Physica C 517 (2015) 5–15

Contents lists available at ScienceDirect

Physica C

journal homepage: www.elsevier.com/locate/physc

Electronic structure of cuprate superconductors in a full charge-spin recombination scheme

Shiping Feng [a,*], Lülin Kuang [a], Huaisong Zhao [b]

[a] Department of Physics, Beijing Normal University, Beijing 100875, China
[b] College of Physics, Qingdao University, Qingdao 266071, China

ARTICLE INFO

Article history:
Received 21 May 2015
Accepted 30 June 2015
Available online 8 July 2015

Keywords:
Electronic structure
Electron Fermi surface
Full charge-spin recombination
Cuprate superconductor

ABSTRACT

A long-standing unsolved problem is how a microscopic theory of superconductivity in cuprate superconductors based on the charge-spin separation can produce a large electron Fermi surface. Within the framework of the kinetic-energy driven superconducting mechanism, a full charge-spin recombination scheme is developed to fully recombine a charge carrier and a localized spin into a electron, and then is employed to study the electronic structure of cuprate superconductors in the superconducting-state. In particular, it is shown that the underlying electron Fermi surface fulfills Luttinger's theorem, while the superconducting coherence of the low-energy quasiparticle excitations is qualitatively described by the standard d-wave Bardeen–Cooper–Schrieffer formalism. The theory also shows that the observed peak-dip-hump structure in the electron spectrum and Fermi arc behavior in the underdoped regime are mainly caused by the strong energy and momentum dependence of the electron self-energy.

1. Introduction

Superconductivity in cuprate superconductors occurs upon charge carrier doping Mott insulators [1]. Experimentally, it is well established that the Mott insulating state at zero doping develops long-range order antiferromagnetism [2,3]. Upon doping the antiferromagnetic (AF) long-range order (AFLRO) disappears rapidly and soon thereafter is replaced by the superconducting (SC) ground-state [2,3]. After intensive investigations over more than two decades, a large body of data available from a wide variety of measurement techniques have introduced important constraints on the microscopic model and SC theory [2–10]. At the temperature above the SC transition-temperature T_c, the electron is in a normal-state, however, the normal-state in the underdoped and optimally doped regimes is not normal at all, since the normal-state of cuprate superconductors exhibits a number of the anomalous properties [7–10] in the sense that they do not fit in with the standard Landau-Fermi liquid theory. The defining characteristic is that the resistivity grows nearly linearly with temperature [8–11]. Infrared measurements confirmed that the resistivity scales similarly with energy and temperature, and that the anomalous energy dependence extends up to an energy equivalent to at least 300 meV [8–11]. More importantly, the conductivity in the underdoped and optimally doped regimes shows a non-Drude behavior (the conductivity decays as $\rightarrow 1/\omega$) at low energies [9,10], and is carried by δ charge carriers, where δ is the charge carrier doping concentration. These are strong experimental evidences supporting the notion of the charge-spin separation [12,13]. Superconductivity is an instability of the normal-state. However, one of the most striking dilemmas is that the SC coherence of the low-energy quasiparticle excitations in cuprate superconductors seems to be described by the standard Bardeen–Cooper–Schrieffer (BCS) formalism [14–18], although the normal-state is undoubtedly not the standard Landau Fermi-liquid on which the conventional electron–phonon theory is based. Angle-resolved photoemission spectroscopy (ARPES) experiments reveal sharp spectral peaks in the single-particle excitation spectrum [4,5,14–22], indicating the presence of quasiparticle-like states, which is also consistent with the long lifetime of the electronic state as it has been determined by the conductivity measurements [9,10]. In particular, as a direct method for probing the electron Fermi surface, the early ARPES measurements indicate that in the entire doping range, the underlying electron Fermi surface satisfies Luttinger's theorem [23–26], i.e., the electron Fermi surface with the area is proportional to $1-\delta$. Later, the ARPES experimental studies show that in the underdoped and optimally doped regimes, although the antinodal region of the electron Fermi surface is gapped out, leading to the notion that only part of the electron Fermi surface survives as the disconnected Fermi arcs around the nodes [27–31], the underlying

