PHYSICAL REVIEW B **81**, 180513(R) (2010)

Lifshitz transition in underdoped cuprates

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(Received 1 April 2010; published 27 May 2010)

Recent studies show that quantum oscillations thought to be associated with a density wave reconstructed Fermi surface disappear at a critical value of the doping for $YBa_2Cu_3O_{6+y}$ and the cyclotron mass diverges as the critical value is approached from the high doping side. We argue that the phenomenon is due to a Lifshitz transition where the pockets giving rise to the quantum oscillations connect to form an open (quasi-one-dimensional) Fermi surface. The estimated critical doping is close to that found by experiment and the theory predicts a logarithmic divergence of the cyclotron mass with a coefficient comparable to that observed in experiment.

DOI: 10.1103/PhysRevB.81.180513 PACS number(s): 74.25.Jb, 72.15.Gd, 75.30.Fv

The unusual doping dependence of the physical properties of the high-T_c cuprate superconductors has been a focus of interest since the beginning of the field. Experiments conducted over the past several years have demonstrated that a crucial aspect of the doping dependence is a Fermi surface reconstruction, most likely due to some form of spin- or charge-density wave order. In overdoped materials, photoemission[1] and quantum oscillation studies[2] have confirmed the existence of a large Fermi surface of size and shape compatible with band theory. As the doping is reduced, the form of the Fermi surface changes. Photoemission data indicate that the Fermi surface breaks up. The initial studies were interpreted in terms of disconnected "Fermi arcs"[3] but some recent studies have argued that what is observed is actually part of a closed hole pocket.[4,5] One issue is that photoemission experiments access the "normal" (nonsuperconducing) state by raising the temperature above the superconducting (SC) transition temperature T_c. Quantum oscillation measurements, on the other hand, are conducted at high magnetic fields which suppress superconductivity, permitting (at least, in principle) access to the low-temperature normal state. As the doping is reduced, unambiguous signatures of the formation of small Fermi pockets are observed,[6,7] in particular, a dominant oscillation frequency of about 530 T, corresponding to a pocket size about 1.9% of the Brillouin zone. The fate of the pocket (or pockets) as the doping is reduced is the subject of intense current interest.[8]

In a very interesting recent experiment, Sebastian *et al.*[9] report that in underdoped $YBa_2Cu_3O_{6+y}$ (YBCO), the cyclotron mass of the Fermi pocket corresponding to the dominant quantum oscillation frequency diverges near y of 6.46.[9] Below this doping, the oscillation frequency is not seen. The critical doping is close to the value at which high-field transport indicates localization[10,11] and also near the doping where inelastic neutron-scattering studies have indicated a collapse of the spin gap[12] with the subsequent appearance of a nematic phase.[13,14] Reference 15 suggests that the mass divergence might be associated with an excitonic instability involving electron and hole pockets.

In this Rapid Communication we propose that the transition observed by Sebastian *et al.*[9] is a Lifshitz transition where the pockets touch and so connect to form an open (quasi-one-dimensional) Fermi surface. The phase diagram resulting from our proposal is shown in Fig. 1. The new feature added to existing phase diagrams such as those of Ref. 16 is the Lifshitz transition, shown as the heavy line with filled circles. We present theoretical calculations showing that for reasonable parameters, such a transition can occur at the experimentally observed doping. In two dimensions, we find that the cyclotron mass diverges logarithmically at the Lifshitz transition. We estimate the doping dependence of the mass and the magnitude of the divergence, finding good agreement with the data. The sensitivity of one-dimensional conductors to localization[17] is consistent with the divergent resistivity observed at lower dopings.[10,11] Our proposal thus naturally explains the main features of the observations near this doping.

Our calculations are based on a linear spin-density wave (SDW) (magnetic stripe) model introduced to account for the first generation of quantum oscillation experiments.[18] The model involves electrons described by a tight-binding band structure believed to be appropriate for hole-doped high-T_c superconductors and subject to a periodic potential appropriate for an antiphase spin-density wave state characterized by the wave vector $q=(1-2\delta,1)\pi$, which we measure in units of $1/a$ where a is the lattice constant. Details of the electronic dispersion used and the form of the secular matrix can be found in Ref. 18. In our previous work,[18,19] we focused on the case of $\delta=0.125$. Electron pockets centered at $(0,\pi)$ and symmetry related points were found, as well as hole pockets and open orbits. The precise fermiology depended on the specific model parameters chosen but the generic features of the calculation were the electron pockets and the open orbits. The hole pockets were less robust in that they existed for smaller ranges of the density wave potential. We therefore argued that the observed quantum oscillation signal[6,7] arose from the electron pocket. We will return to this issue below.

