d-Wave Superconductivity and Pomeranchuk Instability in the Two-Dimensional Hubbard Model

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We present a systematic stability analysis for the two-dimensional Hubbard model, which is based on a new renormalization group method for interacting Fermi systems. The flow of effective interactions and susceptibilities confirms the expected existence of a d-wave pairing instability driven by antiferromagnetic spin fluctuations. More unexpectedly, we find that strong forward scattering interactions develop which may lead to a Pomeranchuk instability breaking the tetragonal symmetry of the Fermi surface.

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The two-dimensional Hubbard model [1] has attracted much interest as a promising prototype model for the electronic degrees of freedom in the copper-oxide planes of high-temperature superconductors, since it has an antiferromagnetically ordered ground state at half-filling and is expected to become a d-wave superconductor for slightly smaller electron concentrations [2].

Although the Coulomb interaction in the cuprate superconductors is rather strong, the tendency towards antiferromagnetism and d-wave pairing is captured already by the 2D Hubbard model at *weak* coupling. Conventional perturbation theory breaks down for densities close to half-filling, where competing infrared divergences appear as a consequence of Fermi surface nesting and Van Hove singularities [3–5]. A controlled and unbiased treatment of these divergencies cannot be achieved by standard resummations of Feynman diagrams but requires a *renormalization group* (RG) analysis which takes into account the particle-particle and particle-hole channels on an equal footing.

Early RG studies of the two-dimensional Hubbard model started with simple but ingenious scaling approaches, very shortly after the discovery of high-T_c superconductivity [3–5]. These studies focused on dominant scattering processes between Van Hove points in k space, for which a small number of running couplings could be defined and computed on the one-loop level. Spin-density and superconducting instabilities where identified from divergencies of the corresponding correlation functions.

A major complication in two-dimensional systems compared to one dimension is that the effective interactions cannot be parametrized accurately by a small number of running couplings, even if irrelevant momentum and energy dependences are neglected, since the *tangential* momentum dependence of effective interactions along the Fermi surface is strong and important in the low-energy limit. This has been demonstrated in particular in a one-loop RG study for a model system with two parallel flat Fermi surface pieces [6]. Zanchi and Schulz [7] have recently shown how modern functional RG methods can be used to treat the full tangential momentum dependence of effective interactions for arbitrary curved Fermi surfaces. Evaluating the corresponding one-loop flow equations for the Hubbard model (with pure nearest-neighbor hopping), antiferromagnetic and d-wave pairing instabilities were found. An improved version of the functional RG derived by Salmhofer [8], which is particularly suitable for a concrete numerical evaluation, has recently been extended for the calculation of susceptibilities and applied to the Hubbard model [9]. Most recently, a third functional RG version has been used to analyze a possible spin liquid regime in the Hubbard model with a sizable next-nearest-neighbor hopping amplitude [10].

In this Letter we present and discuss results obtained from Salmhofer's [8] RG method for the two-dimensional Hubbard model with a small next-nearest-neighbor hopping amplitude on a square lattice. The expected existence of a d-wave pairing instability driven by antiferromagnetic spin fluctuations is confirmed. For a small finite next-nearest-neighbor hopping amplitude the pairing instability dominates over magnetic instabilities in the weak coupling limit for any density. More unexpectedly, we find that strong forward scattering interactions develop which may lead to a Pomeranchuk [11] instability breaking the tetragonal symmetry of the Fermi surface.

The one-band Hubbard model [1]

$$H = \sum_{\mathbf{i},\mathbf{j}} \sum_{\sigma} t_{\mathbf{i}\mathbf{j}} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{j}} n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow} \tag{1}$$

describes tight-binding electrons with a local repulsion $U > 0$. Here $c^{\dagger}_{\mathbf{i}\sigma}$ and $c_{\mathbf{i}\sigma}$ are creation and annihilation operators for fermions with spin projection $\sigma \in \{\uparrow, \downarrow\}$ on a lattice site $\mathbf{i}$, and $n_{\mathbf{j}\sigma} = c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{j}\sigma}$. A hopping amplitude $-t$ between nearest neighbors and an amplitude $-t'$ between next-nearest neighbors on a square lattice leads to the dispersion relation

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y \tag{2}$$

for single-particle states. This dispersion relation has saddle points at $\mathbf{k} = (0, \pi)$ and $(\pi, 0)$, which generate logarithmic Van Hove singularities in the noninteracting density of states at the energy $\epsilon_{\mathrm{VH}} = 4t'$. For $t' = 0$, $\epsilon_{\mathbf{k}}$

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has the nesting property $\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}}$ for $\mathbf{Q} = (\pi, \pi)$, which leads to an antiferromagnetic instability for arbitrarily small $U > 0$ at half-filling [1].

