Momentum dependence of quasiparticle spectrum and Bogoliubov angle in cuprate superconductors

Weifang Wang, Zhi Wang, Jingge Zhang, and Shiping Feng*

Department of Physics, Beijing Normal University, Beijing 100875, China

The momentum dependence of the low energy quasiparticle spectrum and the related Bogoliubov angle in cuprate superconductors are studied within the kinetic energy driven superconducting mechanism. By calculation of the ratio of the low energy quasiparticle spectra at positive and negative energies, it is shown that the Bogoliubov angle increase monotonically across the Fermi crossing point. The results also show that the superconducting coherence of the low energy quasiparticle peak is well described by a simple d-wave Bardeen-Cooper-Schrieffer formalism, although the pairing mechanism is driven by the kinetic energy by exchanging spin excitations.

Keywords: Bogoliubov angle; Quasiparticle spectrum; Cuprate superconductors; Kinetic energy driven superconducting mechanism

After over twenty years of extensive studies, an agreement has emerged that superconductivity in cuprate superconductors results when electrons pair up into Cooper pairs as in the conventional superconductors, then these electron Cooper pairs condensation reveals the superconducting (SC) ground-state. However, as a natural consequence of the unconventional SC mechanism that is responsible for the high SC transition temperatures, the electron Cooper pairs in cuprate superconductors have a dominant d-wave symmetry. However, in spite of the unconventional SC mechanism, the angle-resolved photoemission spectroscopy (ARPES) experimental results have unambiguously established the Bogoliubov quasiparticle nature of the sharp SC quasiparticle peak in cuprate superconductors, then the SC coherence of the low energy quasiparticle peak is well described by a simple d-wave Bardeen-Cooper-Schrieffer (BCS) formalism.

In the framework of the BCS formalism, the Bogoliubov quasiparticle is a coherent combination of particle (electron) and its absence (hole), i.e., its annihilation operator is a linear combination of particle and hole operators as,

$$\gamma_k = U_k \alpha_k + V_k c_k^\dagger,$$

with the constraint for the coherence factors $|U_k|^2 + |V_k|^2 = 1$ for any wave vector $k$ (normalization). In this case, the Bogoliubov quasiparticle do not carry definite charge. This particle-hole dualism of Bogoliubov quasiparticles then is responsible for a variety of profound phenomena in the SC state. In particular, the coherence factors $U_k$ and $V_k$ for cuprate superconductors as a function of momentum have been determined experimentally from the ARPES measurements.

Recently a quantity referred to as the Bogoliubov angle has been introduced in terms of the coherence factors $U_k$ and $V_k$ as,

$$\Theta_k = \arctan \left( \frac{|U_k|^2}{|V_k|^2} \right)^{1/2},$$

which is the manifestation of the particle-hole dualism of the SC quasiparticles, for example, for $\Theta_k = 0$ the Bogoliubov quasiparticle excitation will be a hole-like, whereas in the opposite case of $\Theta_k = \pi/2$ the Bogoliubov quasiparticle is essentially an electron-like. Moreover, the angle that corresponds to the strongest admixture between particle and hole is $\Theta_k = \pi/4$. In a simple BCS formalism, this Bogoliubov angle can be rewritten as,

$$\Theta_k = \arctan \left( \frac{A(k, \omega > 0)}{A(k, \omega < 0)} \right)^{1/2},$$

where $A(k, \omega)$ is the ARPES spectrum of superconductors.

Moreover, this Bogoliubov angle reflects the relative weight of particle and hole amplitudes in the Bogoliubov quasiparticle, and therefore plays an essential role in characterizing the SC state via quantities such as the SC gap and its symmetry. By comparing the ratio of the ARPES spectral intensities at positive and negative energies, the momentum dependence of the Bogoliubov angle increase monotonically across the Fermi crossing point. The results also show that the superconducting coherence of the low energy quasiparticle peak is well described by a simple d-wave Bardeen-Cooper-Schrieffer formalism, although the pairing mechanism is driven by the kinetic energy by exchanging spin excitations.

