaved in the ultra-high vacuum and immediately inserted into the STM head at $T = 4.2K$. To show the BA, we acquired local density of states (LDOS) images by measuring the STM tip-sample differential tunneling conductance $g(r, V) \equiv dI/dV_{\pm}(r, V)$ at each location $r$ and bias voltage $V$. Since LDOS($r, E = eV$) $\propto g(r, V)$, energy and position dependence of the LDOS is obtained.

In Fig. 5, we show 54nm $g(r, V)$ map at $V=-16mV$ measured on the Bi-2212 surface, showing the spatial modulations which is interpreted as an interference of the Bogoliubov quasiparticles. A Fourier transform of $g(r, -18mV)$ in the inset of Fig. 5 exhibits several fourier spots corresponding to the period of modulation in real space. These observations are consistent with previous reports. Although similar modulations are visible in $g(r, +18mV)$ shown in Fig. 5 which is the same FOV (field-of-view) as Fig. 5a, one can notice that the spatial phase of these modulations is different. $dI/dV$-spectra which are averaged over the regions with the same gap size, where $g(r, -18mV)$ in Fig. 5a is slightly higher/lower then the average value, see black/red curves.
in Fig. 3b. Overall feature of the spectra taken with different intensity of $g(\vec{r},-18\text{mV})$ with the same gap are almost identical, however, the significant differences at low energies in the spectra are seen in the Fig. 3a. It is obvious that the spectrum with relatively higher amplitude at the negative sample bias has the relatively smaller amplitude at the positive sample bias (and vice versa). This implies that the particle and the hole in the superconducting state are entangled each other.

In Fig. 3a, we calculate a local BA $\Theta (\vec{r}, V)$ by taking ratio of the positive and the negative sample bias $g(\vec{r}, V)$, using the following simple formulas,

$$Z(\vec{r}, V) \equiv \frac{d\tilde{I}}{d\tilde{V}}(\vec{r}, +V) \quad (14)$$

$$\Theta (\vec{r}, V) = \arctan (\sqrt{Z}). \quad (15)$$

Taking ratio has an advantage to cancel out the unknown matrix element involved in $d\tilde{I}/d\tilde{V}$. Fig. 3a is the BA map at $V = 18\text{mV}$ with its fourier transform, and we found that the $\Theta (\vec{r}, 18\text{mV})$ shows spatial modulations as well as $d\tilde{I}/d\tilde{V}$ map in the Fig. 3 but with more stronger contrast. As seen in the Fig. 3a, amplitude of $d\tilde{I}/d\tilde{V}$ between positive and negative bias are anti-correlated, so that the taking ratio enhances such structure, namely, spatial modulations. BA map is essentially different from the $d\tilde{I}/d\tilde{V}$ map, since BA map exhibits the degree of spatial particle-hole mixture of the Bogoliubov quasiparticles. However, as evidenced by the fourier transform of $\Theta (\vec{r}, 18\text{mV})$ (Fig. 3b), fourier pattern is qualitatively the same as those of Fig. 3a and b, indicating that the period of the existing modulation in the BA map is similar to $d\tilde{I}/d\tilde{V}$ modulations. This similarity supports the claim that the local particle and hole amplitude are modulated by scattering. Taking the ratio of $d\tilde{I}/d\tilde{V}$ in Eq.(14) and taking the BA map in Eq.(15) can therefore be important new tools to search for the true spatial modulations and individual fourier spots in the electron density of states.

In Fig. 3b, we show the distribution of BA at energy $V = 18\text{mV}$ which is peaked at $\Theta = 43^\circ$, not exactly at 45$^\circ$. One possibility is that the apparent shift of the distribution is caused by asymmetric background in the tunneling spectrum that is sampled more at higher voltage as we shall see in the Fig. 5. To visualize the particle- and hole-like regions more clearly, line cuts of BA at $V=18\text{mV}$ as well as $d\tilde{I}/d\tilde{V}$ at $V=+18\text{mV}$ and $-18\text{mV}$, along the trajectory shown in Fig. 4a, are exhibited in Fig. 4b, c, and d. For simplicity, we only focus on the specific $q$-vector in Fig. 4b, so that the line profiles are taken from the fourier-filtered $d\tilde{I}/d\tilde{V}$ and $\Theta (\vec{r}, V=18\text{mV})$ with $q$-vector highlighted by red circle in Fig. 4b. Particle- and hole-like regions are spatially modulating along the line and clearly show the anti-phase behavior in modulation between $d\tilde{I}/d\tilde{V}$ at $+18\text{mV}$ and $-18\text{mV}$.