The RG equations are obtained as follows (for details, see Salmhofer [8] and Ref. [9]). The infrared singularities are regularized by introducing an infrared cutoff $\Lambda > 0$ into the bare propagator such that contributions from momenta with $|\epsilon_{\mathbf{k}} - \mu| < \Lambda$ are suppressed. All Green functions of the interacting system will then flow as a function of Λ, and the true theory is recovered in the limit $\Lambda \to 0$. Salmhofer [8] has recently pointed out that an expansion of the effective action of the theory in powers of *normal ordered* monomials of fermion fields yields differential flow equations with a particularly convenient structure. With the bare interaction as initial condition at the highest scale $\Lambda_0 = \max|\epsilon_{\mathbf{k}} - \mu|$, these flow equations determine the exact flow of the effective interactions as Λ sweeps over the entire Brillouin zone down to the Fermi surface. The effective low-energy theory can thus be computed directly from the microscopic model without introducing any *ad hoc* parameters.

For a weak coupling stability analysis it is sufficient to truncate the exact hierarchy of flow equations at the one-loop level and neglect all components of the effective interaction except the two-particle interaction Γ^{Λ}, whose flow is then determined exclusively by Γ^{Λ} itself. Flow equations for susceptibilities are obtained by considering the exact RG equations in the presence of suitable external fields, which leads to an additional one-particle term in the bare interaction, and expanding everything in powers of the external fields to sufficiently high order [9].

One cannot solve the flow equations with the full energy and momentum dependence of the vertex function, since Γ^{Λ} has three independent energy and momentum variables. The problem can, however, be much simplified by ignoring dependences which are *irrelevant* in the low-energy limit, namely, the energy dependence and the momentum dependence normal to the Fermi surface (for details, see Ref. [9]). This approximation is exact for the bare Hubbard vertex, and asymptotically exact in the low-energy regime. The remaining tangential momentum dependence is discretized for a numerical evaluation. Most of our results were obtained for a discretization with 16 points on the Fermi surface (yielding 880 "running couplings"), and we have checked that increasing the number of points does not change our results too much.

We have computed the flow of the vertex function for many different model parameters t' and U (t just fixes the absolute energy scale) and densities close to half-filling. In all cases the vertex function develops a strong momentum dependence for small Λ with divergencies for several momenta at some critical scale $\Lambda_c > 0$, which vanishes exponentially for $U \to 0$. To see which physical instability is associated with the diverging vertex function we have computed commensurate and incommensurate spin susceptibilities $\chi_S(\mathbf{q})$ with $\mathbf{q} = (\pi, \pi)$, $\mathbf{q} = (\pi - \delta, \pi)$, and $\mathbf{q} = (1 - \delta)(\pi, \pi)$, where δ is a function of density [12], the commensurate charge susceptibility $\chi_C(\pi, \pi)$, and singlet pair susceptibilities with form factors [2]

$$d(\mathbf{k}) = \begin{cases} 1 & (s\text{-wave}), \\ \frac{1}{\sqrt{2}}(\cos k_x + \cos k_y) & (\text{extended } s\text{-wave}), \\ \frac{1}{\sqrt{2}}(\cos k_x - \cos k_y) & (d\text{-wave } d_{x^2-y^2}), \\ \sin k_x \sin k_y & (d\text{-wave } d_{xy}). \end{cases} \quad (3)$$

At least one of these susceptibilities diverges together with the vertex function at the scale Λ_c. Depending on the choice of U, t', and μ, divergencies are found for the commensurate or incommensurate spin susceptibility or for the pair susceptibility with $d_{x^2-y^2}$ symmetry. In Fig. 1 we show a typical result for the flow of susceptibilities as a function of Λ. The *pairing susceptibility* with $d_{x^2-y^2}$ symmetry is obviously *dominant* here (note the logarithmic scale). Following the flow of the two-particle interactions and susceptibilities, one can see that those interaction processes which enhance the antiferromagnetic spin susceptibility (especially umklapp scattering) also generate an attractive interaction in the $d_{x^2-y^2}$ pairing channel. This confirms the spin-fluctuation route to d-wave superconductivity in the Hubbard model [2].