In this paper, we study the momentum dependence of the low energy quasiparticle spectrum and the related Bogoliubov angle for cuprate superconductors based on the kinetic energy driven SC mechanism. We employed the $t$-$J$ model, and then show explicitly that the Bogoliubov angle for cuprate superconductors increase monotonically across the Fermi crossing point.

We start from the two-dimensional $t$-$J$ model on a...
square lattice. The kinetic energy term in the Hamiltonian is
\[ H = -t \sum_{i\bar{\eta}} C_{i\sigma}^\dagger C_{i+\bar{\eta}\sigma} + t' \sum_{i\bar{\eta}} C_{i\sigma}^\dagger C_{i+\bar{\eta}\sigma} + \mu \sum_{i\sigma} C_{i\sigma}^\dagger C_{i\sigma} \]
+ \[ J \sum_{i\bar{\eta}} \mathbf{S}_i \cdot \mathbf{S}_{i+\bar{\eta}}, \]
acting on the Hilbert subspace with no double occupancy, i.e., \( \sum_{\bar{\eta}} C_{i\sigma}^\dagger C_{i\sigma} \leq 1 \), where \( \bar{\eta} = \pm \bar{x}, \pm \bar{y}, \bar{\tau} = \pm \bar{x} \pm \bar{y} \), \( C_{i\sigma}^\dagger \) (or \( C_{i\sigma}^\dagger \)) is the electron creation (annihilation) operator, \( \mathbf{S}_i \equiv (S_{ix}^i, S_{iy}^i, S_{iz}^i) \) are spin operators, and \( \mu \) is the chemical potential. To deal with the constraint of no double occupancy in analytical calculations, the charge-spin separation (CSS) fermion-spin theory has been developed, where the constrained electron operators are decoupled as \( C_{i\uparrow} = h_{i\uparrow}^i S_i^\uparrow \) and \( C_{i\downarrow} = h_{i\downarrow}^i S_i^\downarrow \), with the spinful fermion operator \( h_{i\sigma} \equiv e^{-i\Phi_{\sigma}^i} h_{i\sigma} \) describes the charge degree of freedom together with some effects of the spin configuration rearrangements due to the presence of the doped hole itself (charge carrier), while the spin operator \( S_i \) describes the spin degree of freedom (spin), then the electron local constraint for single occupancy is satisfied in analytical calculations. In particular, it has been shown that under the decoupling scheme, this CSS fermion-spin representation is a natural representation of the constrained electron defined in the Hilbert subspace without double electron occupancy. In the CSS fermion-spin representation, the \( t-J \) Hamiltonian can be expressed as,
\[ \mathcal{H} = t \sum_{i\bar{\eta}} (h_{i+\bar{\eta}\uparrow}^i h_{i\uparrow}^i S_i^\uparrow S_{i+\bar{\eta}}^\uparrow + h_{i+\bar{\eta}\downarrow}^i h_{i\downarrow}^i S_i^\downarrow S_{i+\bar{\eta}}^\downarrow - t' \sum_{i\bar{\tau}} (h_{i+\bar{\tau}\uparrow}^i h_{i\uparrow}^i S_i^\uparrow S_{i+\bar{\tau}}^\uparrow - h_{i+\bar{\tau}\downarrow}^i h_{i\downarrow}^i S_i^\downarrow S_{i+\bar{\tau}}^\downarrow) - \mu \sum_{i\sigma} h_{i\sigma}^i h_{i\sigma}^i + J_{\text{int}} \sum_{i\bar{\eta}} \mathbf{S}_i \cdot \mathbf{S}_{i+\bar{\eta}}, \]
where \( J_{\text{int}} = (1 - \delta^2) J \) and \( \delta = (h_{\uparrow\uparrow}^i h_{\downarrow\downarrow}^i) = (h_{\uparrow\downarrow}^i h_{\downarrow\uparrow}^i) \) is the hole doping concentration. As a consequence, the kinetic energy term in the \( t-J \) model has been transferred as the interaction between charge carriers and spins, which reflects that even the kinetic energy term in the \( t-J \) Hamiltonian has a strong Coulombic contribution due to the restriction of no double occupancy of a given site.

