Truncation of a Two-Dimensional Fermi Surface due to Quasiparticle Gap Formation at the Saddle Points

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We study a two-dimensional Fermi liquid with a Fermi surface containing the saddle points $(\pi, 0)$ and $(0, \pi)$. Including Cooper and Peierls channel contributions leads to a one-loop renormalization group flow to strong coupling for short range repulsive interactions. In a certain parameter range the characteristics of the fixed point, opening of a spin and charge gap, and dominant pairing correlations are similar to those of a two-leg ladder at half-filling. We argue that an increase of the electron density leads to a truncation of the Fermi surface to only four disconnected arcs. [S0031-9007(98)07323-2]

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The origin of the instability of the Landau-Fermi liquid state as the electron density is increased in overdoped cuprates is one of the most interesting open questions in the field. Recently, we proposed that the origin lies in a flow of umklapp scattering to strong coupling [1]. The simpler case with the Fermi surface (FS) extrema at $(\pm\pi/2, \pm\pi/2)$ was considered and not the realistic case for hole-doped cuprates where the leading contribution from umklapp processes comes from scattering at the saddle points $(\pi, 0)$ and $(0, \pi)$. In this Letter we report a one-loop renormalization group (RG) calculation for the realistic case including contributions from both Cooper and Peierls channels. Reasonable conditions can lead to a strong coupling fixed point whose characteristics are similar to those of half-filled two-leg ladders. There, strong coupling umklapp processes lead to spin and charge gaps but only short range spin correlations. A particularly interesting and novel feature is that, although the strongest divergence is in the d-wave pairing channel, the charge gap causes insulating not superconducting behavior.

There have been a number of previous RG investigations for a FS with saddle points. Schulz [2] and Dzyaloshinskii [3] considered the special case with only nearest neighbor (nn) hopping so that the saddle points coincide with a square FS and perfect nesting exactly at half-filling, leading to a fixed point with long range antiferromagnetic (AF) order. Lederer *et al.* [4] and Dzyaloshinskii [5] also considered the same model as we do. There are two fixed points, one at a strong coupling fixed point with d-wave pairing found by Lederer *et al.* [4], and a weak coupling examined by Dzyaloshinskii [5]. A Hubbard parametrization of the repulsive interactions (U) and moderate interaction strength suffices to stabilize the strong coupling fixed point. The new feature we wish to stress is that there can be both spin and charge gaps. The FS is then truncated through the formation of an insulating spin liquid (ISL) with resonance valence bond (RVB) character. We propose that as the hole doping decreases these gaps spread out from the saddle points so the FS consists of a set of arcs, which progressively shrink as the hole doping decreases.

We start with a two-dimensional FS touching the saddle points $(\pi, 0)$ and $(0, \pi)$. Such a FS is realized in the case of the dispersion relation $\varepsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$ with $t > 0$ $(t' < 0)$ as nn [next-nearest neighbor (nnn)] hoppings. Throughout this Letter, we assume t'/t small but nonzero so that we are close to half-filling. Because of the van Hove singularity, the leading singularity arises from electron states in the vicinity of the saddle points. We consider two FS patches at the saddle points and examine the coupling between them using one-loop RG equations, as illustrated in Fig. 1a. k_c is the radius of the patches.

The susceptibility for the Cooper channel at $q = 0$ has a log-square behavior of the form

$$\chi_0^{\mathrm{pp}}(\omega) = -h \ln(\omega/E_0) \ln(\omega/2tk_c^2) . \quad (1)$$

Here, the sum over k is restricted to the patches. E_0 is the cutoff energy and $h = (8\pi^2 t)^{-1}$ for $|t'/t| \ll 1$. The