In Fig. 2 we show the (μ, U) phase diagram for $t' = -0.01t$ obtained by identifying the dominant instability (for $\Lambda \to \Lambda_c$) from the flow for many different values of μ and U. Note that for $U \to 0$ the pairing instability always dominates, because the BCS channel dominates the flow in the limit $\Lambda \to 0$. A spin density wave is the leading instability for $U \to 0$ only in the special case with perfect nesting, $t' = 0$ and $\mu = 0$ (cf. the phase diagram computed from the one-loop flow for $t' = 0$ in Ref. [9]).

How the critical energy scale Λ_c varies as a function of the chemical potential (i.e., as a function of density) is shown in Fig. 3 for an interaction strength $U = 1.5t$. Ob-

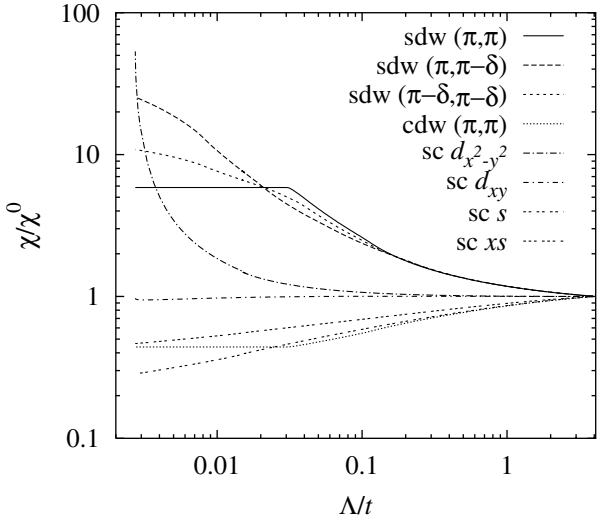

FIG. 1. The flow of the ratio of interacting and noninteracting susceptibilities for $t' = -0.01t$, $U = t$, and $\mu = -0.055t$.

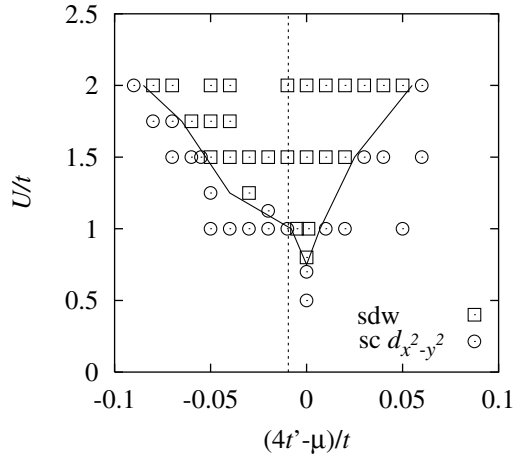

FIG. 2. The one-loop ground state phase diagram for $t' = -0.01t$ near half-filling (marked by the dashed vertical line); the symbols represent the parameter values for which the flow has been computed and whether the dominant instability is magnetic (squares) or superconducting (circles); the solid line separates the spin-density wave regime from the superconducting regime.

viously Λ_c is maximal for μ at the Van Hove energy. Note that Λ_c must not be interpreted as a transition temperature for spin density wave formation or superconductivity, but rather as an energy scale where bound particle-hole or particle-particle pairs are formed.

Since some of the forward scattering interactions grow strong for small Λ, while the Fermi velocity is very small near the saddle points, the Fermi surface may be significantly deformed by interactions, especially for $\mu \approx \epsilon_{\mathrm{VH}}$. Previous investigations of Fermi surface deformations within standard perturbation theory have yielded only very small shifts even for sizable interaction strengths [13], but in these studies the possibility of a spontaneous breaking of the point group symmetry of the square lattice has not been taken into account.

