Topological Transition in the Fermi Surface of Cuprate Superconductors in the Pseudogap Regime

C. M. Varma and Lijun Zhu

Department of Physics and Astronomy, University of California, Riverside, California 92521, USA

(Received 4 August 2006; published 26 April 2007)

The angle-resolved photoemission spectroscopy studies on cuprates in the pseudogap region reveal an extraordinary topological transition in which the ground state changes from one with a normal Fermi surface to one with four Fermi points. Such a state is not possible without some symmetry breaking, which allows interference between one-particle basis states that is normally forbidden. We also show that the experimental results are quantitatively given without any free parameters by a theory and discuss the implications of the results.

DOI: 10.1103/PhysRevLett.98.177004 PACS numbers: 74.25.Jb, 74.20.−z, 74.72.−h

Recently, the single-particle spectral function $A(\mathbf{k}, \omega)$ obtained by angle-resolved photoemission spectroscopy (ARPES) on eight different underdoped BSCCO cuprates with T_c ranging from 25 to 90 K has been systematically analyzed [1]. The principal conclusion is that the angular region in $\hat{\mathbf{k}}$ where $A(\mathbf{k}, \omega)$ has a maxima at the chemical potential μ is a universal function $\Phi(T/T_g(x))$. T is the temperature, and $T_g(x)$ is the pseudogap transition temperature at a given doping level x, the deviation of the density of holes from half-filling. At $T \geq T_g(x)$, $\Phi = 2\pi$, i.e., the angular region encloses an area, while for $T \rightarrow 0$, $\Phi \rightarrow 0$ and the region shrinks to 4 points. $T_g(x)$ is, within the uncertainties of its determination, the same as that obtained from the resistivity or the thermodynamic measurements such as the magnetic susceptibility and the specific heat which also scale as functions of $T/T_g(x)$ [2]. $T_g(x)$ is also consistent with the temperature at which time-reversal symmetry (TRS) breaking is observed by dichroic ARPES experiments [3,4] in the same compounds. Qualitatively similar conclusions were arrived at by Yoshida *et al.* [5].

Recall that in a Fermi liquid [6] [or a marginal Fermi liquid (MFL) [7]], $A(\mathbf{k}, \omega)$ is maximum at $\omega = \mu$ for $\mathbf{k} = \mathbf{k}_F$, thus defining the Fermi surface. The concept of a Fermi surface, properly defined as the nonanalytic surface which separates the area of occupied states from the unoccupied states in a Fermi liquid, is strictly meaningful only at $T \rightarrow 0$. This is merely a technicality in the usual metallic states. But for underdoped cuprates, the proper definition of a Fermi surface is essential. The experimental results suggest that for $x > x_c$, such that $T_g(x_c) = 0$, the extrapolated $T = 0$ nonsuperconducting ground state has a Fermi surface, whereas for $x < x_c$, the concept of a Fermi surface is lost.

It has become the custom to call the angular region $\Phi(T/T_g)$ a *Fermi arc*. This is harmless only if the empirical procedure used to derive $\Phi(T/T_g)$ from the experiments is kept in mind.

The truly new physics is the deduction that, at $T \rightarrow 0$, a gap in the single-particle excitation spectra develops at the chemical potential for a range of electronic densities at all angles on the Fermi surface except four nodal points. Of course, this deduction is based on extrapolating data (available from about $T = 400$ to 25 K) down to $T = 0$, but the data (reproduced in Fig. 3 below) are persuasive. It joins the list of novel concepts brought to physics by the cuprates because it does not obey Bloch's counting theorem for periodic systems that gaps can occur only at Brillouin zone boundaries, i.e., for integer fillings [8,9]. The theorem originally derived for noninteracting electrons also holds for interacting systems in which there is a one-to-one correspondence between particles and quasiparticles. But the derivation implies an even greater generality, because it depends only on the (usually safe) assumption that the excitation energy of one-particle states is a single-valued continuous function of their momentum quantum number except at the zone boundaries, where multiple energies are obtained for a given momentum due to interference.