Figures 5a-e show the $\Theta (\vec{r}, V)$ maps for various bias voltages and their fourier transforms. With increasing energy, the periods of modulation in real space change, and corresponding fourier spots in the inset of the Fig. 5a-e move, following the octet model and these observations are consistent with previous reports. In addition to the period of modulation, one can immediately notice that the pattern of the spatial modulation changes. At low energies (Fig. 5a and b), spatial modulations are visible all over the field of view. On the other hand, at $V = 34\text{mV}$ (or $V > 34\text{mV}$), such modulations tend to be visible in the restricted area. This difference implies that the different type of scattering might kick in at $V = 34\text{mV}$ (or $V > 34\text{mV}$).

In Fig. 5, we show the 2D distribution of the BA and spatial modulations are normalized at each energies. The spatial change in the BA map seems to occur as a crossover, and it can be realized by deviation of the BA from $\Theta = 45^\circ$ in the Fig. 5. The energy which differentiates the spatially coherent excitations and the localized excitations is estimated as $\sim 26\text{mV}$ (less than mean $\Delta \sim 40\text{mV}$) where BA starts to monotonically decrease.

The visualization of the BA shed light to understand the quasiparticle excitations in the superconducting state. The interferences of the Bogoliubov quasiparticles can be understood as a spatial variation of relative weight of the particle and the hole amplitude which is represented by the BA. The BA can be a measure of the energy scale of the coherent excitations which split the type of the modulation structure in real space. And, since the spatial modulations in the electronic structure are revealed much more clearly in the BA map, this provides an excellent new technique to determine the momentum space ($q$-space) electronic structure using STM. Hanaguri et al. have recently demonstrated the power of this technique with the discovery of the interference of the Bogoliubov quasiparticles in Na-CCOC.

V. NUMERICAL SIMULATIONS

We implement simple but realistic model of the optimally doped cuprate superconductor with disorder. We use a simple BCS solution to illustrate the approach on how one can visualize the superconducting admixture of particles and holes in the natural Bogoliubov excitations in superconducting state. Even though the model is simplistic the approach itself is quite general.

To model the high-temperature superconductors we utilize the highly-anisotropic structure of the cuprates and focus on a single layer of the material. In the simplified model, the conduction electrons live on the copper sites, $i$, and can hop to the neighboring sites, $j$, with a certain probability measured by the quantity $t$. In addition to that, the electrons that occupy the neighboring sites feel mutual attraction of a strength $V_{\text{int}}$. Formally, this model is represented by the Hamiltonian,

$$H_0 = -t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^\dagger c_{j\sigma} - V_{\text{int}} \sum_{\langle i,j\rangle} n_i n_j, \quad (16)$$

were a quantum-mechanical operator $c_{i\sigma}^\dagger$ creates an elec-
tron on site \( i \), the operator \( c_{ij}^\dagger c_{ij} \) eliminates an electron from the site \( j \), and \( n_i = c_{ij}^\dagger c_{ij} \) represents the electron density on site \( i \). The electron spin, \( \sigma \), can point up or down. This model, referred to as the \( t-V \) model, is known to produce the \( d \)-wave pairing for the electron densities close to one electron per lattice site, and has been successfully used to describe strong impurities in a \( d \)-wave superconductor\cite{12}. The local impurity is introduced by modifying the electron energy on a particular site. The corresponding correction to the Hamiltonian is
\[
H_{\text{imp}} = V_{\text{imp}}(n_{i\uparrow} + n_{i\downarrow}).
\] (17)
This term is the potential part of the impurity energy that couples to the total electronic density on site \( i \). We solve the impurity problem in the Hartree-Fock approximation, which replaces the two-body interaction in \( H_0 \) with an effective singe-electron potential. Our goal is to use \( V_{\text{imp}} \) to investigate the spatial distribution of BA as a function of position and energy.