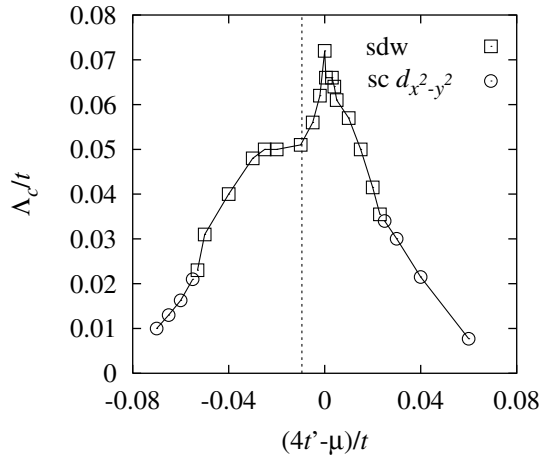

FIG. 3. The critical energy scale Λ_c as a function of the chemical potential μ for $U = 1.5t$ and $t' = -0.01t$. The different symbols indicate whether the leading instability is a spin-density wave or d-wave pairing instability.

To analyze systematically the stability of the Fermi surface shape, we define a susceptibility $\kappa_{\mathbf{k}_F\mathbf{k}'_F} = \delta s_{\mathbf{k}_F}/\delta\mu_{\mathbf{k}'_F}$, which measures the size of Fermi surface shifts $\delta s_{\mathbf{k}_F}$ for small momentum dependent shifts of the chemical potential $\delta\mu_{\mathbf{k}'_F}$ at points $\mathbf{k}'_F$ on the Fermi surface. The matrix $\kappa_{\mathbf{k}_F\mathbf{k}'_F}$ defines a linear integral operator acting on functions of $\mathbf{k}_F$. A simple consideration in the spirit of phenomenological Fermi liquid theory shows that the corresponding inverse operator is given by

$$(\kappa^{-1})_{\mathbf{k}_F\mathbf{k}'_F} = v_{\mathbf{k}_F}\delta(\mathbf{k}_F - \mathbf{k}'_F) + 2f^c_{\mathbf{k}_F\mathbf{k}'_F}, \qquad (4)$$

where $v_{\mathbf{k}_F}$ is the Fermi velocity and $f^c_{\mathbf{k}_F\mathbf{k}'_F}$ is the Landau function in the charge (spin-symmetric) channel. It is now obvious that the matrix $\kappa_{\mathbf{k}_F\mathbf{k}'_F}$ is symmetric. The Fermi surface is stable, if all eigenvalues of κ (or κ^{-1}) are positive. Landau's energy functional can be written as a quadratic form in $\delta s_{\mathbf{k}_F}$, with κ^{-1} as the kernel [14], and negative eigenvalues would imply that this energy can be lowered by a suitable deformation of the Fermi surface. In isotropic Fermi liquids such instabilities occur for strongly negative Landau parameters, as first pointed out by Pomeranchuk [11].

We have computed the renormalization group flow of the eigenvalues and eigenvectors of the operator κ^{-1} from the flow of the Landau function $f^{c\Lambda}_{\mathbf{k}_F\mathbf{k}'_F}$, which is given directly by the vertex function in the forward scattering channel [15]. For various choices of the model parameters we have always found that κ acquires a negative eigenvalue at a scale Λ^P_c above the scale Λ_c where the vertex function diverges. Usually Λ^P_c is only slightly above Λ_c, but Λ^P_c/Λ_c becomes large when the Fermi surface is close to the Van Hove points. In all cases the corresponding eigenvector signals a deformation of the Fermi surface which breaks the point group symmetry of the square lattice, as shown schematically in Fig. 4. The instability is mainly driven by a strong attractive interaction between particles (or holes) on opposite corners of the Fermi surface near the saddle points and a repulsive interaction between particles on neighboring corners.

