Pomeranchuk and other instabilities in the t-t' Hubbard model at the Van Hove filling

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We present a stability analysis of the two-dimensional t-t' Hubbard model for various values of the next-nearest-neighbor hopping t', and electron concentrations close to the Van Hove filling by means of the flow equation method. For $t' \geqslant -t/3$ a $d_{x^2-y^2}$-wave Pomeranchuk instability dominates (apart from antiferromagnetism at small t'). At $t' < -t/3$, the leading instabilities are a g-wave Pomeranchuk instability and p-wave particle-hole instability in the triplet channel at temperatures $T < 0.15t$, and an s^*-magnetic phase for $T > 0.15t$; upon increasing the electron concentration, the triplet analog of the flux phase occurs at low temperatures. Other weaker instabilities are also found.

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In recent years, the two-dimensional (2D) Hubbard model has been used[1,2] as the simplest model that maps the electron correlations in the copper oxide planes of high-temperature superconductors since experimental data suggest that superconductivity in cuprates basically originates from the CuO_2 layers.[3] Although electron-electron interactions are strong in the high-temperature cuprate superconductors some important features of these systems (in particular, antiferromagnetic and d-wave superconducting instabilities) are captured already by the 2D Hubbard model at weak to moderate Coulomb coupling.

Apart from the antiferromagnetism and $d_{x^2-y^2}$-wave superconductivity mentioned above [for review, see Refs. 1,2,4, and references therein], a few other instabilities related to symmetry-broken states[5–11] in the 2D t-t' Hubbard model with next-nearest-neighbor hopping t' have been reported recently. Specially, much interest of researchers has been attracted by the case when the Fermi surface passes through the saddle points of the single-particle dispersion (Van Hove filling). One of the instabilities found in such a case is a d-wave Pomeranchuk instability breaking the tetragonal symmetry of the Fermi surface, i.e., a spontaneous deformation of the Fermi surface reducing its symmetry to orthorhombic. It has been recently observed for small values of t' from renormalization-group calculations by Halboth and Metzner.[5] They argued that the Pomeranchuk instability occurs more easily if the Fermi surface is close to the saddle points with a sizable t' (reducing nesting that leads to antiferromagnetism). However, within their technique it is difficult to compare the strength of the Fermi-surface deformation with other instabilities and to conclude which one dominates. The authors of Ref. 10 have investigated the interplay of d-density wave[12,13] and Fermi-surface deformation tendencies with those towards d-wave pairing and antiferromagnetism by means of a similar temperature-flow renormalization-group approach. They have found that the d-wave Pomeranchuk instability never dominates in the 2D t-t' Hubbard model (even under the conditions mentioned above).

On the other hand, Vollhardt *et al.*[14] showed that the t'-hopping term destroys the antiferromagnetic nesting instability at weak interactions in two and three dimensions, and supports the stabilization of metallic ferromagnetism in infinite dimensions away from half filling. Therefore, one could expect also the stabilization of ferromagnetism by a sizable t' in two dimensions. Indeed, in the t-t' Hubbard model on a 2D square lattice at weak to moderate Coulomb coupling, a projection quantum Monte Carlo calculation with 20×20 sites and the T-matrix technique,[6] a generalized random-phase approximation including particle-particle scattering[7] point towards a ferromagnetic ground state for large negative values of t'/t in a density range around the Van Hove filling. Similar tendencies have been found by the authors of Ref. 8 within the renormalization group and parquet approaches. Honerkamp and Salmhofer recently studied[9] the stability of this ferromagnetic region at finite temperatures by means of the temperature-flow renormalization-group technique. They have found that ferromagnetic instability is the leading one at $t' < -0.33t$ and Van Hove filling with critical temperatures depending on the value of t'. When the electron concentration is increased slightly above the Van Hove filling, the ferromagnetic tendencies get cut off at low temperatures, and a triplet p-wave superconducting phase dominates. However, they did not consider the Pomeranchuk instability (which could have the most favorable conditions to occur) and other ones apart from antiferromagnetism, d- and p-wave superconductivity, and ferromagnetism.

Therefore, the investigation of interplay and rivalry between the Pomeranchuk instability and ferromagnetism, and other phases in the 2D $t-t'$ Hubbard model at the Van Hove filling, is a considerable task. We will consider the leading instabilities depending on the ratio U/t (in all papers cited above it was fixed). The main goal of this paper is such a study. We also report on a few instabilities in a range of electron concentration around the Van Hove filling.