The only previously known state [10], in the absence of disorder, where a gap (or a gap with nodal points or lines as in anisotropic superconductors) occurs tied to the chemical potential independent of band filling is superconductivity. In that case, the energy of states is a double valued function of momentum for states near $\mathbf{k}_F$ with a gap. Bloch's theorem is circumvented in this case only because the single-particle excitations near $\mathbf{k} = \mathbf{k}_F$ are linear combinations of electrons and holes and, therefore, are not eigenstates of charge. A gap occurs due to an interference between basis states of different charges. Circumventing Bloch's counting theorem in other circumstances requires that some other normally sacrosanct quantum number be no longer protected, which allows interference between basis states that is usually forbidden [11].

Bloch's theorem is circumvented in a theory of the pseudogap state [14,15] for reasons not having to do with BCS pairing. This theory predicts that the pseudogap state breaks time-reversal symmetry below $T_g(x)$ without

changing the translational symmetry. This aspect has been tested in BSCCO by dichroic ARPES [3,4] and in YBCO by polarized neutron scattering [16]. The statistical mechanical model derived to obtain such a symmetry breaking [17] is the Ashkin-Teller model, which in the relevant range of parameters has a smooth change in specific heat at the transition with the entropy released over a temperature range typically more than twice the transition temperature [18]. It is also shown that a normal Fermi surface cannot exist in such a TRS breaking state. The order parameter is not a conserved quantity; therefore, fermions with crystal momentum $\mathbf{k}$ have a finite coupling $g(\mathbf{k})$ to the order parameter fluctuations in the long wavelength limit. Since in this limit the energy of the order parameter fluctuations goes to 0, a Fermi surface instability with no change in translational symmetry but in the harmonic of $g(\mathbf{k})$ accompanies the broken TRS. A stable state is found with an anisotropic gap in the excitation spectra. In the new state, the single-particle excitations are not eigenstates of crystal momentum but formed from the linear combination of states of momentum in a small region around a given momentum [14]. Interference between basis states of crystal momentum leads to the anisotropic gap at the erstwhile Fermi surface with four Fermi points left intact. The ground state itself is perfectly periodic and, therefore, an eigenstate of crystal momentum. This is not new conceptually; recall that in superconductivity the ground state conserves charge although the single-particle excitations do not.

The purpose of this Letter is to show that the predictions of such a state agree quantitatively with the new experimental results. To show this, we calculate the evolution of the single-particle spectral function as a function of temperature and define the Fermi arc in the same way that the experimentalists have done. We calculate the function $\Phi(T/T_g(x))$, defined above and compare it with the experiments [1]. An independent experimental result consistent with the underlying ideas is that the linewidth of the single-particle spectra of the cuprates abruptly acquires a large elastic part in going from the overdoped cuprates [19] to the underdoped cuprates.

The single-particle states at $T \to 0$ in the stable TRS breaking state in the absence of impurity scattering have been derived [14,15] to have energies given by

$$E_{\mathbf{k}}^{\gtrless} = \epsilon_{\mathbf{k}} \pm D(\mathbf{k}) \quad \text{for } E_{\mathbf{k}} \gtrless \mu, \tag{1}$$

where $D(\mathbf{k}) \approx D_0(1 - T/T_g)^{1/2}\cos^2(2\phi)/[1 + (\epsilon_{\mathbf{k}}/\epsilon_c)^2]$ is the gap function, which is anisotropic and temperature-dependent. ϕ is the angle of $\hat{\mathbf{k}}$, and $\epsilon_{\mathbf{k}}$ is the "band-structure" energy of a tight-binding model to fit the Fermi surface [20] found by ARPES for $x \leq x_c$, with effective nearest-neighbor and next-nearest-neighbor Cu-Cu hopping parameters t and t', respectively:

$$\epsilon_{\mathbf{k}} = -2t[\cos k_x + \cos k_y] - 4t' \cos k_x \cos k_y, \tag{2}$$

where $t'/t = -0.35$. ϵ_c is a cutoff of order D_0. The simple theory [15] gives $D_0 \approx \sqrt{6}T_g$.