The above diagnosis of Pomeranchuk instabilities would be rigorous for a normal Fermi liquid with finite renormalized interactions in the infrared limit. In the present system, however, the vertex function diverges at a finite scale

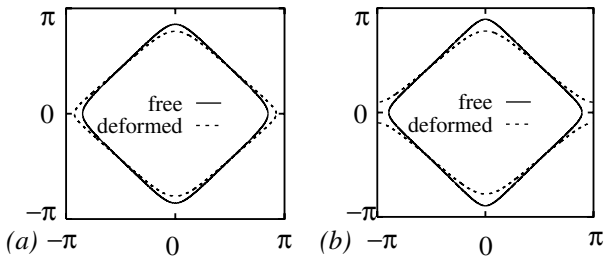

FIG. 4. Schematic plot of Fermi surface deformations breaking the square symmetry; the deformed surface may be closed (a) or open (b).

and possible Pomeranchuk-type instabilities compete with magnetic and superconducting instabilities. Note that Λ_c^P is not the energy scale at which a Pomeranchuk instability sets in, but only the scale at which the (flowing) Landau function has become big enough to destabilize the Fermi surface in a putative Fermi liquid ground state. Since we have no quantitative theory of the strong coupling physics near and below the scale Λ_c, we can discuss only two possible scenarios: (i) Energy gaps due to particle-particle or particle-hole binding may stop the flow of forward scattering interactions before a Pomeranchuk instability sets in. (ii) The Pomeranchuk instability is not blocked by binding phenomena. In that case one would have a finite temperature phase transition with a spontaneous breaking of the (discrete) tetragonal symmetry of the square lattice and subsequent continuous symmetry breaking associated with magnetic order or superconductivity in the ground state.

The Pomeranchuk instability occurs more easily if the Fermi surface is close to the saddle points of $\epsilon_{\mathbf{k}}$. On the other hand, nesting raises the scale for particle-hole binding (leading ultimately to magnetic order). The best candidate is therefore the Hubbard model with a sizable t' (reducing nesting) and $\mu = \epsilon_{\mathrm{VH}}$.

We emphasize that the Pomeranchuk instability does not cut off the singularity in the Cooper channel since it does not break the reflection invariance. Hence, at sufficiently large doping away from half-filling, d-wave superconductivity will set in in any case, with an order parameter that may be slightly distorted away from perfect d-wave symmetry. The Pomeranchuk instability would also not destroy the umklapp scattering route to an insulating spin liquid discussed recently by Furukawa *et al.* [10].

To our knowledge a Pomeranchuk instability has not yet been observed in numerical solutions of the two-dimensional Hubbard model. Of course this may be due to finite size limitations or too high temperatures in Monte Carlo simulations. It would thus be interesting to compute the Fermi surface susceptibility $\kappa_{\mathbf{k}_F\mathbf{k}'_F}$ by Monte Carlo methods. In real systems a Pomeranchuk instability as in Fig. 4 may lead to an orthorhombic lattice distortion, as a consequence of the coupling of electronic and lattice degrees of freedom.

In conclusion, modern renormalization group methods establish the expected d-wave pairing instability in the two-dimensional Hubbard beyond doubt. Note that for small bare interactions and in a parameter regime where only particle-particle pairing fluctuations grow strong, the strong coupling problem associated with the formation of a superconducting state can be treated rigorously [16]. In addition to magnetic or superconducting instabilities, a Pomeranchuk instability breaking the tetragonal symmetry of the Fermi surface is likely to occur for a Fermi surface near the saddle points in the absence of perfect nesting. A quantitative analysis of this instability requires the inclusion of spontaneous symmetry breaking and self-energy terms into the RG scheme (work in progress). Self-energy contributions are usually small and regular at weak coupling, but they become important near the Van Hove points [17]. Although our one-loop RG is *a priori* controlled only at weak coupling, the experience with many other systems shows that qualitative features of a theory emerging in a loop expansion usually survive for quite strong interactions.

When this work was completed we were informed that a Pomeranchuk instability leading to an open Fermi surface as in Fig. 4b has also been found within a mean-field theory for the t-J model, and it has been pointed out that an alternate stacking of such Fermi surfaces in the cuprate planes may explain angle-resolved photoemission data in $La_{2-x}Sr_xCuO_4$ [18].

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