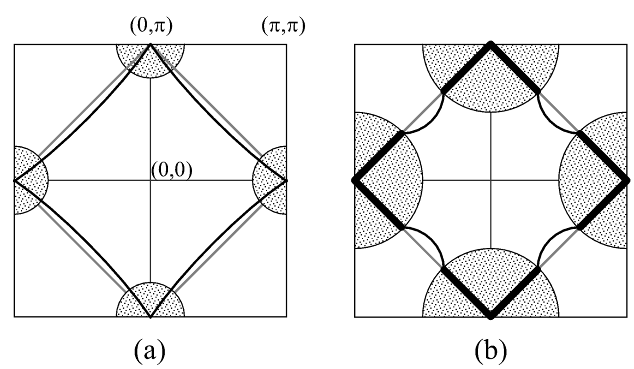

FIG. 1. Fermi surface (FS). (a) Two patches of the FS at the saddle points. (b) Truncated FS as electron density is increased.

Peierls channel at $Q = (\pi, \pi)$ diverges as

$$\chi_Q^{\rm ph}(\omega) = \begin{cases} h \ln(\omega/E_0)\ln(\omega/2tk_c^2) & \omega \gg |t'| \\ 2h \ln|t'/t| \ln(\omega/E_0) & \omega \ll |t'| \end{cases}. \quad (2)$$

The susceptibilities for the Peierls channel at $q = 0$ ($\chi_0^{\rm ph}$) and the Cooper channel at $q = Q$ ($\chi_Q^{\rm pp}$) also diverges as

$$\chi_0^{\rm ph} \sim -\chi_Q^{\rm pp} \sim 2h \ln(E_0/\omega), \quad (3)$$

but the coefficients of $\ln(\omega)$ are smaller than that of $\chi_Q^{\rm ph}$.

In Fig. 2 we define the interaction vertices g_i ($i = 1 \sim 4$). Normal and umklapp processes are indistinguishable since the patches are at the zone edge. We use a Wilson RG flow, parametrized by a decreasing energy scale, in which all degrees of freedom above that energy scale are integrated out. Wilson's effective action at scale E_0 has the dual interpretation that (a) it generates the interaction vertices, and thus an effective Hamiltonian, for the particles with energy below E_0 and (b) these vertices are also the connected correlation functions with the infrared cutoff E_0. We consider only the four-point function and include only the one-loop terms. The one-loop RG was justified as the leading behavior at low energies and weak coupling for a class of FS in Ref. [6], which includes those with nonzero curvature ($t' \neq 0$ in our case). It leads to the flow equations (see also Lederer *et al.* [4])

$$\dot g_1 = 2d_1 g_1(g_2 - g_1) + 2d_2 g_1 g_4 - 2d_3 g_1 g_2, \quad (4)$$

$$\dot g_2 = d_1(g_2^2 + g_3^2) + 2d_2(g_1 - g_2)g_4 - d_3(g_1^2 + g_2^2), \quad (5)$$

$$\dot g_3 = -2g_3 g_4 + 2d_1 g_3(2g_2 - g_1), \quad (6)$$

$$\dot g_4 = -(g_3^2 + g_4^2) + d_2(g_1^2 + 2g_1 g_2 - 2g_2^2 + g_4^2). \quad (7)$$

Here, we introduced the normalization$g_i \to h g_i$, to give dimensionless couplings, and $\dot g_i \equiv (dg_i)/(dy)$, where $y \equiv \ln^2(\omega/E_0) \propto \chi_0^{\rm pp}(\omega)$. We define functions which describe the relative weight of $q = 0$ Cooper channel contribution and those of other channels,

$$d_1(y) = d\chi_Q^{\rm ph}/dy, \quad (8)$$

$$d_2(y) = d\chi_0^{\rm ph}/dy, \quad (9)$$

$$d_3(y) = -d\chi_Q^{\rm pp}/dy. \quad (10)$$

Their asymptotic forms are $d_1(y) \to 1$ at $y \approx 1$ and $d_1(y) \sim \ln|t/t'|/\sqrt{y}$ as $y \to \infty$, while $d_2(y) \sim d_3(y) \sim 1/\sqrt{y}$ throughout the region of interest.