In this Rapid Communication we extend our analysis to lower dopings, $x<0.125$. Neutron-scattering data[20] indicate that the stripe wave vector $\delta=x$ and we make this assumption

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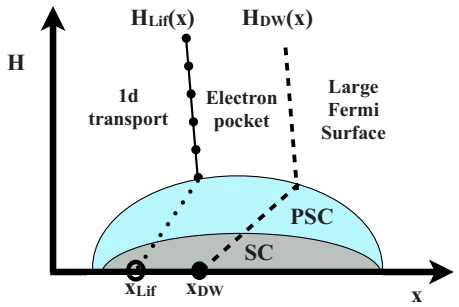

FIG. 1. (Color online) Schematic phase diagram at zero temperature in the plane of doping x and applied magnetic field H suggested by quantum oscillation experiments and the present work. Shaded regions: SC (zero resistance) phase and regime of precursor (fluctuating) superconductivity (PSC). $H_{DW}(x)$ (dashed line): onset of density wave order (broken lattice translation symmetry). At fields above the PSC boundary, the Fermi surface is well defined and, in the presence of density wave order, is reconstructed as indicated in the figure. $H_{Lif}(x)$ (solid line with filled circles): Lifshitz transition proposed in the present work at which the dominant Fermi pockets connect to form an open Fermi surface. Light dotted line indicates the continuation of the Lifshitz transition into the PSC/SC regimes, where the gapping of the Fermi surface converts it to a crossover.

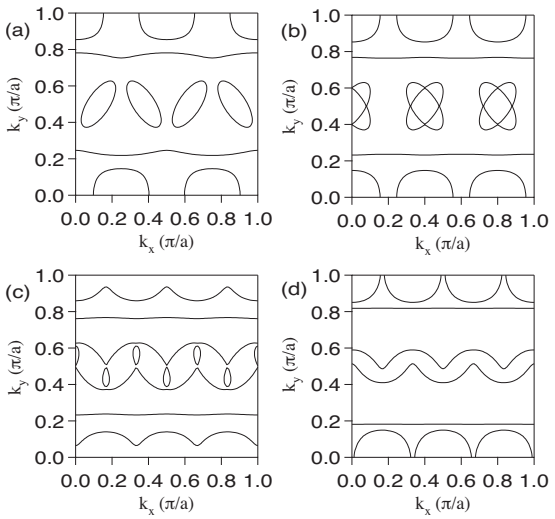

FIG. 2. Fermi surface for (a) V_s=0.178 eV and $x=\delta=1/8$, (b) V_s=0.204 eV and $x=\delta=1/10$, (c) V_s=0.233 eV and $x=\delta=1/12$, and (d) V_s=0.25 eV, V_c=−0.12 eV, and $x=\delta=1/12$, where V_s is the spin potential, V_c the charge potential, x the doping, and δ the incommensurability.

in the calculations presented in this Rapid Communication. For simplicity, we include in most of our calculations only the fundamental harmonic of the spin potential (V_s) but do show one example with a nonzero second-harmonic (charge) potential (V_c). Representative results are shown in the four panels of Fig. 2. Figure 2(a) reproduces our previous results for $x=1/8$.[18] The subsequent panels show the evolution of the Fermi surface as the doping is reduced. In these calculations V_s was adjusted so that the area of the electron pocket corresponds to an oscillation frequency of 530 T as observed by experiment (experiment indicates only a weak doping dependence of the frequency[9]). One sees that between $\delta=1/10$ and $\delta=1/12$, the pockets touch, resulting in a Lifshitz transition. The critical δ can be easily estimated. In a repeated zone scheme, the pocket centers are separated by a momentum 2δ, so if δ is decreased while the pocket area is held fixed, the pockets must touch. If we assume a circular pocket, which is consistent with a recent quantum oscillation study where the field angle was swept,[15] then for a pocket radius corresponding to the oscillation frequency of 530 T, and with the lattice constant, a, of 3.85 Å, implies a critical value of δ equal to 0.078, corresponding to a period just beyond 12. The parameters used to construct Fig. 2 lead to pockets slightly elongated along the k_x direction and the critical δ in our calculation is correspondingly slightly greater than 1/12. The critical doping can be changed by introducing a second-harmonic (charge) potential (V_c). Figure 2(d) shows that a negative value of V_c makes the pocket shape more circular, stabilizing a closed pocket for the 12 period case (a positive V_c would act oppositely by further elongating the pocket along k_x).

