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Fermi-surface instabilities of a generalized two-dimensional Hubbard model

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Possible Fermi-surface-related instabilities in a Hubbard model, generalized so as to include finite-range and exchange interactions, are studied in the weak-coupling limit. In addition to the usual instabilities of superconducting, charge- or spin-density-wave type, two new types of instability are found. The first state is an orbital antiferromagnet, with currents circulating around each elementary plaquette. In the second phase, a *spin* current flows around the plaquettes. In both cases, there are low-temperature power laws in thermodynamic and transport properties. Two-dimensional fluctuation effects are shown to lead, for weak interactions, to a sharp crossover from a Fermi-liquid state to a regime governed by orientational fluctuations of the order parameter at fixed amplitude.

The high-temperature superconducting oxides[1,2] like $La_{2-x}Sr_xCuO_4$ or $YBa_2Cu_3O_{6+x}$ exhibit a number of interesting physical phenomena. According to a simple electron count (or more sophisticated band-structure calculations[3,4]) at $x=0$ these compounds should be metals, whereas experimentally they are found to be antiferromagnetic insulators.[5-7] By analogy with transition-metal oxides like NiO (Ref. 8) this behavior can be explained assuming electron correlations sufficiently strong to localize the electrons (a Mott-Hubbard insulator).[9] Moreover, rather small changes in x lead to a high-temperature superconducting state, and it is therefore tempting to explain the properties of both the insulating and superconducting states in the framework of the same model. Finally, both the crystallographic[10,11] and electronic[3,4] structure strongly suggest that the properties of these compounds are dominated by CuO_2 layers. Consequently, the two-dimensional Hubbard model can be assumed to constitute a reasonable starting point for the understanding of these compounds.[9]

Even though in the real compounds electron correlation energies are probably at least comparable to the bandwidth, in the present paper I will study the different possible phases occurring for rather weak interactions in the two-dimensional Hubbard model, generalized so as to include finite-range and exchange interactions. It is hoped that this investigation will help to shed some light on possible phases occurring for intermediate and strong coupling (in one dimension phases occurring for weak and strong electron-electron interactions are identical).[12] These questions seem to be of special importance considering the rather unusual properties of the resonating-valence-bond (RVB) state proposed by Anderson,[9,13] as well as some other possibilities.[14-16] As will be seen below, some states with rather unusual properties can occur the existence of which seem (to my knowledge) not to have been realized before.

I consider the generalized Hubbard model, described by the Hamiltonian

$$H=-t\sum_{\langle i,j\rangle s}(a_{is}^{\dagger}a_{js}+a_{js}^{\dagger}a_{is})+U\sum_i n_{i\uparrow}n_{i\downarrow}+H'. \tag{1}$$

Here $a_{is}^{\dagger}$ creates an electron at site i with spin projection s, $n_{is}=a_{is}^{\dagger}a_{is}$, $n_i=n_{i\uparrow}+n_{i\downarrow}$, and $\langle i,j\rangle$ indicates summation over nearest-neighbor pairs in a square lattice, each pair being counted once. H' contained finite-range direct and exchange interactions to be specified below.

The single-particle eigenstates of (1) have energy $\varepsilon(\mathbf{k})=-2t(\cos k_x+\cos k_y)$. I will consider here the case of a half-filled band. Then the Fermi surface is a perfect square: $|k_{F,y}|=\pi-|k_{F,x}|$, and the Fermi surface is perfectly nested, with nesting wave vector $(\pm\pi,\pi)$. The single-particle density of states per site and spin orientation is

$$N(\varepsilon)=\frac{1}{2\pi^2 t}K\{[1-(\varepsilon/4t)^2]^{1/2}\}\approx\frac{1}{2\pi^2 t}\ln(16t/|\varepsilon|), \tag{2}$$

where $K(k)$ is the complete elliptic integral of the first kind, and the approximate formula in (2) is valid for small ε. The logarithmic divergence in (2) is due to saddle points in $\varepsilon(\mathbf{k})$ at $\mathbf{k}_{1,2}=(\pm\pi,0)$, $(0,\pm\pi)$. As here I am interested in instabilities of the model for weak interactions, it will be mainly the states close to the *two* saddle points which will be involved. It is then convenient to introduce a continuum representation of the fermion operators by