Using the Bogoliubov-Valatin transformation to the quasi-particles operators \( \gamma \)
\[
c_{i\uparrow} = \sum_n [\gamma_{n\uparrow} u_n(r_i) - \gamma_{n\uparrow}^\dagger v_n(r_i)],
\]
\[
c_{i\downarrow} = \sum_n [\gamma_{n\downarrow} u_n(r_i) - \gamma_{n\downarrow}^\dagger v_n(r_i)],
\] (18)
and the mean-field approximation, one can diagonalize the Hamiltonian Eq. (16). The quasiparticle amplitudes on lattice sites \( (u_n(r_i), v_n(r_i)) \) have to satisfy inhomogeneous Bogoliubov-de Gennes equations\cite{20}:
\[
\begin{pmatrix}
\hat{\xi} & \hat{\Delta} \\
\hat{\Delta}^* & -\hat{\xi}^*
\end{pmatrix}
\begin{pmatrix}
u_n(r_i) \\
u_n^*(r_i)
\end{pmatrix} = E_n
\begin{pmatrix}
u_n(r_i) \\
u_n^*(r_i)
\end{pmatrix},
\] (19)
where the kinetic operator \( \hat{\xi} \) and superconducting order parameter \( \hat{\Delta} \) can be represented as:
\[
\hat{\xi} u_n(r_i) = -t \sum_\delta u_n(r_i + \delta) + (V_{\text{imp}}(r_i) - \mu) u_n(r_i),
\]
\[
\hat{\Delta} v_n(r_i) = \sum_\delta \Delta(r_i) v_n(r_i + \delta),
\] (20)
where \( \delta = \pm \hat{x}, \pm \hat{y} \) are nearest neighbor vectors for a square lattice.

We solve Eq.(19) together with the self-consistency condition:
\[
\Delta(r_i) = \frac{V_{\text{int}}}{2} \sum_n (u_n(r_i + \delta) v_n^*(r_i) + u_n(r_i) v_n^*(r_i + \delta)) \tanh(E_n/2k_B T),
\] (21)
where the summation is over the positive eigenvalues \( E_n \) only.

For a square lattice system with \( L \times L \) lattice sites, the solution of the Bogoliubov-de Gennes equations Eq.(21) is equivalent to the eigenproblem for a \( 2L^2 \times 2L^2 \) matrix.

In order to minimize the boundary effects we assume periodic boundary conditions in both \( x \) and \( y \) directions.

We have performed numerical simulations on a square lattice \( 32 \times 32 \) at \( T = 0 \). We assume 40 impurities randomly placed on the lattice, each impurity has strength \( V_{\text{imp}} = 1t \). It corresponds to approximately 3% doping. We set \( V_{\text{int}} = -2t \) and a half-filled band \( \mu = 0 \).

The results of our numerical simulations are summarized in Figs.\cite{10,11} where we show three panels of plots for calculated local tunneling conductance \( dI/dV \) at positive and negative bias, the corresponding Bogoliubov angle \( \Theta(x, y) \), and the logarithm of the absolute value of its Fourier transform. We consider the following values for the bias: \( V = \pm 0.4t, \pm 0.8t, \pm 1.2t \). Note, that at bias \( V = \pm 0.4t \), that is under the gap value \( \Delta \approx 0.8t \), the pattern of the local Bogoliubov angle (see Fig.\cite{10}) is rotated 45 degrees with respect to the patterns calculated at higher biases \( V = \pm 0.8t \) (near the gap, see Fig.\cite{11}, and \( V = \pm 1.2t \) (above the gap, see Fig.\cite{12}). The sites on the lattice where there is a large particle-like component of the Bogoliubov excitation, hole component is small. Complementary pattern is observed on opposite bias. This “rotation” is commonly present in the whole field of view.

We also present BA along the diagonal line cut for our numerical calculation to compare with experimental results. We observe an out-of-phase angle change for low energy vs high energy BA, Fig.\cite{13}. This out of phase behavior is consistent with the behavior seen in Fig.\cite{14}.

VI. CONCLUSION

In conclusion, we have introduced a new spectroscopic measure, Bogoliubov angle \( \Theta(r, E) \). This measure allows one to image local particle-hole admixture in the superconducting state and in the normal state with superconducting correlations.

Bogoliubov angle can be studied as a function of position. It can also contain nontrivial Fourier components. This could allow us to make connection with the spatial interference of quasiparticles in superconducting state\cite{19,24,27,28}. Complementary to the momentum space information one can look at the energy dependence of BA. Energy dependence observed experimentally clearly indicates that there is a change in behavior in \( \Theta(r, E) \) at \( E \approx 20 - 25mV \), Figs.\cite{15}. This energy range clearly correlates with the changes in the interference patterns. We interpret these changes as an evidence for a change in the superconducting coherence that is weakened at higher energies.