The single-particle spectrum is given by the spectral function $A^{\gtrless}(\mathbf{k}, \omega)$

$$-\frac{1}{\pi}\frac{\mathrm{Im}\Sigma(\mathbf{k}, \omega)}{[\omega - E_{\mathbf{k}}^{\gtrless} - \mathrm{Re}\Sigma(\mathbf{k}, \omega)]^2 + [\mathrm{Im}\Sigma(\mathbf{k}, \omega)]^2}, \tag{3}$$

where $\Sigma(\mathbf{k}, \omega)$ is the self-energy, which is the sum of the contributions due to electron-electron scattering and impurity scattering. We present here results in the pure limit as well as including small angle impurity scattering. If $-\mathrm{Im}\Sigma \gtrsim D(\hat{\mathbf{k}}_F)$, the spectrum $A^{>}(\mathbf{k}, \omega)$ has finite weight in the $\omega < \mu$ region. So the total spectrum measured by ARPES (at $\omega \leq \mu$) is

$$A(\mathbf{k}, \omega \leq \mu) = A^{<}(\mathbf{k}, \omega) + A^{>}(\mathbf{k}, \omega). \tag{4}$$

$\Sigma(\mathbf{k}, \omega)$ close to the maximum of $D(\hat{\mathbf{k}})$ or far away from the *nodal* region can be calculated in the pure limit from the fact that, due to momentum and energy conservation, decay of a particle requires three intermediate-state particles, at least one of which must also be close to the maximum of the gap function. Using these kinematical constraints and that for ω, $T \gtrsim D(\hat{\mathbf{k}})$, the decay rate must revert to the state without the pseudogap (i.e., the MFL state). So

$$-\mathrm{Im}\Sigma_{\mathrm{in}}(\mathbf{k}, \omega, T) \approx \mathrm{sech}\left(\frac{D(\hat{\mathbf{k}})}{\sqrt{\omega^2 + \pi^2 T^2}}\right)\tau_M^{-1}(\omega, T), \tag{5}$$

where τ_M^{-1} is the MFL relaxation rate:

$$\tau_M^{-1} = \lambda\sqrt{\omega^2 + \pi^2 T^2}. \tag{6}$$

λ is the dimensionless coupling constant used to fit ARPES data for $x \geq x_c$ by the MFL spectral function.

Near the zeros of $D(\hat{\mathbf{k}})$ (nodal region), one can again use momentum and energy conservation to calculate the phase space for decay. One easily finds that the self-energy for $\omega \ll D(\hat{\mathbf{k}})$ is

$$-\mathrm{Im}\Sigma_{\mathrm{in}}(\mathbf{k}, \omega, T) = \lambda\{(\omega^2 + \pi^2 T^2)/D_0\}, \tag{7}$$

while for $\omega \gg D_0$, it reverts to the MFL form τ_M^{-1}. Another interpolation form, such as in Eq. (5), is used to connect the nodal region and the antinodal region. In our calculations below, we have used Eq. (7) in an angular region extending to $\delta\phi = \pi/20$ from the nodal point and Eq. (5) elsewhere. Similar results are obtained for factors of 2 variations about this partitioning. For the low energy region of interest, $\mathrm{Re}\Sigma$ produces negligible corrections and has been ignored.

The spectral function is calculated using Eqs. (3) and (4). The parameters used in the evaluation are $D_0/T_g = 2.5$, and λ is fixed by the value determined by the MFL fits to the spectral function for $x \geq x_c$ to be ≈ 0.5. Earlier, the specific heat and the magnetic susceptibility in the underdoped cuprates were fitted [15] to experiments with $D_0/T_g \approx 2.5$. Thus, there are no free parameters left to fit.