$$a_{is}=(-1)^{x_i}\psi_{1s}(\mathbf{r})+(-1)^{y_i}\psi_{2s}(\mathbf{r}), \tag{3}$$

where $\psi_{1,2}$ are slowly varying functions, describing electrons close to $\mathbf{k}_{1,2}$. In terms of these operators the Hamiltonian can be rewritten as

$$\begin{aligned}H=&\,t\int d^2r\sum_s[\psi_{1s}^{\dagger}(\partial_x^2-\partial_y^2)\psi_{1s}+\psi_{2s}^{\dagger}(\partial_y^2-\partial_x^2)\psi_{2s}]\\&+4\pi t\int d^2r\Big[\sum_{s,t}(G_1\psi_{1s}^{\dagger}\psi_{2t}^{\dagger}\psi_{1t}\psi_{2s}+G_4\psi_{1s}^{\dagger}\psi_{2t}^{\dagger}\psi_{2t}\psi_{1s})\\&+G_2(\psi_{1\uparrow}^{\dagger}\psi_{1\downarrow}^{\dagger}\psi_{1\downarrow}\psi_{1\uparrow}+\psi_{2\uparrow}^{\dagger}\psi_{2\downarrow}^{\dagger}\psi_{2\downarrow}\psi_{2\uparrow})+G_3(\psi_{1\uparrow}^{\dagger}\psi_{1\downarrow}^{\dagger}\psi_{2\downarrow}\psi_{2\uparrow}+\psi_{2\uparrow}^{\dagger}\psi_{2\downarrow}^{\dagger}\psi_{1\downarrow}\psi_{1\uparrow})\Big].\end{aligned} \tag{4}$$

One easily sees that this form of the Hamiltonian conserves the nesting property of the lattice version (1). Choosing a circular cutoff in momentum space around $\mathbf{k}_{1,2}$, so that the total number of states is the same as in (1), the single-particle density of states is $N(\epsilon) = (\frac{1}{2}\pi^2 t)\ln(\pi^2 t/|\epsilon|)$, i.e., the logarithmic singularity in (2) is also reproduced, and consequently I expect the weak-coupling physics of the lattice model to be correctly reproduced by (4). However, mainly due to different numerical factors in the lattice and continuum forms for the density of states, the precise numerical factors in formulas like (12) or (19) are slightly different.

Using (3) the coupling constants in (4) can be related to those in the lattice Hamiltonian (1). For H' I chose the most general form involving nearest-neighbor terms only:[17]

$$H' = \tfrac{1}{2}\sum_{i,\delta,s,t}(Vn_{is}n_{i+\delta,t} + Wa_{is}^{\dagger}a_{it}^{\dagger}a_{i+\delta,t}a_{i+\delta,s} + Ja_{is}^{\dagger}a_{i+\delta,t}^{\dagger}a_{it}a_{i+\delta,s}) . \tag{5}$$

Here δ is summed over the four nearest neighbors of site i. The continuum coupling constants then are

$$4\pi t G_1 = U-4V-4W+4J,\quad 4\pi t G_2 = U+4V+4W+4J,$$
$$4\pi t G_3 = U-4V+4W-4J,\quad 4\pi t G_4 = U+4V-4W-4J. \tag{6}$$

Of course, other lattice parametrizations of the constants in (4) are also possible.

Due to the perfectly nested Fermi surface, in addition to the usual pairing instability, a number of electron-hole-type Fermi-surface instabilities can occur in the model,[18,19] depending on the values of the coupling constants. The operators taking nonzero expectation values in the ordered phases are, for a charge-density wave (CDW) or a spin-density wave, polarized along direction α (SDW_α, $\alpha = x,y,z$)

$$O_{\mathrm{CDW}} = \psi_{1s}^{+}\psi_{2s} + \psi_{2s}^{+}\psi_{1s},$$
$$O_{\mathrm{SDW}_\alpha} = \psi_{1s}^{+}\sigma_\alpha^{st}\psi_{2t} + \psi_{2s}^{+}\sigma_\alpha^{st}\psi_{1t}, \tag{7}$$

where the σ_α are the Pauli matrices and summation over repeated spin indices is implied; and for s-wave or d-wave superconductivity (SC) (i.e., same or opposite sign of the gap parameter in the two corners of the Fermi surface)

$$O_{\mathrm{SC}_s} = \psi_{1\uparrow}\psi_{1\downarrow} + \psi_{2\uparrow}\psi_{2\downarrow},\quad O_{\mathrm{SC}_d} = \psi_{1\uparrow}\psi_{1\downarrow} - \psi_{2\uparrow}\psi_{2\downarrow}. \tag{8}$$