* Corresponding author. Tel.: +86 10 58806408; fax: +86 10 58801764.
E-mail address: spfeng@bnu.edu.cn (S. Feng).

http://dx.doi.org/10.1016/j.physc.2015.06.017
0921-4534/

electron Fermi surface determined from the low-energy spectral weight still fulfills Luttinger's theorem in the entire doping range [31]. These ARPES experimental facts [14–31] on the other hand provide strong evidences supporting the notion of the charge-spin recombination [12,13]. Since the electron Fermi surface is a fundamental property of interacting electron systems, the study of the nature of the electron Fermi surface should be crucial for understanding the electronic structure of cuprate superconductors.

Theoretically, it is generally agreed that the strong electron correlation plays a dominant role in the description of the anomalous normal-state properties of cuprate superconductors and the related SC mechanism [32,33]. This strong electron correlation originates from a large on-site repulsion between two electrons occupying the same site, which effectively translates into an elimination of double electron occupancy. Apart from the numerical techniques, an intuitively appealing approach to implement this elimination of double electron occupancy and the charge-spin separation is the slave-particle approach [13,34,35], where the constrained electron operator $C_{l\sigma}$ is given by a composite operator as $C_{l\sigma}=a^{\dagger}_{l}f_{l\sigma}$, with $a^{\dagger}_{l}$ as the slave boson and $f_{l\sigma}$ as the fermion or *vice versa*, i.e., $a^{\dagger}_{l}$ as the fermion and $f_{l\sigma}$ as the boson. In this slave-particle approach, the operator $f_{l\sigma}$ carries spin index (spinon) and the operator $a^{\dagger}_{l}$ is interpreted as creating a vacancy (holon). The elimination of double electron occupancy is presented by the requirement that $a^{\dagger}_{l}a_{l}+\sum_{\sigma}f^{\dagger}_{l\sigma}f_{l\sigma}=1$ which can be enforced by introducing a Lagrangian multiplier. Moreover, the doped holes are mainly responsible for the charge transport, and the relaxation time of the excitation from the spin degree of freedom is mainly responsible for the spin response, while the SC-state is characterized by the charge-spin recombination, forming SC quasiparticles [13,35]. In the conventional charge-spin recombination scheme, the electron Green's function in space–time is a product of the holon and spinon Green's functions [12,13,35,36]. The resulting Fourier transform is a convolution of the holon and spinon Green's functions. However, in the early days of superconductivity, we [36] have formally proved that the electron Fermi surface observed experimentally from the ARPES experiments cannot be restored based on the conventional charge-spin recombination. In this case, a long-standing unsolved problem is how a microscopic theory based on the charge-spin separation can give a consistent description of the electronic structure of cuprate superconductors in terms of a full charge-spin recombination. By the *full charge-spin recombination* we refer to the obtained electron propagator that can produce a large electron Fermi surface with an area proportional to $1-\delta$. For a proper treatment of the strong electron correlation in cuprate superconductors, we [37,38] have developed a fermion-spin theory based on the charge-spin separation, where the constrained electron operator is decoupled as a product of a charge carrier and a localized spin, and then the electron motion is restricted in the restricted Hilbert space without double electron occupancy. Within the framework of the fermion-spin theory, we [38–40] have established a kinetic-energy driven SC mechanism, where the charge-carrier pairing state is conventional BCS-like with the d-wave symmetry, although the pairing mechanism is driven by the kinetic-energy by the exchange of spin excitations in the higher powers of the doping concentration. In particular, this kinetic-energy driven charge-carrier pairing state is controlled by both the charge-carrier pair gap and charge-carrier quasiparticle coherence, which leads to that the charge-carrier pair transition-temperature T_c takes a domelike shape with the underdoped and overdoped regimes on each side of the optimal doping, where T_c reaches its maximum. Following this kinetic-energy driven SC mechanism, we in this paper develop a *full charge-spin recombination scheme*, and then show that although the electron Cooper pairing state (then the SC-state) originates from the charge-carrier pairing state, the low-energy excitation of cuprate superconductors in the SC-state resembles the BCS-Bogoliubov quasiparticle. In particular, we show that the obtained formalism for the electron pairing can be used to compute the electronic structure of cuprate superconductors on the first-principles basis much as can be done for conventional superconductors. Moreover, the theory produces a large electron Fermi surface with the area that is given by $1-\delta$, while the striking feature of the peak-dip-hump structure in the single-particle excitation spectrum around the antinodal point and remarkable Fermi arc behavior in the underdoped and optimally doped regimes are mainly caused by the strong energy and momentum dependence of the electron self-energy.