For the understanding of the physical properties of cuprate superconductors in the SC state, we have developed a kinetic energy driven SC mechanism, where the interaction between charge carriers and spins from the kinetic energy term in the \( t-J \) model induces the charge carrier pairing state with the \( d \)-wave symmetry by exchanging spin excitations, then the electron Cooper pairs originating from the charge carrier pairing state are due to the charge-spin recombination, and their condensation reveals the SC ground-state. In particular, this \( d \)-wave SC state is controlled by both the SC gap function and the quasiparticle coherence, which leads to a fact that the maximal SC transition temperature occurs around the optimal doping, and then decreases in both underdoped and overdoped regimes. Furthermore, it has been shown that this SC state is a conventional BCS-like with the \( d \)-wave symmetry so that the basic BCS formalism with the \( d \)-wave SC gap function is still valid in discussions of the low energy electronic structure of cuprate superconductors, although the pairing mechanism is driven by the kinetic energy by exchanging spin excitations, and other exotic magnetic scattering is beyond the \( d \)-wave BCS formalism. Following the previous discussions, the charge carrier diagonal and off-diagonal Green’s functions can be obtained as,
\[ g(k, \omega) = Z_{hF} \left( \frac{U_{hk}^2}{\omega - E_{hk}} + \frac{V_{hk}^2}{\omega + E_{hk}} \right), \]
\[ \Im(k, \omega) = -Z_{hF} \frac{\Delta_{hZ}(k)}{2E_{hk}} \left( \frac{1}{\omega - E_{hk}} - \frac{1}{\omega + E_{hk}} \right), \]
where the charge carrier quasiparticle spectrum \( E_{hk} = \sqrt{k_x^2 + |\Delta_{hZ}(k)|^2} \) with the renormalized \( d \)-wave charge carrier pair gap function \( \Delta_{hZ}(k) = \Delta_{hZ}^\tau \cos k_x - \cos k_y \), and the charge carrier quasiparticle coherence factors \( U_{hk}^2 = (1 + \xi_k/E_{hk})/2 \) and \( V_{hk}^2 = (1 - \xi_k/E_{hk})/2 \), while the charge carrier quasiparticle coherent weight \( Z_{hF} \) and other notations are defined as same as in Ref. 14, and have been determined by the self-consistent calculation.

In the CSS fermion-spin theory, the electron diagonal and off-diagonal Green’s functions are the convolutions of the spin Green’s function and charge carrier diagonal and off-diagonal Green’s functions in Eqs. [5] and [6], respectively. Following the previous discussions, we can obtain the electron diagonal and off-diagonal Green’s functions in the present case, and then the electron spectral function from electron diagonal Green’s function is obtained as,
\[ A(k, \omega) = 2\pi \frac{1}{N} \sum_p Z_F \frac{B_p}{2\omega_p} \times \left[ U_{hp+k}^2 L_1(k, p) \delta(\omega + E_{hp+k} - \omega_p) + U_{hp+k}^2 L_2(k, p) \delta(\omega + E_{hp+k} + \omega_p) + V_{hp+k}^2 L_1(k, p) \delta(\omega - E_{hp+k} + \omega_p) + V_{hp+k}^2 L_2(k, p) \delta(\omega - E_{hp+k} - \omega_p) \right], \]
where the electron quasiparticle coherent weight \( Z_F = Z_{hF}/2 \), \( L_1(k, p) = \coth(\beta E_{hp+k}/2) - \tanh(\beta E_{hp+k}/2) \) and \( L_2(k, p) = \coth(\beta E_{hp+k}/2) + \tanh(\beta E_{hp+k}/2) \), and the spin excitation spectrum \( \omega_p \) and \( B_p \) have been given in Ref. 14. For the convenience of discussions, the electron spectral function in Eq. [7] also can be rewritten formally as,
\[ A(k, \omega) = 2\pi Z_F [U_{k}^2 \delta(\omega - E_k) + V_{k}^2 \delta(\omega + E_k)], \]
obtained as,
\[ U_k^2 \delta(\omega - E_k) = \frac{1}{N} \sum_p \frac{B_p}{2\omega_p} [L_1(k, p) \delta(\omega - E_{hp+k} + \omega_p) \]
\[ + L_2(k, p) \delta(\omega - E_{hp+k} - \omega_p)] V_{hp+k}^2, \]  
(9)
\[ V_k^2 \delta(\omega + E_k) = \frac{1}{N} \sum_p \frac{B_p}{2\omega_p} [L_1(k, p) \delta(\omega + E_{hp+k} - \omega_p) \]
\[ + L_2(k, p) \delta(\omega + E_{hp+k} + \omega_p)] U_{hp+k}^2, \]  
(10)
with the electron quasiparticle spectrum \( E_k \). With the help of the spectral function \( \gamma \), the Bogoliubov angle in the present case for cuprate superconductors is expressed explicitly as,
\[ \Theta_k = \arctan \left[ \frac{A(k, \omega > 0)}{A(k, \omega < 0)} \right]^{1/2}. \]  
(11)
In particular, this Bogoliubov angle \( \Theta_k \) can be used to determined the Fermi surface as it has been done in the experiments. This follows from a fact that at the Fermi crossing point \( k_F \), the electron coherence factors \( U_{k_F}^2 = V_{k_F}^2 \), and then the Bogoliubov angle \( \Theta_{k_F} = \pi/4 \).