We identify the Lifshitz transition at which the electron pockets vanish with the transition observed by Sebastian *et al.*[9] This argument relies on the identification of the $(0,\pi)$ pocket as the one which gives rise to the dominant 530 T quantum oscillation frequency. In the calculation this pocket is an electron pocket. The first quantum oscillation study[6] of underdoped $YBa_2Cu_3O_{6+y}$ detected only the dominant oscillation frequency but interpreted it as a hole pocket (as suggested also by the photoemission experiments). However, the subsequent observation of a negative Hall number in this doping range[7] led to the suggestion that the observed frequency originated from an electron pocket near the $(0,\pi)$ point of the Brillouin zone.[7,18] Recently, multiple frequencies have been seen.[21,22] The smaller ones, near the originally observed frequency, have been interpreted as arising from bilayer splitting and warping of the two-dimensional Fermi cylinders associated with the $(0,\pi)$ pocket,[21] although a recent proposal suggests electron and hole cylinders of comparable size,[15] one of them warped and the other not.

Further support for an electron pocket comes from the fact that a π phase shift is observed between the longitudinal and Hall Shubnikov-de Haas oscillations as expected for an electron pocket.[23] Recently, it has been determined that the transport data are most consistent with a coherent electron contribution and an incoherent hole contribution.[24] As the doping is reduced, the coherent electron contribution is lost.[25] Also, the Shubnikov-de Haas oscillations associated with this oscillation frequency are largest for the c-axis resistance,[26] suggesting again an electron pocket since the c-axis hopping is largest in the $(0,\pi)$ region of the zone.[27]

A difficulty with an interpretation of the dominant frequency in terms of electron pockets is that photoemission experiments at these dopings indicate a large energy gap in this region of the Brillouin zone[1,3–5] suggesting that an electron pocket would not exist. However, the photoemission and quantum oscillation experiments are not in direct contradiction. The photoemission experiments are conducted at zero magnetic field and at temperatures above T_c [below T_c, one observes a d-wave superconducting gap which is maximal at the $(0,\pi)$ points]. On the other hand, quantum oscillation experiments are conducted at high fields and at low tempera-

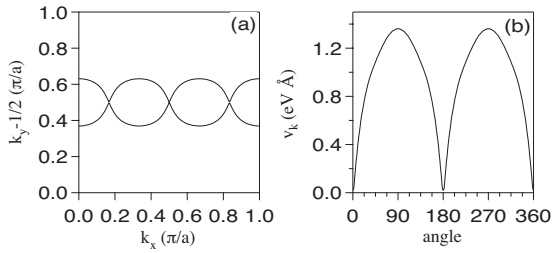

FIG. 3. (a) Electron Fermi surface for V_s=0.235 eV, μ=−0.35466 eV, and δ=1/12, where μ is the chemical potential (for clarity, the rest of the bands are not shown). (b) Fermi velocity around the Fermi surface from (a). 0° and 180° correspond to the touching points.

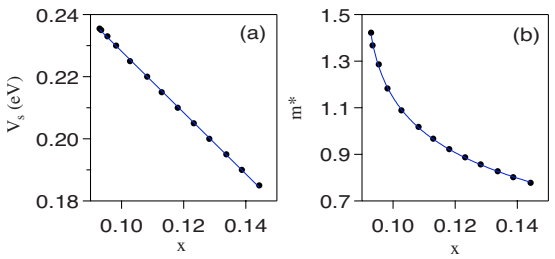

FIG. 4. (Color online) (a) V_s and (b) cyclotron mass versus doping, x, for δ=1/12. Note the actual cyclotron mass will be renormalized upward by about a factor of 3 due to many-body correlations not included in the present calculation. Points: results of calculations using the stripe SDW model. Curves: fits to linear (panel a) and logarithmic (panel b) functions. $V_s(x)$ is determined by requiring that the area of the electron pocket be doping independent. Obtaining an area corresponding to a quantum oscillation frequency of 530 T at a critical doping of 9% requires a nonzero V_c as in Fig. 2(d). To reduce the number of varying parameters, we set V_c=0 in this calculation; the V_s-only model for δ=1/12 gives a frequency of 447 T.