The rest of this paper is organized as follows. Since the work in this paper builds on the kinetic-energy driven SC mechanism, a short summary of the formalism of the kinetic-energy driven SC mechanism is first given in Section 2, and then based on this kinetic-energy driven SC mechanism, the basic formalism of the full charge-spin recombination is presented, which is manifested itself by the self-consistent equations that are satisfied by the full electron diagonal and off-diagonal Green's functions. Moreover, we confirm that the SC transition-temperature T_c obtained from this full charge-spin recombination scheme is identical to the charge-carrier pair transition-temperature. In Section 3, the full electron diagonal Green's function is employed to study the electronic structure of cuprate superconductors in the SC-state, and then some main features of the ARPES measurements on cuprate superconductors in the SC-state are qualitatively reproduced. Finally, we give a summary in Section 4.

2. Theoretical framework

Superconductivity in cuprate superconductors is found in copper oxide-based compounds with a layered crystal structure consisting of the two-dimensional CuO_2 planes separated by insulating layers [1–5]. The key element shared by all such structure is the CuO_2, and then it seems evident that the relatively high T_c in cuprate superconductors is dominated by this CuO_2 plane [1–5]. Immediately following the discovery of superconductivity in cuprate superconductors, Anderson [32] argued that the essential physics of the doped CuO_2 plane is contained in the t–J model on a square lattice,

$$H=-t\sum_{l\hat{\eta}\sigma}C^{\dagger}_{l\sigma}C_{l+\hat{\eta}\sigma}+t'\sum_{l\hat{\tau}\sigma}C^{\dagger}_{l\sigma}C_{l+\hat{\tau}\sigma}+\mu\sum_{l\sigma}C^{\dagger}_{l\sigma}C_{l\sigma}+J\sum_{l\hat{\eta}}\mathbf{S}_{l}\cdot\mathbf{S}_{l+\hat{\eta}}, \quad (1)$$

where the summation is over all sites l, and for each l, over its nearest-neighbors $\hat{\eta}$ or the next nearest-neighbors $\hat{\tau}$, $C^{\dagger}_{l\sigma}$ ($C_{l\sigma}$) is electron creation (annihilation) operator with spin σ, $\mathbf{S}_{l}=(S^{x}_{l},\ S^{y}_{l},\ S^{z}_{l})$ are spin operators, and μ is the chemical potential. In spite of its simple form, the t–J model (1) is proved to be very difficult to analyze, analytically as well as numerically. However, the most difficult in the analytical treatment of the t–J model (1) comes mainly from the local constraint of no double electron occupancy, i.e., $\sum_{\sigma}C^{\dagger}_{l\sigma}C_{l\sigma}\leqslant 1$, while the strong electron correlation manifests itself by this local constraint of no double electron occupancy, and therefore the crucial requirement is to impose this local constraint. In order to satisfy this local constraint, we employ the fermion-spin formalism [37,38], in which the electron operators $C_{l\uparrow}$ and $C_{l\downarrow}$ are replaced by,

$$C_{l\uparrow}=h^{\dagger}_{l\uparrow}S^{-}_{l},\quad C_{l\downarrow}=h^{\dagger}_{l\downarrow}S^{+}_{l}, \quad (2)$$

respectively. The spinful fermion operator $h_{l\sigma}=e^{-i\Phi_{l\sigma}}h_{l}$ keeps track of the charge degree of freedom of the constrained electron together with some effects of spin configuration rearrangements due to the