In cuprate superconductors, although the values of \( J \) and \( t \) is believed to vary somewhat from compound to compound, however, as a qualitative discussion, the commonly used parameters in this paper are chosen as \( t/J = 2.5, \ t'/t = 0.3 \). We are now ready to discuss the energy and momentum dependence of the SC quasiparticle spectral function \( A(k, \omega) \) in Eq. (7) and the related Bogoliubov angle \( \Theta_k \) in Eq. (11). In Fig. 1, we plot \( A(k, \omega) \) as a function of energy along the cut direction \([0.776\pi, 0.651\pi] \) to \([0.786\pi, 0.661\pi] \) crossing the Fermi surface with temperature \( T = 0.002J \) at the doping concentration \( \delta = 0.15 \) in comparison with the corresponding experimental results for the optimally doped cuprate superconductor \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) (inset). The thick solid curve is the momentum distribution curve where the electron coherence factors \( U_k^2 = V_k^2 \) and has been defined as the Fermi crossing point just as it has been done in the experiments. Obviously, the spectral weight of the two branches is momentum dependent. These two sharp quasiparticle peaks in each energy distribution curve exhibit a evolution of the relative peak height at different momentum positions. Moreover, the quasiparticle spectral intensity of the two bands show an opposite evolution as a function of \( k \) along the cut direction \([0.82\pi, 0.57\pi] \) to \([0.83\pi, 0.58\pi] \). This is a common feature of the momentum dependence of the SC quasiparticle spectral function along the cut direction crossing the Fermi surface. For a better understanding of the momentum dependence of the SC quasiparticle spectral function, we have made a series of calculations for the momentum dependence of the SC quasiparticle spectral function along different cut directions crossing the Fermi surface at different doping
concentration levels, and the result of $A(k,\omega)$ as a function of energy along the cut direction $[0.776\pi,0.651\pi]$ to $[0.786\pi,0.661\pi]$ crossing the Fermi surface with temperature $T = 0.002J$ at the doping concentration $\delta = 0.12$ is plotted in Fig. 2. The quasiparticle peak below the Fermi surface has a higher intensity than that above the Fermi surface. However, after passing the Fermi surface, the quasiparticle peak above the Fermi surface has a higher intensity than that below the Fermi surface. This crossover behavior near the Fermi surface, a characteristic of the Bogoliubov quasiparticle dispersion in the conventional superconductors in the SC state, appears in cuprate superconductors. To show this point clearly, we plot the quasiparticle peak intensity along the cut direction $[0.65\pi,0.4\pi]$ to $[\pi,0.75\pi]$ crossing the Fermi surface with temperature $T = 0.002J$ at the doping concentration $\delta = 0.15$ in Fig. 3. For comparison, the corresponding experimental results$^{12}$ for the optimally doped cuprate superconductor Bi$_2$Sr$_2$CaCu$_2$O$_8$+\delta is also plotted in Fig. 3 (inset). In comparison with the results in Fig. 1 and Fig. 2, we therefore confirm that (i) although the dispersive feature in Fig. 1 and Fig. 2 is almost symmetrical with respect to the Fermi surface, the SC quasiparticle peak intensity is not; (ii) the quasiparticle spectral intensity break near the Fermi surface shows the existence of a gap and two branches of dispersion centered at the Fermi surface; (iii) both bands show the bending back effect at the Fermi surface. All these theoretical results are qualitatively consistent with the ARPES experimental data of cuprate superconductors$^{5,9}$. Incorporating our previous results$^{3,4}$, we therefore confirming that the basic $d$-wave BCS formalism under the kinetic energy driven SC mechanism can correctly reproduce some low energy features of the SC coherence of the quasiparticle peaks observed in cuprate superconductors$^{5,9}$, including the doping and temperature dependence of the electron spectral function at the antinodal point and the momentum dependence of the electron spectral function along the cut direction crossing the Fermi surface.