That there are actually more possible Fermi-surface instabilities in the model can be seen applying the electron-hole transformation $a_{i\downarrow} \rightarrow (-1)^i a_{i\downarrow}^{\dagger}$ to the different operators above. The continuum version of this transformation is

$$\psi_{1\downarrow} \rightarrow \psi_{2\downarrow}^{+},\quad \psi_{2\downarrow} \rightarrow \psi_{1\downarrow}^{+}. \tag{9}$$

Under the transformation, O_{CDW}, O_{SDW_α}, and O_{SC_s} transform amongst themselves; however O_{SC_d} transforms into the x and y component of the operator

$$O_{\mathrm{JS}_\alpha} = \psi_{1s}^{+}\sigma_\alpha^{st}\psi_{2t} - \psi_{2s}^{+}\sigma_\alpha^{st}\psi_{1t}, \tag{10}$$

whereas O_{JS_z} transforms into

$$O_{\mathrm{JC}} = \psi_{1s}^{+}\psi_{2s} - \psi_{2s}^{+}\psi_{1s}. \tag{11}$$

It should now be apparent that there are *two groups* of instabilities, each of them transforming amongst itself under (9); (CDW, SC_s, SDW_α) and (JC, SC_d, JS_α). The successive members of each group represents states with a broken Z(2), O(2), and O(3) symmetry, respectively.

In the Hartree-Fock approximation the different phases become stable below a critical temperature given by

$$T_{c\lambda} = 2\pi e^{\gamma} t \exp(-2\sqrt{\pi/G_\lambda}), \tag{12}$$

where $e^{\gamma} = 1.781\ldots$ and λ designates the different phases: CDW, SDW, etc. The corresponding coupling constants are

$$G_{\mathrm{CDW}} = -2(2G_1 + G_3 - G_4),$$
$$G_{\mathrm{SC}_s} = -2(G_2 + G_3), \tag{13}$$
$$G_{\mathrm{SDW}} = 2(G_3 + G_4),$$

and the constants for the second group are obtained from their counterparts in the first group by the replacement $G_3 \rightarrow -G_3$. For given coupling constants the phase with the highest T_c will be realized.

What is the nature of the new JC and JS_α phases? To answer this question rewrite O_{JC} in terms of the original lattice operators:

$$O_{\mathrm{JC}} \approx \frac{1}{N}\sum_{i,s}(-1)^i(a_{is}^{\dagger}a_{i+\hat{\mathbf{x}},s} - a_{i+\hat{\mathbf{x}},s}^{\dagger}a_{is} - a_{is}^{\dagger}a_{i+\hat{\mathbf{y}},s} + a_{i+\hat{\mathbf{y}},s}^{\dagger}a_{is}), \tag{14}$$

where $\hat{\mathbf{x}}$ is the unit lattice vector along x. Now, the operator $a_{is}^{\dagger}a_{i+\hat{\mathbf{x}},s} - a_{i+\hat{\mathbf{x}},s}^{\dagger}a_{is}$ is the *charge current* through the bond $i \rightarrow i+\hat{\mathbf{x}}$, and consequently a finite expectation value of O_{JC} represents a state with a nonzero current flowing around each plaquette of the square lattice, alternatively clockwise and anticlockwise. The current leads to a magnetic moment perpendicular to the plane, i.e., the JC phase represents an *orbital antiferromagnet,* which is, in principle, observable in a neutron-scattering experiment.