The case $d_1 = 1$ and $d_2, d_3 \ll d_1$ was studied by Schulz [2], Dzyaloshinskii [3], and Lederer *et al.* [4] which arises at $t' = 0$ as well as in a sufficiently large U region where t' is irrelevant. Spin-density wave (SDW) susceptibility has the same exponent as d-wave pairing but is dominant due to the next leading divergent terms. The fixed point is understood as a Mott insulator with long range AF order. The limit $d_1 = d_2 = d_3 = 0$ was treated by Dzyaloshinskii [5]. In this case, (6) and (7) combine to give $\dot g_- = -g_-^2$ with $g_- = g_4 - g_3$. Dzyaloshinskii considered the weak-coupling fixed point $g_- \to 0$ which arises when $g_- \geq 0$, and discussed the resulting Tomonaga-Luttinger liquid behavior.

In this Letter we examine the RG equations with $0 < d_1(y) < 1$ which enables us to consider nonzero values of the ratios t'/t and U/t. Since $d_2, d_3 \ll d_1$, we neglect d_2 and d_3 in RG equations for simplicity. Note the terms involving d_1 act to enhance the basin of attraction for the strong coupling fixed point, $g_- \to -\infty$ [4]. The one-loop RG equations are solved numerically. Starting from a Hubbard-model initial value $g_i = U$ ($i = 1 \sim 4$), the vertices flow to strong coupling fixed points with $g_2 \to +\infty$, $g_3 \to +\infty$, and $g_4 \to -\infty$, with the asymptotic form

$$g_i(y) = g_i^0/(y_c - y). \quad (11)$$

Here $y_c \sim t/U$ is the critical point of one-loop RG equations. The divergence of $g_1(y)$ with respect to $y_c - y$ is only logarithmic. To analyze this fixed point more precisely, we substitute the asymptotic form (11) into Eqs. (4)–(7) and obtain polynomial equations

$$g_1^0 = 2d_1(y_c)g_1^0(g_2^0 - g_1^0), \quad (12)$$

$$g_2^0 = d_1(y_c)[(g_2^0)^2 + (g_3^0)^2], \quad (13)$$

$$g_3^0 = -2g_3^0 g_4^0 + 2d_1(y_c)g_3^0(2g_2^0 - g_1^0), \quad (14)$$

$$g_4^0 = -[(g_3^0)^2 + (g_4^0)^2]. \quad (15)$$

Figure 3 shows the solution of these equations g_i^0 for the initial values $g_i = U$. The coefficients g_i^0 are determined as a function of $d_1(y_c) \sim \sqrt{U/t}\,\ln|t/t'|$, i.e., the critical behavior of the fixed point is a function of U.

Although one cannot solve for the strong coupling fixed point using only one-loop RG equations, a qualitative description comes from the susceptibilities. Using these coefficients g_i^0, exponents for various susceptibilities are

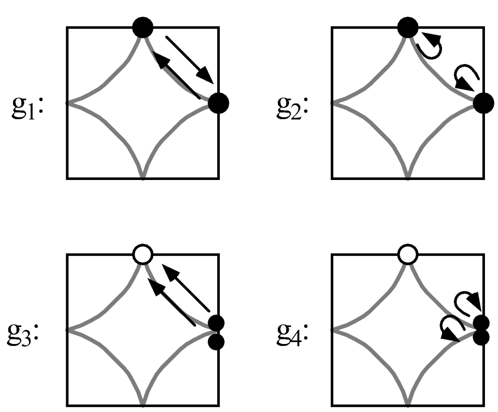

FIG. 2. The definitions of vertices for the two-patch model.