We start from the Hamiltonian of the t-t' Hubbard model,

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\substack{\mathbf{k}_1\mathbf{k}'_1 \\ \mathbf{k}_2\mathbf{k}'_2}} c^{\dagger}_{\mathbf{k}_1\uparrow} c_{\mathbf{k}'_1\uparrow} c^{\dagger}_{\mathbf{k}_2\downarrow} c_{\mathbf{k}'_2\downarrow} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}'_1+\mathbf{k}'_2}, \tag{1}$$

where $\varepsilon_{\mathbf{k}}$ is the Bloch electron energy with the momentum $\mathbf{k}$, $c^{\dagger}_{\mathbf{k}\sigma}(c_{\mathbf{k}\sigma})$ is the creation (annihilation) operator for the elec-

trons with spin projection $\sigma \in \{\uparrow,\downarrow\}$, U is the local Coulomb repulsion of two electrons of opposite spins, N is the number of lattice points, and the lattice spacing equals unity.

By means of the flow equation method,[15] the Hamiltonian is transformed into one of molecular-field type. This Hamiltonian is calculated in second order in the coupling U.[11] Adopting the notations of Ref. 11, the expression for the free energy has the form

$$\beta F = \frac{1}{N}\sum_{\mathbf{kq}} \beta U\left(1+\frac{U}{t}V_{\mathbf{k},\mathbf{q}}\right)\Delta_{\mathbf{k}}^{*}\Delta_{\mathbf{q}} + \sum_{\mathbf{k}} f_{\mathbf{k}}\Delta_{\mathbf{k}}^{*}\Delta_{\mathbf{k}}, \quad (2)$$

where the first term is the energy contribution and the second term is the entropy contribution, $\beta = 1/(k_B T)$, T is the temperature, t is the hopping integral of electrons between nearest neighbors of the lattice, $V_{\mathbf{k},\mathbf{q}}$ is effective second-order interaction, $f_{\mathbf{k}}$ is an entropy coefficient, and $\Delta_{\mathbf{k}}$ are the order parameters. For example, $\Delta_{\mathbf{k}\sigma,-\mathbf{k}\sigma'} = \langle c_{\mathbf{k}\sigma} c_{-\mathbf{k}\sigma'}\rangle = (\sigma_y)_{\sigma\sigma'}\Delta_{\mathbf{k}}^{s} + \Sigma_\alpha (\sigma_y\sigma_\alpha)_{\sigma\sigma'}\Delta_{\mathbf{k}}^{t\alpha}$, where σ_α is a Pauli spin matrix ($\alpha = x,y,z$) and $\Delta_{\mathbf{k}}^{s}(\Delta_{\mathbf{k}}^{t\alpha})$ is the singlet (triplet) amplitude. An expression similar to Eq. (2) is obtained for particle-hole channels with the order parameters ν instead of Δ. In this case, for example, we have $\nu_{\mathbf{k}\sigma,\mathbf{k}\sigma'} = \langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{Q}\sigma'}\rangle = \nu_{\mathbf{k}}^{s}\delta_{\sigma,\sigma'} + \Sigma_\alpha \nu_{\mathbf{k}}^{t\alpha}(\sigma_\alpha)_{\sigma\sigma'}$, with $\mathbf{Q} = (\pi,\pi)$. All quantities of Eq. (2) are defined in Ref. 11. For a square lattice, the single-particle dispersion has the form

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y . \quad (3)$$

The spectrum (3) contains Van Hove singularities in the density of states at the energy $\varepsilon_{VH} = 4t'$ related to the saddle points of the Fermi surface at $\mathbf{k} = (0,\pm\pi)$ and $(\pm\pi,0)$. For $t' = 0$ and half filling, the Fermi surface is nested, $\varepsilon_{\mathbf{k}+\mathbf{Q}} = -\varepsilon_{\mathbf{k}}$, which leads to an antiferromagnetic instability for $U > 0$. The nesting is removed for $t'/t \neq 0$.