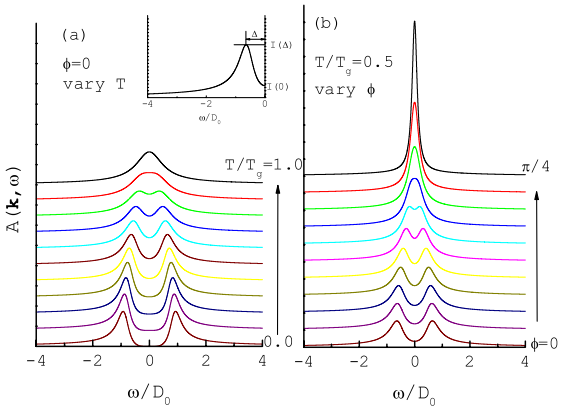

FIG. 1 (color online). The spectral functions (energy-distribution curves) for (a) the antinodal angle at various temperatures and (b) fixed temperature ($T/T_g = 0.5$) while varying angles from antinode to node. Here $D_0 = 2.5T_g$. As shown in the inset, we have followed the representation of the data as in experiments, explained in the main text.

In Fig. 1, the calculated spectral function is plotted at the antinodal point for various T/T_g and for various angles at $T/T_g = 0.5$. The inset shows the definition of various quantities used to represent the experiments in Ref. [1]. $\Delta(\phi)$ is defined as the energy at which the spectral function peaks below the chemical potential at the angle ϕ, while $I(0, \phi)$ and $I(\Delta, \phi)$ are the intensities at the chemical potential (set to $\omega = 0$) and at Δ, respectively. Either $\Delta(\phi) = 0$ or $1 - I(0, \phi)/I(\Delta, \phi) = 0$ implies that $A(\mathbf{k}_F, \omega)$ peaks at the chemical potential, giving the impression of a "Fermi surface." The angular region where these quantities vanish are defined as "Fermi arcs."

The experimental results and the calculated values of $\Delta(\phi)/\Delta(0)$ and of $1 - I(0, \phi)/I(\Delta, \phi)$ are shown in Fig. 2. The central aspect of the experimental results deduced from the experiments is shown in Fig. 3 together with the results of calculations. Figure 3 shows that the Fermi arc length $\Phi(T/T_g(x))$ for a whole range of underdoped cuprates at various dopings x is a universal function of $T/T_g(x)$ and that at $T \to 0$, $\Phi \to 0$. The theory in the pure limit is in quantitative accord with the experimental curve without any free parameters except for the region of $T/T_g \approx 1$. This disagreement may be traced to the fact that the experimental gap rises below T_g much faster than the mean-field theory. The qualitatively new physics in the results deduced from the experiments is, however, in the low temperature limit.

The agreement actually is a little worse if we include impurity scattering; see also Fig. 3. We have calculated the spectral function including the effects of small angle scattering due to impurities between the Cu-O planes [21,22]. Because of the anisotropy of the density of states in the pseudogap state, the impurity scattering rate becomes anisotropic as well as frequency-dependent. With the impurity scattering estimated from experiments, which gives an elastic scattering rate of about 200 K at the nodal point

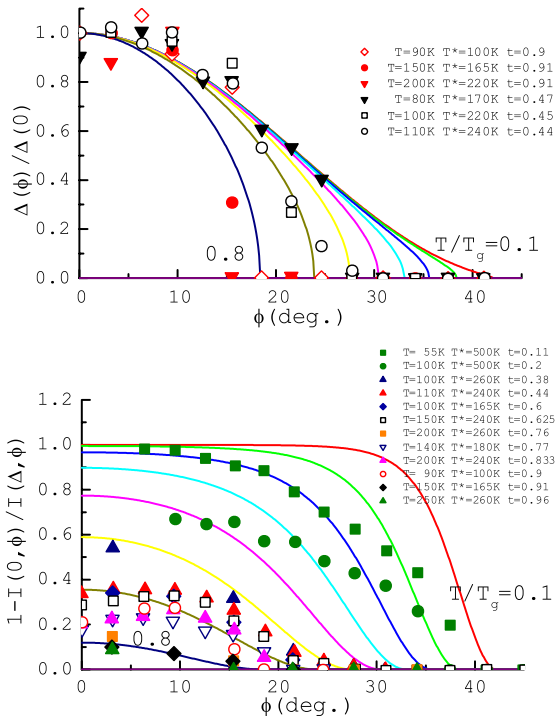

FIG. 2 (color online). The gap function and the peak intensity $1 - I(0, \phi)/I(\Delta, \phi)$ as functions of the angle. The solid lines are theoretical results for $T/T_g = 0.1$–0.8 (in sequence from right to left).