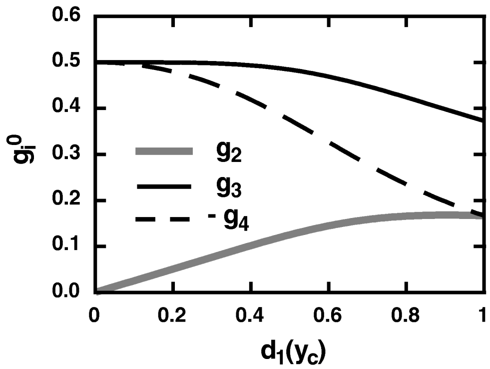

FIG. 3. The fixed point values for g_i^0.

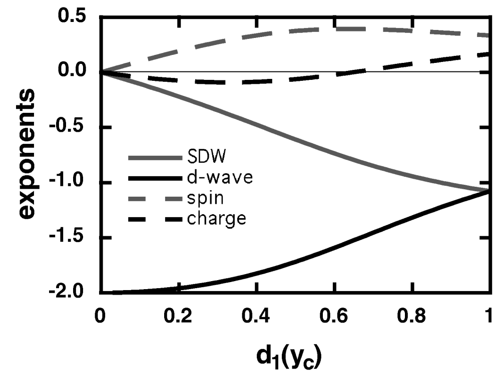

FIG. 4. Exponents for various susceptibilities. For uniform spin and charge susceptibilities, exponents are scaled by d_2/d_1.

calculated as follows. The one-loop RG equation for the d-wave pairing is

$$\dot{\bar{\chi}}_{\mathrm{dP}} = 2(g_4 - g_3), \tag{16}$$

where $\bar{\chi}_{\mathrm{dP}} = (\partial \chi_{\mathrm{dP}}/\partial \omega)/(\partial \chi_0^{\mathrm{pp}}/\partial \omega)$. From Eq. (11), we obtain a divergence $\chi_{\mathrm{dP}} \propto (y_{\mathrm{c}} - y)^{\alpha}$ with exponent $\alpha = \alpha_{\mathrm{dP}} = 2(g_4^0 - g_3^0)$. Similarly, exponents for s-wave pairing, charge density waves (CDW), SDW, as well as uniform spin, charge compressibilities, and finite momentum π pairing, are given by

$$\alpha_{\mathrm{sP}} = 2(g_3^0 + g_4^0), \tag{17}$$

$$\alpha_{\mathrm{CDW}} = (2g_1^0 - g_2^0 + g_3^0)d_1(y_{\mathrm{c}}), \tag{18}$$

$$\alpha_{\mathrm{SDW}} = -2(g_2^0 + g_3^0)d_1(y_{\mathrm{c}}), \tag{19}$$

$$\alpha_{\mathrm{s}} = -2(g_1^0 + g_4^0)d_2(y_{\mathrm{c}}), \tag{20}$$

$$\alpha_{\kappa} = (-g_1^0 + 2g_2^0 + g_4^0)d_2(y_{\mathrm{c}}), \tag{21}$$

$$\alpha_{\pi} = 2(-g_1^0 + g_2^0)d_3(y_{\mathrm{c}}), \tag{22}$$

respectively. For weak coupling, we have $d_2(y_{\mathrm{c}}) \sim d_3(y_{\mathrm{c}}) \sim \sqrt{U/t}$. Uniform susceptibilities are calculated in the limit $\omega, q \to 0$ with q/ω held fixed.

In Fig. 4 we show the exponents for d-wave pairing, SDW, uniform spin, and charge compressibility. Comparison of the values of the exponents shows us that the most divergent susceptibility is d-wave pairing throughout the parameter region of $0 < d_1(y_{\mathrm{c}}) < 1$ [4]. The SDW susceptibility shows a weaker divergence, and the exponent vanishes in the limit $d_1(y_{\mathrm{c}}) \to 0$ or $U/t \to 0$. The exponents for uniform spin as well as s-wave pairing, CDW, and π pairing are always positive; i.e., these susceptibilities are suppressed at low frequency.