We start from the symmetric state and investigate whether this state is stable against fluctuations of the order parameters Δ and ν. As soon as a nonzero Δ or ν yields a lower free energy in comparison with the symmetric state with all vanishing Δ and ν, the symmetric state becomes unstable and the system will approach a symmetry broken state. This indicates a phase transition. We perform numerical calculation on a square lattice with 24×24 points in the Brillouin zone for the various representations under the point group C_{4v}. The representations of the even-parity states are one dimensional. We denote them by $s_+ = s_1, s_- = s_{xy(x^2-y^2)}, d_+ = d_{x^2-y^2}, d_- = d_{xy}$. The odd-parity representation is two dimensional, and is denoted by p. Initially, such numerical calculations have been performed in Refs. 11 and 16, but they were sensitive to the lattice size at low temperatures. Here we use an improved scheme (for details, see Ref. 17). Within this scheme we take the average value of entropy coefficients instead of the value calculated at a point in the Brillouin zone. A similar procedure is applied to the chemical-potential calculation. One should also perform the averaging in determination of effective interactions, but it would take much more time. We have checked the size effects, performing some calculations also for 16×16 and 32×32 lattices, and found that the differences are very small and unessential.

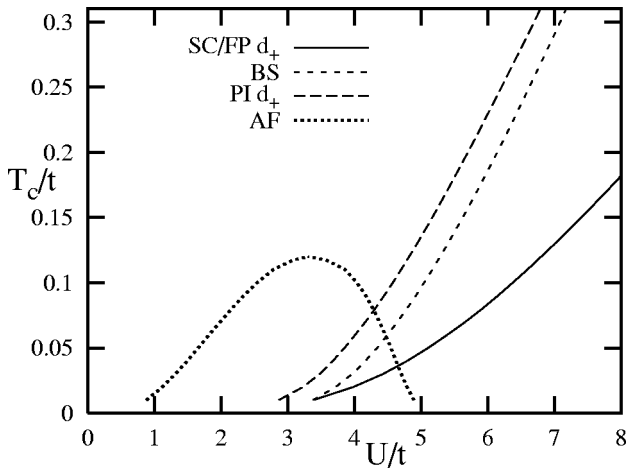

FIG. 1. Temperature phase diagram of the 2D t-t' Hubbard model for $n = 1$ and $t' = 0$. Chemical potential $\mu = 0$. SC stands for superconductivity, FP for flux phase, BS for band splitting, PI for Pomeranchuk instability, and AF for antiferromagnetism.

Although size effects increase at low-temperatures in the low-density region, they do not touch and change the leading instabilities essentially.

We start from $t' = 0$ and half filling ($n = 1$) (see Fig. 1). As expected in this case, the leading instability is the antiferromagnetic one that disappears at the temperature $T \approx 0.1t$ or doping $\delta \equiv n - 1 = 0.06$. As the second-order contribution suppresses antiferromagnetism, it decays rapidly at larger values of U/t. Remarkably, since we work with a weak-coupling calculation, we obtain at intermediate couplings the same tendency as it is expected at strong interactions, although we do not reproduce the Neél temperature behavior $T_c \sim t^2/U$. We take the decrease of the Neél temperature as an indication that the calculation in second order in U yields reasonable results even for intermediate values $U \sim 4t$. For stronger couplings, higher-order contributions will become important. However, it is of interest to see which instabilities emerge within our approximation for larger values of U/t, since this gives a hint of the types of ordering to be investigated for stronger couplings. Therefore, we discuss the phase diagram obtained from the second-order calculation also for larger values U/t.

The next instability is a Pomeranchuk instability with $d_{x^2-y^2}$-wave symmetry in the singlet channel. The corresponding eigenvectors signal a deformation of the Fermi surface, which breaks the point-group symmetry of the square lattice. For negative $t' \geqslant -t/3$, the Pomeranchuk instability dominates at the Van Hove filling (see Fig. 2). The $d_{x^2-y^2}$-wave Pomeranchuk instability competes with other instabilities at $t' < -t/3$, and it is not the leading one (Fig. 3). In agreement with the ideas of Ref. 5 the instability is mainly driven by a strong attractive interaction between particles on opposite corners of the Fermi surface near the saddle points and a repulsive interaction between particles on neighboring corners. To favor such a behavior we need a sizable t' reducing antiferromagnetic correlations. At half filling and $t' = 0$, the next instability is a particle-hole instability of singlet type with staggered p-wave symmetry. It