above T_g [19], we have to use $D_0/T_g \approx 3$ to get agreement with the experiments. With small angle scattering, only four Fermi points remain at $T \to 0$, but a weak smooth bump develops for these values at around $T/T_g \approx 0.1$, which, however, continues to give a theoretical curve within the experimental error bars. The impurity scattering, of course, varies also from sample to sample. We should also mention that if the large angle impurity scattering in the unitary limit were important, say, due to impurities in the plane, we expect an impurity resonance at the nodal points, so that the Fermi points are smeared out.

We are not aware of any other theory giving the results of the experiments, specifically a scaling form for the Fermi arc $\Phi(T/T_g(x))$, with $\Phi(0) \to 0$. There exist theories which generate anisotropic reduction of the density of states in the underdoped state without generating Fermi points at $T = 0$, such as approximate solutions of the Hubbard model with dynamical mean-field theory and its extensions [23]. There is no indication that the Fermi surface shrinks to four Fermi points in such calculations at $T \to 0$. This is consistent with the general arguments given in this Letter that this is not possible without some symmetry breaking. On the other hand, experiments must be done in materials where the extrapolation to the ground state of the pseudogap phase can be done more precisely. This necessitates experiments in high quality underdoped samples just at the boundary to superconductivity. Another prediction of the theory which awaits more precise mea-

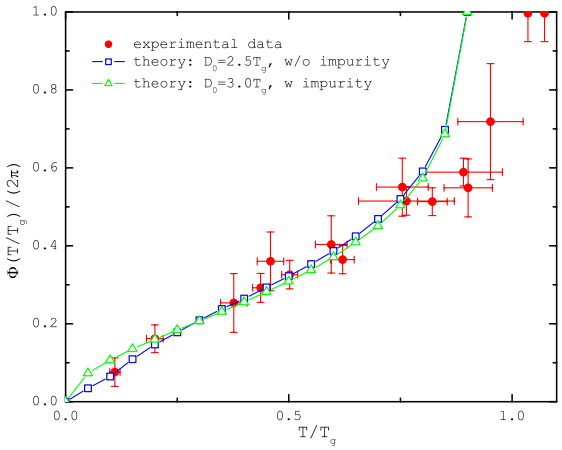

FIG. 3 (color online). The Fermi arc length as a function of T/T_g. The experimental data from Ref. [1] are shown as red dots with error bars. The solid lines are theoretical results: one in the pure limit with $D_0 = 2.5T_g$; another with small angle impurity scattering, fitted with $D_0 = 3T_g$ and $1/\tau_0 = T_g$, where $1/\tau_0$ is the impurity scattering rate at the nodal point, and its magnitude can be estimated from the normal state data, such as in Ref. [19].

surements through higher energy and momentum resolution is that the angular dependence of the pseudogap is $\propto (\phi - \phi_0)^2$ near the points ϕ_0 at which it is 0 [see the expression for the pseudogap following Eq. (1)]. This is important to conclude that there is no phase associated with the pseudogap, unlike superconducting gaps or gaps due to a change in translational symmetry due to charge or spin-density waves or staggered flux phases.

In conclusion, we would like to reemphasize that the scaling of the Fermi arc is a new phenomenon in condensed matter physics and that it requires a broken symmetry. We have presented the results of a theory, one of whose consequences is a Fermi surface with only four points. With two parameters taken to fit thermodynamic measurements, we have been able to account for the details of the Fermi arcs. The same theory has predicted a time-reversal violating state in the pseudogap region and the theory of quantum critical fluctuations [17], which gives the phenomenological spectrum [7] with which the "strange metal" phase is understood. These fluctuations also give rise to attractive pairing interaction in the "d-wave" symmetry [24].