As O_{JC} is related to O_{SC_d} by symmetry transformations [Eq. (9) and spin rotation], the structure of the gap parameter on the Fermi surface is the same in both cases: $\Delta(\mathbf{k}) = \Delta_0(\cos k_x - \cos k_y)$, and therefore the quasiparticle density of states has a V-shaped zero at the Fermi level,[20] $N(\varepsilon) \approx |\varepsilon|$. Consequently, there will be a rather abrupt decrease of conductivity below $T_{c,\mathrm{JC}}$, but at low temperature the carrier density and therefore the conductivity behave as T^2, instead of the exponential decrease in the CDW and SDW states. Similarly the spin susceptibility behaves as $\chi_{\mathrm{spin}} \propto T$.

The lattice version of O_{JS_α} is obtained from (14) by inserting the appropriate Pauli matrix [see (10)]. Therefore, a state with a nonzero JS_α order parameter has a *spin current* around each elementary plaquette. For example, for $\alpha = z$ $\uparrow$ and $\downarrow$ electrons circulate in opposite directions. Such a current obviously does not induce any magnetic moment, and consequently a JS phase will be

completely featureless in a scattering experiment (notice that neither O_{JC} nor its spin equivalent couple directly to the lattice, so there will be no lattice deformation associated with any of these phases). On the other hand, the quasiparticle density of states is the same in the JC state, and consequently the temperature dependence of the conductivity and of the spin susceptibility for a field parallel to the direction α have the behavior discussed in the preceding paragraph. Finally, applying a magnetic field perpendicular to α does not destroy the nesting properties of the Fermi surface, and consequently there is a finite spin susceptibility for $\mathbf{H}\perp\alpha$.

The CDW instability considered here implies a modulation of the charge density on the lattice *sites*. One might also consider a modulation of the bond lengths ["bond-order wave" (BOW)], with order parameter

$$O_{\mathrm{BOW}}=\frac{1}{N}\sum_{is}(-1)^i[a_{is}^\dagger a_{i+\hat{\mathbf{x}},s}+a_{i+\hat{\mathbf{x}},s}^\dagger a_{is} \pm (a_{is}^\dagger a_{i+\hat{\mathbf{y}},s}+a_{i+\hat{\mathbf{y}},s}^\dagger a_{is})]\,. \tag{15}$$

Going over to k space, one finds however that the corresponding gap function has zero amplitude in the corners of the Fermi surface, and therefore the square root in (12) is replaced by the coupling constant itself. Consequently, at least for weak coupling, a BOW phase does not occur, as has been noticed previously.[21] Similarly, triplet superconductivity does not occur either: such a state would imply opposite signs of $\Delta(\mathbf{k})$ at $(\pm\pi,0)$, whereas these two points are connected by a reciprocal lattice vector, requiring $\Delta(\pi,0)=\Delta(-\pi,0)$. Again one has zero amplitude in the corners of the Fermi surface.

The mean-field approach used here has to be taken with some caution. First, there are competing electron-hole and electron-electron instabilities in the model, so that a RPA-like calculation of critical temperatures is not valid. A more involved treatment of the coupled-singularity problem seems however to indicate that for half-filling differences are minor.[18,19] A second problem arises from thermal fluctuations which in two dimensions do not allow an ordered state with a broken continuous symmetry,[22] i.e, of the SC_s, SC_d, SDW, or JS type in the present case. To assess more qualitatively the meaning of the critical temperature calculated here, I use a Ginzburg-Landau functional

$$F[\{\Delta(\mathbf{r})\}]=\int d^2r\{a|\Delta|^2+b|\Delta|^4+c|\nabla\Delta|^2\}\,, \tag{16}$$

where $\Delta(\mathbf{r})=\Delta(\mathbf{r})\mathbf{n}(\mathbf{r})$ is an n-component vector order parameter, $\mathbf{n}(\mathbf{r})$ is a unit vector, $a(T)=a'(T-T_c^{\mathrm{MF}})$, and T_c^{MF} is the mean-field transition temperature given in Eq. (12). Writing $\Delta(\mathbf{r})=\Delta_0(T)+\delta(\mathbf{r})$, where $\Delta_0^2=-a/2b$ minimizes F, one straightforwardly calculates the fluctuations of the amplitude of the order parameter around Δ_0:

$$\langle\delta^2\rangle=\frac{T}{4\pi c}\ln(1+\xi^2\Lambda^2)\,, \tag{17}$$

where $\xi^2=c/|a|$ and Λ is an ultraviolet cutoff. Clearly, when $\langle\delta^2\rangle<\Delta_0^2$ the fluctuations in the model are essentially orientational, with fixed $|\Delta|$, and one has

$$F[\{\Delta(\mathbf{r})\}]\approx c\Delta_0(T)^2\int d^2r|\nabla\mathbf{n}|^2+\mathrm{const}\,. \tag{18}$$

This is the energy functional of the $O(n)$ nonlinear σ model.[23] In the opposite case, both amplitude and orientation fluctuations are important.