Now we turn to discuss the momentum dependence of the electron coherence factors in Eq. (11) and Eq. (10) and the related Bogoliubov angle Eq. (11). From Eq. (11), we can find that the SC quasiparticle peak height of the peak below the Fermi surface in Fig. 1 and Fig. 2 is assigned a weight $Z_FV^2_k$, while that of the peak above the Fermi surface is assigned a weight $Z_FU^2_k$, therefore the coherence factors describe the relative intensity of the Bogoliubov quasiparticle bands above and below the Fermi surface. In Fig. 4, we plot $U^2_k$ (solid line) and $V^2_k$ (dashed line) along the cut direction $[0.82\pi,0.57\pi]$ to $[0.83\pi,0.58\pi]$ with $T = 0.002J$ at the doping concentration $\delta = 0.15$ in comparison with the corresponding experimental results$^{12}$ for the optimally doped cuprate superconductor Bi$_2$Sr$_2$CaCu$_2$O$_8$+\delta (inset), where the particle-hole mixing takes place due to the pairing, leading to a transfer of weight between the electron and hole bands. In particular, the electron coherence factors $U^2_k$ and $V^2_k$ have contrary evolution, and they are equivalent at the Fermi wave vector $k_F$, then $V^2_k + U^2_k = 1$ is always satisfied, showing good agreement in the band dispersion between the experiment$^{5,9}$ and the present theoretical calculation. For a further confirmation of the conventional Bogoliubov quasiparticle behaviors in cuprate superconductors, we have employed the ratio of the low energy quasiparticle spectra at positive and negative energies as a measure of the Bogoliubov angle $\Theta_k$ (11) at each momentum just as

FIG. 3: A color plot of the quasiparticle peak intensity along the cut position $[0.65\pi,0.4\pi]$ to $[\pi,0.75\pi]$ with $T = 0.002J$ for $t/J = 2.5$ and $t'/t = 0.3$ at $\delta = 0.15$. Inset: the corresponding experimental results taken from Ref. [3].

FIG. 4: The quasiparticle coherence factors $U^2_k$ (solid line) and $V^2_k$ (dashed line) along the cut position $[0.82\pi,0.57\pi]$ to $[0.83\pi,0.58\pi]$ with $T = 0.002J$ for $t/J = 2.5$ and $t'/t = 0.3$ at $\delta = 0.15$. Inset: the corresponding experimental results taken from Ref. [3].
it has been done in the experiments\textsuperscript{9}. The result for the extracted the Bogoliubov angle $\Theta_k$ along the cut direction $[0.82\pi, 0.57\pi]$ to $[0.83\pi, 0.58\pi]$ with temperature $T=0.002J$ at the doping concentration $\delta=0.15$ is plotted in Fig. 5 in comparison with the corresponding experimental result\textsuperscript{12} for the optimally doped cuprate superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (inset). We therefore find that $\Theta_k$ increase monotonically across the Fermi crossing point $k_F$ suggesting a continuously evolution of the particle and hole mixing within this momentum range. As we expect, $\Theta_k = \pi/4$ at $k_F$, indicating that the particle and hole mix equally at $k_F$ for cuprate superconductors, since in this case the weight of the SC quasiparticle peak below the Fermi surface $Z_FV_k^2$ is the same as the weight of the peak above the Fermi surface $Z_FU_k^2$ as mentioned above. Our this result is qualitatively consistent with the experimental data for cuprate superconductors\textsuperscript{9}.