As a future application we propose that BA be studied as a function of doping and temperature. One can use to investigate BA and particle-hole at temperatures above \( T_c \) for studies of the nature of the pseudogap phase. Using Bogoliubov angle one could be able to identify how robust the particle-hole mixture is in the normal state and therefore be able to differentiate between different
The effective spin model is:

\[ \text{in a range near Fermi surface. Excitation spectrum for } n \text{ and they represent a complete spin algebra over space} \]

\[ \text{defined particle number and } \]

\[ \text{BCS solution, once we assume } \]

\[ \text{BCS Hamiltonian is taken to be} \]

\[ \text{Office of Naval Research.} \]

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APPENDIX A: Anderson Mapping

Here we recall the Anderson mapping of reduced BCS Hamiltonian on the effective spin model. The reduced BCS Hamiltonian is taken to be

\[ H_{\text{red}} = - \sum_{k} (\epsilon_{k} - \mu)(1 - n_{k} - n_{-k}) - \sum_{k \neq k'} V_{kk'} c_{k}^{+} c_{k'}^{+} c_{-k'} c_{-k} = (A-1) \]

\[ -2 \sum_{k} (\epsilon_{k} - \mu) s_{z,k} - 1/2 \sum_{k,k'} (s_{k}^{+} s_{k'}^{-} + s_{k}^{-} s_{k'}^{+}) = (A-2) \]

where we assumed translational invariance for simplicity and omit spin indexes. Spin operators are defined as:

\[ s_{z,k} = 1 - n_{k} - n_{-k}, \quad (A-3) \]

\[ s_{k}^{+} = b_{k}^{+} = c_{k}^{+} c_{-k}^{+}, \quad (A-4) \]

\[ s_{k}^{-} = b_{k} = c_{k} c_{-k} \quad (A-5) \]

and they represent a complete spin algebra over space \[ n_{k} - n_{-k} = 0 \], the so called hard core boson constraint. \[ z \] component of the spin corresponds to state with well defined particle number and \[ s_{\pm} \] corresponds to pairing correlations. Anderson showed that this reduced Hamiltonian describes the spin \[ s_{k} \] in an “external” field pointing at an angle \[ \Theta_{k} \]

\[ \Theta_{k} = 1/2 \sum_{k'} \frac{V_{kk'} \sin \Theta_{k}}{\epsilon_{k} - \mu} \quad (A-6) \]

One immediately recognizes this a self-consistency equation for BCS solution, once we assume \[ V_{kk'} \] to be constant in a range near Fermi surface. Excitation spectrum for the effective spin model is:

\[ E_{k} = ((\epsilon_{k} - \mu)^2 + 1/4 \sum_{k'} V_{kk'} \sin \Theta_{k'})^{1/2} \quad (A-7) \]

Complete identification with Bogoliubov quasiparticles is clear if one identifies

\[ \sin \Theta_{k} = 2u_{k} v_{k}, \cos \Theta_{k} = u_{k}^2 - v_{k}^2 \quad (A-8) \]

To make a contact with BA we notice that in case of broken translational symmetry we can work out exactly the same representation based on eigenfunctions in real space \[ u_{n}(r_{i}), v_{n}(r_{i}) \]. Then the mapping on the spin problem will be done in real space, angle \[ \Theta_{k} \] is proportional to the BA defined in the Introduction, and we will have \[ \Theta_{E}(r_{i}) \] as defined in Eq. (2). One can immediately see the direct connection with the Anderson angle used in this effective spin model.

Appendix B: Numerical details

The numerical solution of Eq. (20) together with the self-consistency condition Eq. (21) requires iterative solution and it is organized as follows:

1. For a reasonable initial value of the order parameter \[ \Delta_{s}(r_{i}) \] we solve the eigenproblem Eq. (20) to obtain the quasiparticle amplitudes \( (u_{n}(r_{i}), v_{n}(r_{i})) \) and the quasiparticle spectrum \( E_{n} \).

2. Then, substituting \( (u_{n}(r_{i}), v_{n}(r_{i})) \) and \( E_{n} \) into Eq. (21) we compute a new approximation of the order parameter \( \Delta_{s}^{\text{appr}}(r_{i}) \).

3. In order to avoid numerical instabilities during iterations, we use a mixing scheme \[ \Delta_{s}^{(n+1)}(r_{i}) = \alpha \Delta_{s}^{\text{appr}}(r_{i}) + (1 - \alpha) \Delta_{s}^{(n)}(r_{i}) \] where \[ \Delta_{s}^{(n)}(r_{i}) \] is the order parameter at the previous iteration step. Adjustable parameter \( \alpha \) is a number between 0 and 1. To insure convergence, we increase the current value of \( \alpha \) by 5% if the relative deviation between two consequent steps \[ S_{n} = \max_{i,\delta} |\Delta_{s}^{(n)}(r_{i}) - \Delta_{s}^{(n-1)}(r_{i})|/\max_{i,\delta} |\Delta_{s}^{(n)}(r_{i})| \] has decreased, \( S_{n} < S_{n-1} \). And we decrease \( \alpha \) by 20% in the opposite case, \( S_{n} > S_{n-1} \).