A microscopic calculation, based on the model (4) gives the following expressions for the coefficients in F, in the case of a SDW instability (the results are analogous for the other cases):

$$a'=\frac{1}{2\pi^2tT}\ln\left(\frac{2\pi e^\gamma t}{T}\right),\qquad b=\frac{7\zeta(3)}{32\pi^2tT^2}\ln\left(\frac{\pi^2t}{2T}\right),\qquad c=\frac{7\zeta(3)t}{32\pi^2T^2}\,, \tag{19}$$

where $\zeta(3)=1.202\ldots$. Furthermore, the ultraviolet cutoff is $\Lambda\approx 1/\xi(T=0)$. One then finds from (17) that the amplitude fluctuations are comparable to Δ_0^2 at a temperature T_x given by

$$T_x=T_c^{\mathrm{MF}}(1-\pi T_c^{\mathrm{MF}}/t)\,, \tag{20}$$

and decrease rapidly below T_x. Consequently, in the weak-coupling limit $T_c^{\mathrm{MF}}\ll t$ the temperatures given in Eq. (12) mark a sharp crossover from a metallic state with small antiferromagnetic correlations to a state with a rather well-defined SDW order-parameter amplitude, described by a (fixed-length spin) nonlinear σ model, with a temperature-dependent stiffness constant. Physical properties of that model are well known.[23] With increasing T_c^{MF} the width of the crossover region increases, and for large values of U the calculated T_c^{MF} only sets the temperature scale of the crossover from a region with charge fluctuations on each site to the fixed-length spin region, with exactly one electron per site. Finally, one may notice that the singular density of states gives rise to the logarithmic factors in the coefficients a' and b, and in particular the resulting correlation length are only shortened by a rather small factor, unless $\ln(t/T_c^{\mathrm{MF}})$ becomes very large.

In conclusion, I have studied here the different possible phases occurring in a generalized two-dimensional Hubbard model. Specifically I have found two new phases, JC and JS, characterized by charge (JC) or spin (JS) currents circulating around the elementary plaquettes of the lattice. Even though both phases are characterized by a broken translational symmetry, they are expected to be rather featureless in scattering experiments (apart from a weak orbital antiferromagnetism for JC). They do however show unusual behavior in the low-temperature conductivity ($\propto T^2$), spin susceptibility ($\propto T$), or specific heat ($\propto T^2$). In analogy with d-type superconductors,[20] one can expect that impurity scattering can lead to a finite (but reduced) density of states at the Fermi level even in the ordered state, which then will give rise to apparently metallic properties, in spite of the Fermi-surface induced order. The JC state discussed here bears some resemblance with the "flux phase" discussed by Affleck and Marston for the large-n limit of the Heisenberg model.[15]

In particular, extending the present mean-field theory to (infinitely) strong coupling, the excitation spectrum becomes $E(\mathbf{k}) \approx \pm (\cos^2 k_x + \cos^2 k_y)^{1/2}$ as proposed in Ref. 15. In contrast to the flux phase, however, the JC phase is not stable for a pure Hubbard model.

Finally, I have shown that for weak coupling the mean-field critical temperature corresponds to a sharp crossover from a Fermi-liquid state to a state with a well-defined order-parameter amplitude. One therefore can expect Schottky-type anomalies close to T_c^{MF} in thermodynamic quantities as the specific heat. With increasing T_c^{MF} these anomalies progressively widen and vanish.

Note added in proof. After submission of this paper I became aware of an article by B. I. Halperin and T. M. Rice [*Solid State Physics, Vol. 21,* edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1968), p. 115], which discusses states analogous to JC and JS. These states are also discussed in unpublished works by A. A. Nersesyan and A. Luther, and by I. E. Dzyaloshinskii and V. M. Yakovenko.

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