The essential physics of the momentum dependence of the quasiparticle spectrum and the related Bogoliubov angle in cuprate superconductors in the SC state is the same as in the case of Ref. \textsuperscript{14}, where the doping and temperature dependence of the low energy electron spectral function at the antinodal point are discussed within the kinetic energy driven SC mechanism, and the results are qualitatively consistent with the corresponding ARPES experimental data\textsuperscript{15}. Incorporating these previous results\textsuperscript{14}, the good agreement between the ARPES experimental data\textsuperscript{15} and the present theoretical results within the kinetic energy driven superconductivity is further confirmation of the conventional Bogoliubov quasiparticle concept for cuprate superconductors.

In conclusion we have shown very clearly in this paper that the basic d-wave BCS formalism under the kinetic energy driven SC mechanism can correctly reproduce some low energy features found in ARPES measurements on cuprate superconductors. Our results show that the Bogoliubov quasiparticle intensity break near the Fermi surface shows the existence of a gap and two branches of dispersion centered at the Fermi surface. By calculation of the ratio of the low energy quasiparticle spectra at positive and negative energies, we show that the Bogoliubov angle increase monotonically across the Fermi crossing point.

Acknowledgments

This work was supported by the National Natural Science Foundation of China under Grant No. 10774015, and the funds from the Ministry of Science and Technology of China under Grant Nos. 2006CB601002 and 2006CB921300.
Lan, and Li Cheng, Int. J. Mod. Phys. B 22 (2008) 3757-3811, and references therein.

14 Huaiming Guo and Shipping Feng, Phys. Lett. A 361 (2007) 382-390; Shipping Feng and Tianxing Ma, Phys. Lett. A 350 (2006) 138-146; Yu Lan, Jihong Qin, and Shipping Feng, Phys. Rev. B 76 (2007) 014533.

15 K. Yamada, C. H. Lee, K. Kurahashi, J. Wada, S. Wakimoto, S. Ueki, H. Kimura, Y. Endoh, S. Hosoya, G. Shirane, R. J. Birgeneau, M. Greven, M. A. Kastner, and Y. J. Kim, Phys. Rev. B 57 (1998) 6165-6172; P. Dai, H. A. Mook, R. D. Hunt, and F. Dogan, Phys. Rev. B 63 (2001) 054525; P. Bourges, B. Keimer, S. Pailhés, L. P. Regnault, Y. Sidis, and C. Ulrich, Physica C 424 (2005) 45-49; C. Stock, W. J. Buyers, R.A. Cowley, P. S. Clegg, R. Coldea, C. D. Frost, R. Liang, D. Peets, D. Bonn, W. N. Hardy, and R. J. Birgeneau, Phys. Rev. B 71 (2005) 024522.

16 B. O. Wells, Z.-X. Shen, A. Matsuura, D. M. King, M. A. Kastner, M. Greven, and R. J. Birgeneau, Phys. Rev. Lett. 74 (1995) 964-967; C. Kim, P. J. White, Z.-X. Shen, T. Tohyama, Y. Shibata, S. Maekawa, B. O. Wells, Y. J. Kim, R. J. Birgeneau, and M. A. Kastner, Phys. Rev. Lett. 80 (1998) 4245-4248.

17 K. Tanaka, T. Yoshida, A. Fujimori, D. H. Lu, Z.-X. Shen, X.-J. Zhou, H. Eisaki, Z. Hussain, S. Uchida, Y. Aiura, K. Ono, T. Sugaya, T. Mizuno, and I. Terasaki, Phys. Rev. B 70 (2004) 092503.

18 J. Campuzano, H. Ding, M. Norman, H. Fretwell, M. Ran- deira, A. Kaminski, J. Mesot, T. Takeuchi, T. Sato, T. Yokoya, T. Takahashi, T. Mochiku, K. Kadowaki, P. Gup- tasarma, D. Hinks, Z. Konstantinovic, Z. Li, and H. Raffy, Phys. Rev. Lett. 88 (2002) 107001.