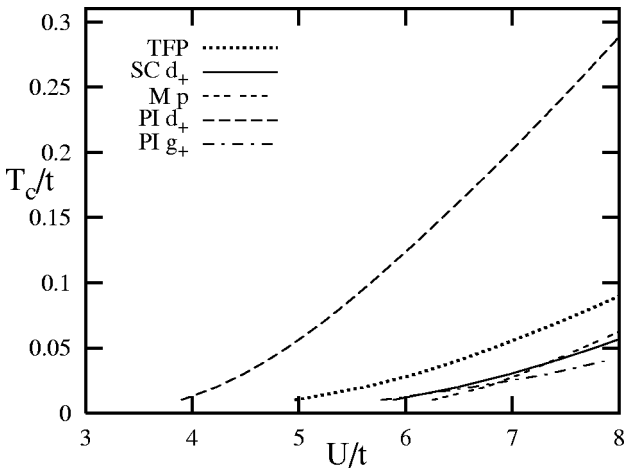

FIG. 2. Temperature phase diagram of the 2D t-t' Hubbard model for $t'=-t/3$ and $n=0.68$ (the Van Hove filling). Chemical potential varies in the range of $\mu/t=-(1.317-1.339)$. TFP stands for triplet flux phase, M for magnetic particle-hole instability in triplet channel, and other notations are the same as in Fig. 1.

yields[11] a splitting into two bands and may lead to an energy gap in the charge excitation spectrum. Another mechanism for a charge gap formation has been proposed[18,19] recently in the 2D Hubbard model with $t'=0$ at weak coupling. The band splitting phase is developed in the region of electron concentration around half filling, and is one of the strongest in that region. Then the superconducting $d_{x^2-y^2}$ instability follows, which coincides with the $d_{x^2-y^2}$-wave staggered flux phase (the flux phase has been proposed by the authors of Refs. 20 and 21 and discussed recently in Refs. 12,13, and 22). Away from half filling, the degeneration disappears, and d-wave superconductivity dominates at low temperatures in certain regions of electron concentration around half filling, which depends on the value of $t'\neq 0$. Even large values of $|t'|$ do not destroy the dominant low-temperature behavior of $d_{x^2-y^2}$-wave superconductivity at doping.[17] One phase may

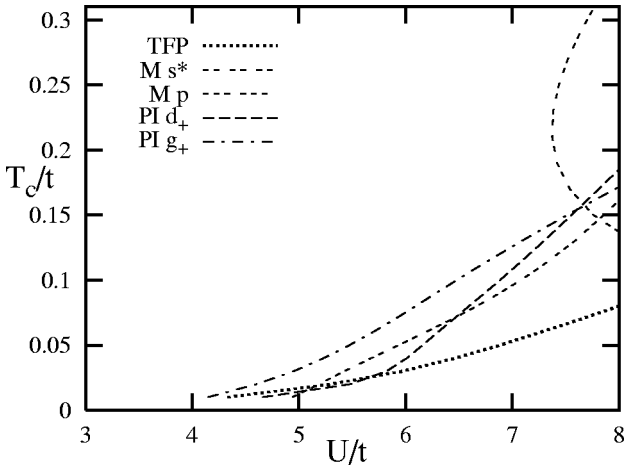

FIG. 3. Temperature phase diagram of the 2D t-t' Hubbard model for $t'=-5t/12$ and $n=0.55$ (the Van Hove filling). Chemical potential varies $\mu/t=-(1.666-1.632)$. Notations are the same as in Fig. 2.

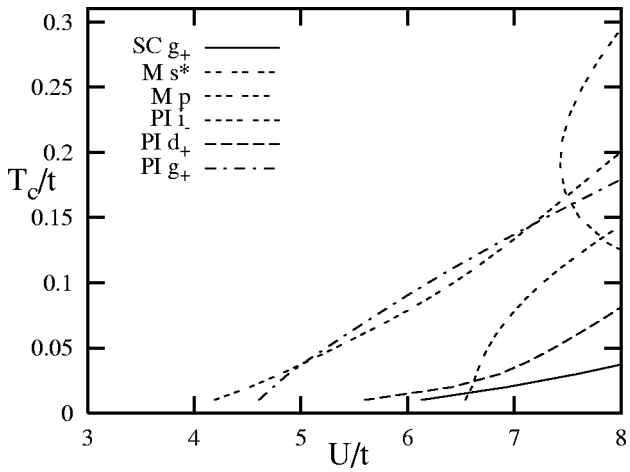

FIG. 4. Temperature phase diagram of the 2D t-t' Hubbard model for $t'=-5t/12$ and $n=0.50$ (slightly below the Van Hove filling). Chemical potential varies in the range of $\mu/t=-(1.709-1.713)$. Notations are the same as in Fig. 2.