One of us (C. M. V.) is grateful to Leon Balents for a discussion of the Bloch's counting theorem.

[1] A. Kanigel *et al.*, Nature Phys. **2**, 447 (2006).
[2] J. W. Loram *et al.*, J. Phys. Chem. Solids **62**, 59 (2001); see also Fig. 8 in Ref. [15].
[3] A. Kaminski *et al.*, Nature (London) **416**, 610 (2002). There has been some controversy about the results of this paper; see S. V. Borisenko *et al.*, *ibid.* doi:10.1038/nature02931 (2004); J. C. Campuzano *et al.*, *ibid.* doi:10.1038/nature02932 (2004); C. M. Varma, Phys. Rev. B **73**, 233102 (2006).
[4] M. E. Simon and C. M. Varma, Phys. Rev. Lett. **89**, 247003 (2002).
[5] T. Yoshida *et al.*, cond-mat/0610759.
[6] See, e.g., D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1966).
[7] C. M. Varma, P. B. Littlewood, S. Schmitt-Rink, E. Abrahams, and A. E. Ruckenstein, Phys. Rev. Lett. **63**, 1996 (1989).
[8] F. Bloch, Z. Phys. **52**, 555 (1928).
[9] The theorem continues to hold for gaps which are zero on points and lines, because, when integrating over the Brillouin zone, points or lines contribute negligibly to the number of total states.
[10] The ground state of Mott insulators is antiferromagnetic. Therefore, their gap is consistent with Bloch's theorem. Even ignoring antiferromagnetism, the Mott gap occurs only for integer filling of a band. The Efros-Shklovskii gap [B. I. Shklovskii and A. L. Efros, *Electronic Properties of Amorphous Semiconductors* (Springer-Verlag, Berlin, 1984)] in disordered insulators is indeed tied to the chemical potential but occurs only due to the unscreened Coulomb interaction associated with the localization of states.
[11] A change of the connectivity of the Fermi surface without a change of symmetry was described by Lifshitz [12,13] many years ago. Clearly, the shrinking of the Fermi surface to four points while retaining all of the symmetries is a topological transition. But in a Lifshitz transition, the total volume of the Fermi surface (taking into account the "sign" of the Fermi surface, positive for electrons and negative for holes) is conserved. The (extrapolated) ground state in the underdoped cuprates encloses no electrons or holes.
[12] I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **38**, 1569 (1960) [Sov. Phys. JETP **11**, 1130 (1960)].
[13] G. E. Volovik, *The Universe in a Helium Droplet* (Clarendon, London, 2003).
[14] C. M. Varma, Phys. Rev. Lett. **83**, 3538 (1999).
[15] C. M. Varma, Phys. Rev. B **73**, 155113 (2006). The spectral functions were also calculated here and shown in a dimensionless form.
[16] B. Fauqué *et al.*, Phys. Rev. Lett. **96**, 197001 (2006).
[17] V. Aji and C. M. Varma, cond-mat/0610646.
[18] It is known from L. P. Kadanoff and A. C. Brown [Ann. Phys. (N.Y.) **121**, 318 (1979)] that the specific heat in the Ashkin-Teller model has no singularity; A. Sudbo (private communication) has explicitly calculated the specific heat for this model by Monte Carlo methods.
[19] A. Kaminski *et al.*, Phys. Rev. B **71**, 014517 (2005).
[20] See, e.g., O. Andersen *et al.*, J. Phys. Chem. Solids **56**, 1573 (1995).
[21] E. Abrahams and C. M. Varma, Proc. Natl. Acad. Sci. U.S.A. **97**, 5714 (2000).
[22] E. Abrahams and C. M. Varma, Phys. Rev. B **68**, 094502 (2003); C. M. Varma and E. Abrahams, Phys. Rev. Lett. **86**, 4652 (2001).
[23] B. Kyung *et al.*, Phys. Rev. B **73**, 165114 (2006), and references therein.
[24] C. M. Varma, BAPS (March 2007), Session L8 1.