tures. In that context, it is known that application of a magnetic field stabilizes the formation of the density wave state as observed by neutron scattering,[28] as indicated in Fig. 1. Moreover, quantum oscillations can exist in the presence of an energy gap. For instance, oscillations are observed in type-II superconductors well below the upper critical field.[29] For all of these reasons, we argue that the main quantum oscillation frequency arises from the electron pocket located near the $(0,\pi)$ region of the Brillouin zone, as found in our calculations.[18]

To study the Lifshitz transition in more detail, we tune the system to the Lifshitz point and present in Fig. 3 the Fermi surface and the variation around the Fermi surface of the Fermi velocity. One can see the linear variation in the Fermi contour about the touching point. This is reflected in a linear variation in the Fermi velocity, v_k, about the touching point. As a consequence, the cyclotron mass, which is defined by the line integral along the orbit, $\int dk/v_k$ (equivalent to the energy derivative of the cyclotron area), is logarithmically divergent. This divergence can be seen analytically by noting that the touching point corresponds to a saddle point in the dispersion, which also leads to a logarithmically divergent density of states in two dimensions. This divergence will be cutoff by doping away from the Lifshitz point or by any c-axis warping of the Fermi cylinders, although we note that the oscillation studies have not been able to resolve the multiple frequencies expected from warping as the critical doping is approached. The divergence with doping is illustrated in Fig. 4(b). Note that we plot the band mass; the actual mass will be renormalized by about a factor of 3 due to many body correlations as observed in photoemission. The observed mass variation with doping is stronger than what we calculate, presumably due to an increase of this renormalization with underdoping. In this plot, we take a simplified approach of working at fixed wave vector and fixed area of the cyclotron orbit. This leads to a linear variation in V_s with x, as illustrated in Fig. 4(a). This increase of the potential with underdoping is expected in a density wave scenario. If instead V_s was held fixed to its value at the critical doping (0.235 eV), the pocket area would decrease by a factor of 3 over the doping range indicated.

A more detailed connection with experiment requires a knowledge of the true dependence of the wave vector on doping. In zero-field neutron-scattering data, it is difficult to determine what the actual δ is because of the presence of the spin gap. Quoted values of δ are typically obtained from the momentum dependence of the neutron-scattering intensity at an energy near the spin gap energy, but as the spin branch below the resonance energy has a significant dispersion, these quoted values are underestimates of the zero energy value. It is also possible (Fig. 1) that δ will change in a magnetic field. The other issue is that the relation of y, T_c, and the doping, x, is complicated because of the presence of chains in the YBCO structure, with differences depending on whether the sample is stabilized in the ortho-I or ortho-II structure.[30] Measurements made at y=6.45 where no spin gap is present[12,31] find δ=0.054, which would be a lower bound. An upper bound would be near 0.1, the expected value for y=6.5 where quantum oscillations have been seen. This indicates a rapid change in δ between these values of y. Our estimated δ_c and therefore y_c is safely within this range. The bounds could be tightened significantly from neutron-scattering data near y_c if a magnetic field is applied to induce an elastic signal.[28] A more decisive test of this scenario would be to use field angle sweeps[15] to look for the expected deviation of the orbit cross section from circular behavior as the proposed Lifshitz transition is approached. One could also look for whether the field dependence of the transport indicates the presence of open orbits for $y<y_c$.

To summarize, we have proposed a simple explanation for the disappearance of quantum oscillations near y=6.46 in YBCO as due to a Lifshitz transition of electron pockets. For y less than this value, we propose that the Fermi surface is quasi-one dimensional (Fig. 1), and thus subject to localization. This would then account for the well-known metal-insulator transition observed in high magnetic fields near this doping value.[10,11]

We thank Louis Taillefer and Cyril Proust for sharing with us their unpublished data, and Suchitra Sebastian and Neil Harrison for discussions. A.J.M. was supported by the U.S. NSF under Grant No. DMR-0705847, and M.R.N. and J.L. by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357.

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