suppress another phase. To which extent the two order parameters can coexist with each other is a question, which has to be investigated in the future.

For $t'=0$, the singlet and triplet T_c of the particle-hole instabilities with staggered symmetry of d_+ wave character (that is the flux phase) are degenerate. If $t'\neq 0$, they are different, and the triplet one is higher. Moreover, the triplet analog of flux phase dominates at low temperatures, and $t'=-5t/12$ when the electron concentration is slightly above the Van Hove filling, in contrast to the results of Ref. 9 which point out the occurrence of triplet superconductivity with p-wave symmetry in this region. The triplet flux phase is also one of the leading instabilities for $t'\geqslant -t/3$ and certain region of electron concentrations (see Fig. 2). It has been considered by Nayak[12] as a density wave order parameter potentially relevant to the cuprates, but to our knowledge a triplet version of the flux phase has not yet been observed in numerical solutions of the 2D t-t' Hubbard model. We shall discuss this state in more details elsewhere.[17]

At $t'=-5t/12$, a few other instabilities appear to compete at the Van Hove filling and low temperatures (Fig. 3), in disagreement with the conclusions of Ref. 9 on the occurrence of ferromagnetism. The leading one is a Pomeranchuk instability in the s_+ channel with $g_+=g_{x^4+y^4-6x^2y^2}$ wave character (four node lines in **k** space). This phase occurs more easily if the electron concentration is close to or slightly smaller than the Van Hove filling (Figs. 3 and 4). It also requires sufficiently large absolute values of t'. When the electron concentration is decreased below the Van Hove density, a particle-hole instability of p-wave symmetry in triplet channel dominates at low temperatures (see Fig. 4), which gives rise to a phase of magnetic currents. In the d_- channel, an i-wave (six node lines in **k** space) Pomeranchuk instability appears when electron concentration n is smaller than the Van Hove filling (Fig. 4). It is a leading one at small values of the electron concentration.[17] We observe (Fig. 4) in the s_+ channel a g_+ wave superconductivity below the Van Hove filling, but it requires strong coupling.

At $t'=-5t/12$ and $T>0.15t$ close to the Van Hove filling, one observes for the couplings $U\geqslant 7t$ a particle-hole instability with s^*-wave character (its order parameter changes sign close to the Fermi edge) in the triplet channel (Figs. 3 and 4). It is likely that the order parameter contributions do not compensate exactly, so that a weak ferromagnetism appears. This s^*-magnetic phase shows a reentrant behavior. Since at lower temperatures only a smaller region in **k** space around the Fermi edge contributes, the sign change of the order parameter reduces the effective interaction, which leads to the disappearance of this phase.

In conclusion, we have presented a stability analysis of the 2D t–t' Hubbard model on a square lattice by means of the flow equations approach in second order in U for various values of the next-nearest-neighbor hopping t' and electron concentrations close to the Van Hove filling. A surprising large number of phases has been observed. Some of them have an order parameter with many nodes in the **k** space. For $t'\geqslant -t/3$, the $d_{x^2-y^2}$-wave Pomeranchuk instability dominates. At $t'<-t/3$, the leading instabilities are a g_+ wave Pomeranchuk instability and p-wave particle-hole instability in triplet channel at temperatures $T<0.15t$, and s^*-magnetic phase for $T>0.15t$; upon increasing the electron concentration, the triplet flux phase occurs at low temperatures. We have found other weaker instabilities also. Most instabilities develop at $U>4t$, which are not small values. Therefore, flow equation calculations beyond second order would be desirable. Nevertheless, as we have found most commonly discussed types of order, and since some effects obtained in the intermediate to strong couplings are reproduced reasonably well by means of the flow equations, we suggest that our calculations give an estimate of the most important instabilities.

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