4. The computed \[ \Delta_{s}^{(n+1)}(r_{i}) \] is used for the next iteration step.

We repeat iterations until we achieve the acceptable level of accuracy \( \epsilon = 10^{-3} \). After the end of the procedure, we perform an additional step with \( \alpha = 1 \) to ensure convergence of the obtained solution. It usually takes 20 – 40 iterations to converge.

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FIG. 2: (Color online) BCS coherence factors $u^2(k)$ (blue), $v^2(k)$ (red) are shown as functions of energy. The function $C(k) = |u^2(k) - v^2(k)| = |\cos 2\Theta(k)|$ (black), 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.
FIG. 3: (Color online) $g(\vec{r}, V)$ with 54nm FOV at $V = -18\text{mV}$ (a) and $V = +18\text{mV}$ (b) with their fourier transforms in the insets. The modulations are visible and consist of several wave vectors. c, Typical averaged spectra taken at different area. d, same spectra as c, but zoomed at the low energy feature below the maximum gap. Systematic deviation in spectra between the negative and the positive sample bias is seen, as indicated by arrows.
FIG. 4: (Color online) a, $\Theta(x, V)$ with 54nm FOV at $V = 18mV$. b, fourier transform of $\Theta(x, V)$ in a. c, Distribution of $\Theta(x, V)$ at $V = 18mV$. d, Spatial evolution of the fourier filtered $dI/dV$ at 18mV and -18mV (black, darker) and $\Theta(x, V = 18mV)$ (red, lighter) with $2\pi/q_T$ modulation along the red (light solid) line starting from the solid (red) circle in a.
FIG. 5: (Color online) a, b, c, d, e, images of the BA at each bias voltages \((V = 10, 18, 26, 34, \text{ and } 42\text{mV})\) and their fourier transforms. f, distributions of the BA at each bias voltages from 0 to 90mV. Peak positions of the histogram are traced by black line.
FIG. 6: (Color online) a, b, c, d, calculated LDOS on a square $32 \times 32$ lattice at $T = 0$. We assume 40 randomly placed impurities with individual impurity strength $V_{imp} = 1t$. The pairing strength is set $V_{int} = -2t$ and chemical potential $\mu = 0$ (see text). a, calculated local $dI/dV$ tunneling conductance at positive bias $V = 0.4t$. b, calculated local $dI/dV$ tunneling conductance at negative bias $V = -0.4t$. c, corresponding Bogoliubov angle $\Theta(x,y)$. d, logarithm of the absolute value of Fourier transform of $\text{BA log}_{10}(|\Theta(x,y)|)$ with subtracted average value $<\Theta(x,y)> = 45^\circ$. 
FIG. 7: (Color online) a,b,c,d, calculated LDOS on a square $32 \times 32$ lattice at $T = 0$. We assume 40 randomly placed impurities with individual impurity strength $V_{\text{imp}} = 1t$. The pairing strength is set $V_{\text{int}} = -2t$ and chemical potential $\mu = 0$ (see text). a, calculated local $\frac{d}{dV}$ tunneling conductance at positive bias $V = 0.8t$. b, calculated local $\frac{d}{dV}$ tunneling conductance at negative bias $V = -0.8t$. c, corresponding Bogoliubov angle $\Theta(x, y)$. d, logarithm of the absolute value of Fourier transform of $\text{BA log}_{10}(|\Theta(k_x, k_y)|)$ with subtracted average value $<\Theta(x, y)> = 45^\circ$. 
FIG. 8: (Color online) a, b, c, d, calculated LDOS on a square $32 \times 32$ lattice at $T = 0$. We assume 40 randomly placed impurities with individual impurity strength $V^{imp} = 1t$. The pairing strength is set $V_{int} = -2t$ and chemical potential $\mu = 0$ (see text). a, calculated local $\frac{dI}{dV}$ tunneling conductance at positive bias $V = 1.2t$. b, calculated local $\frac{dI}{dV}$ tunneling conductance at negative bias $V = -1.2t$. c, corresponding Bogoliubov angle $\Theta(x, y)$. d, logarithm of the absolute value of Fourier transform of $BA \log_{10}(|\Theta(k_x, k_y)|)$ with subtracted average value $<\Theta(x, y)> = 45^\circ$. The Fourier transform we obtain is consistent with FT intensity us seen in the experiment, see inset in Fig. 8e. Please note rotation of $(q_x, q_y)$ basis.
FIG. 9: (Color online) Profile of the Bogoliubov angle $\Theta$ along the line cut for bias values $0.4t$, red (dashed) line; and $1.2t$, black (solid) line. The line cut is taken along the direction $[1,1]$. Note the angle inversion effect with respect to the optimal mixing angle value of $45^\circ$ for low energy and high energy BA.