The exponent for the charge compressibility changes sign at $d_1(y_{\mathrm{c}}) \sim 0.6$. Namely, there exists a critical interaction strength U_{c} such that for $U > U_{\mathrm{c}}$ the charge compressibility is suppressed to zero. The critical value U_{c} is determined by t' in the form $U_{\mathrm{c}}/t \propto \ln^{-2}|t/t'|$. This implies a transition from a superconducting phase at $U < U_{\mathrm{c}}$ with its origin in enhanced Cooper pairing due to the van Hove singularity, to a charge-gapped phase at $U > U_{\mathrm{c}}$ which can be regarded as a precursor of the Mott transition. The fixed point at $U > U_{\mathrm{c}}$ resembles that of the half-filled two-leg ladder which has spin and charge gaps but the most divergent susceptibility is d-wave pairing. This fixed point (C0S0 in the Balents-Fisher [7] notation) is well understood as an ISL of short range RVB form. The close similarity between the fixed points leads us to assign them to the same universality class.

The fixed point for $0 < d_1 < 1$ with d-wave pairing as the leading divergence differs from the case $d_1 \equiv 1$, where SDW correlation is dominant when the next leading term is included [2], and from the weak-coupling fixed point for $d_1 \equiv 0$ [5]. The contribution of the particle-particle channel of the part of the Fermi surface away from the saddle points was not discussed here for brevity; one can show that it gives a non-negative contribution to $\dot{g}_-$ and thus even enhances the asymmetry that drives the flow to strong coupling $g_- \to -\infty$. The present result for the saddle point model with $t' < 0$ is in good accordance with the case $t' > 0$ (or $t' < 0$ with electron doping) previously studied by the authors [1]. There, four patches at the zone diagonals were considered. For interaction U larger than a critical value determined by the infrared cutoff due to finite curvature, the charge compressibility renormalizes to zero due to the umklapp scattering.

Next we consider increasing the electron density. One possibility is to follow the noninteracting FS which expands beyond the saddle points. But the flow to strong coupling and the opening of a charge and spin gap lead us to consider a second possibility, namely, that the FS is pinned by umklapp processes and does not expand beyond the saddle points. This proposal was put forward in Ref. [1] after an examination of eight FS patches located on the umklapp surface (US) which is defined by lines joining saddle points. The leading contribution from umklapp processes comes from scattering between points on this US. Support for this proposal comes from the lightly doped three-leg ladder [8,9], where in strong coupling a C1S1 phase occurs with an ISL with exactly half-filling in the even parity channels and an open FS only in the odd parity channel. This contrasts with the one-loop RG results which gives a C2S1 phase [7] with holes immediately entering both odd and even parity channels. Our proposal, sketched in Fig. 1b, is based on a lateral spread of the spin and charge gaps along the US leading to four open FS segments consisting of arcs centered at the points $(\pm\pi/2, \pm\pi/2)$. Such behavior can be viewed as a sort of phase separation in $\vec{k}$ space in that in some directions an ISL forms but others remain metallic. Note that the area enclosed by the surface defined by the US and these four arcs contains the full electron density, consistent with a generalized form of Luttinger's theorem.

Note that, since the ISL is not characterized by any simple broken symmetry or order parameter, the resulting state cannot be described by a simple mean field or Hartree-Fock factorization. Our proposal of a FS consisting of four disconnected arcs has strong parallels to recent gauge theory calculations for the lightly doped strong coupling t-J model by Lee and Wen [10]. Signs of such behavior are also evident in a recent analysis of the momentum distribution using a high temperature series by Putikka *et al.* [11]. Note that models which include only nn hoppings $(t' = 0)$ are a special limit from the present point of view.

The development of ISL near the saddle points is related to the gap formation of the high-T_c cuprates. In the normal state of the underdoped cuprates, the ARPES experiments [12,13] show a single particle gap opening and a loss of quasiparticle weight in the vicinity of the saddle points below the pseudogap temperature. Tunneling experiment [14] also shows a quasiparticle gap formation above T_c. These results are quite similar to those we propose in Fig. 1b. Systematics of the loss of quasiparticle weights in electron- and hole-doped cuprates [15] are also consistent with our results for four-patch and two-patch models.

The proposal that an ISL truncates the FS along the US in the vicinity of the saddle points has very interesting consequences. There will be a coupling to the open segments in the Cooper channel through the scattering of electron pairs out of the ISL to the open FS segments. This process is reminiscent of the coupling of fermions to bosonic preformed pairs in the Geshkenbein-Ioffe-Larkin model [16]. They argued for an infinite mass for such pairs to suppress their contribution to transport properties. Such scattering processes will be an efficient mechanism for d-wave pairing on the open FS segments.

We also see a close similarity to a phenomenological model by Ioffe and Millis [17], to explain the anomalous transport properties in the normal state. They assumed that the FS segments have the usual quasiparticle properties without spin-charge separation but the scattering rate to vary strongly along the FS arcs. They justified the model by comparison to ARPES and tunneling experiments [12–14]. In our case, the scattering rate varies strongly due to the strong umklapp scattering at the end of the FS arcs where they meet the ISL region. Lastly, we refer the reader to the recent paper by Balents, Fisher, and Nayak [18] which introduces the concept of a nodal liquid with properties similar to the ISL discussed above.

In conclusion, we have shown that, when the Fermi surface approaches the saddle points, umklapp scattering drives the system into a strong coupling fixed point which can cause a breakdown of the Landau Fermi liquid state. The Fermi surfaces near the saddle points $(\pi, 0)$ and $(0, \pi)$ are truncated by the formation of a pinned and insulating condensate, while the zone diagonal regions around $(\pm\pi/2, \pm\pi/2)$ remain metallic. We have given arguments that the spin properties are those of an insulating spin liquid. This microscopic model has a lot in common with the results of ARPES experiments and some recent phenomenological models so that we believe it can form the basis for a theory of the cuprates.

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[1] N. Furukawa and T. M. Rice, J. Phys. Condens. Matter **10**, L381 (1998).
[2] H. J. Schulz, Europhys. Lett. **4**, 609 (1987).
[3] I. Dzyaloshinskii, Sov. Phys. JETP **66**, 848 (1987).
[4] P. Lederer, G. Montambaux, and D. Poilblanc, J. Phys. (Paris) **48**, 1613 (1987).
[5] I. Dzyaloshinskii, J. Phys. I (France) **6**, 119 (1996).
[6] J. Feldman, M. Salmhofer, and E. Trubowitz, J. Stat. Phys. **84**, 1209 (1996).
[7] L. Balents and M. P. A. Fisher, Phys. Rev. B **53**, 12 133 (1996); H.-H. Lin, L. Balents, and M. P. A. Fisher, Phys. Rev. B **56**, 6569 (1997).
[8] T. M. Rice, S. Haas, M. Sigrist, and F. C. Zhang, Phys. Rev. B **56**, 14 655 (1997).
[9] S. R. White and D. J. Scalapino, Phys. Rev. B **57**, 3031 (1998).
[10] P. A. Lee and X. G. Wen, Phys. Rev. Lett. **78**, 4111 (1997).
[11] W. O. Putikka, M. U. Luchini, and R. R. P. Singh, cond-mat/9803141.
[12] A. G. Loeser *et al.*, Science **273**, 325 (1996).
[13] M. R. Norman *et al.*, Nature (London) **392**, 157 (1998).
[14] Ch. Renner *et al.*, Phys. Rev. Lett. **80**, 149 (1998).
[15] C. Kim *et al.*, Phys. Rev. Lett. **80**, 4245 (1998).
[16] V. B. Geshkenbein, L. B. Ioffe, and A. I. Larkin, Phys. Rev. B **55**, 3173 (1997).
[17] L. B. Ioffe and A. J. Millis, cond-mat/9801092.
[18] L. Balents, M. P. A. Fisher, and C. Nayak, cond-mat/9803086.