Deformation of the Fermi surface in the extended Hubbard model

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The deformation of the Fermi surface induced by Coulomb interactions is investigated in the \(t - t'\)-Hubbard model. The interplay of the local \(U\) and extended \(V\) interactions is analyzed. It is found that exchange interactions \(V\) enhance small anisotropies producing deformations of the Fermi surface which break the point group symmetry of the square lattice at the Van Hove filling. This Pomeranchuck instability competes with ferromagnetism and is suppressed at a critical value \(U(V)\). The interaction \(V\) renormalizes the \(t'\) parameter to smaller values what favors nesting. It also induces changes on the topology of hole of the Fermi surface which can go from hole to electron-like what may explain recent ARPES experiments.

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The shape of the Fermi surface plays a crucial role in determining the instabilities of interacting Fermi systems. The importance of Fermi surface deformations by interaction in the non-spherical case was already recognized in the early papers on the foundation of the Fermi liquid concept \([1, 2]\), and remains a central question both under a fundamental point of view as well as for the phenomenological implications.

The physics of the cuprates and the recent ARPES experiments has renewed interest on the anisotropic Fermi surfaces. Main questions are how close is the measured Fermi surface from the non–interacting?, how much can the Fermi surface be deformed before it breaks down driving the system to a broken symmetry phase?, does the deformation always respect the point group symmetry of the lattice?

In this paper we address the former questions in a very simplified model of the cuprates. We study the Fermi surface deformation in the \(t - t'\)-Hubbard model on the squared two–dimensional lattice in the presence of weak to moderate Coulomb interactions. We include an on-site coupling \(U\) to take account of the magnetic interactions and an extended exchange interaction \(V\) which can be as large as \(t\) \([3]\) and is widely used recently to account for the stripe feature and the possible phase separated phase in the cuprates. It will be seen that the \(V\) interaction plays a crucial role when the shape of the Fermi surface does not have special features favoring magnetic instabilities.

The deformation of the Fermi surface in the Hubbard and \(t - J\) models has been studied recently \([4–7]\) with a variety of methods. In most of these approaches attention is centered on the influence of magnetic interactions so the exchange interaction \(V\) is not taken into account. Our results show that, even at the mean field level, this interaction has a strong influence on the Fermi surface renormalization.

In a very recent paper \([8]\) it was argued that the Fermi surface of the \(t - t'\)-Hubbard model may undergo a deformation breaking the point symmetry of the underlying lattice (Pomeranchuck instability) driven by the renormalization of the forward channel. A deformation of this type seems to be observed in recent ARPES experiments \([9]\). Ferromagnetic instabilities which would directly compete with the Pomeranchuck instability were not taken into account. We investigate the conditions for the formation of Pomeranchuck instabilities and the competition with ferromagnetism. We argue that the instability is a fine tuning effect which only takes place at the Van Hove filling and is suppressed by ferromagnetism.

Our analysis provides also interesting results concerning the renormalization of the \(t'\) parameter which is shown to decrease with \(V\).

The hamiltonian that we shall use is

\[
H = -\sum_{i,j,\sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_{<ij>, \sigma\sigma'} n_{is} n_{js'},
\]

where \(t_{ij} = t\) for nearest neighbors, \(t_{ij} = t'\) for next nearest neighbors, and it is zero otherwise, and where we have included an extended Coulomb interaction \(V\).

The non-interacting band structure of (1) in the squared lattice is
\[ \varepsilon^0(k) = -2t \cos k_x - 2t' \cos k_x \cos k_y + 4t' \cos k_x \cos k_y \]  

(2)

what originates the constant energy contours shown in fig. 1.

The shape of the interacting Fermi surface is encoded in the two–point Green’s function of the interacting system

\[ G(\omega, k) = \frac{1}{\omega - (\varepsilon^0(k) - \mu) - \Sigma(\omega, k)}, \]  

(3)

where \( \Sigma(\omega, k) \) is the fermion self–energy. The Fermi surface of the interacting system is defined by the equation \[ \mu - \varepsilon^0(k) - \Re \Sigma(\omega, k) = 0, \]  

(4)

where \( \Re \Sigma \) stands for the real part of the electron self–energy. A mean field decoupling of the interacting term in (1) gives rise to an exchange interaction

\[ V(k_x, k_y) = 2V \sum_{k'_x, k'_y} \left[ \cos(k_x - k'_x) + \cos(k_y - k'_y) \right] n(k'), \]  

(5)

where \( n(k) \) is the occupation of the site \( k \) in momentum space. The \( k \) dependence of the interaction \( V \) in (5) is the key point of the results.

The diagrams contributing to the electron self–energy in perturbation theory are shown in fig. 2.

FIG. 1. Fermi surface of the free system for \( t=1, t'=0.3 \) and various densities around the Van Hove filling.

Local interactions \( U \) do not change the shape of the Fermi surface at the one loop level. Diagrams in fig. 2a) and fig. 2b) give rise to a constant that is absorbed in the chemical potential so as to keep the system at constant density. The first contribution to the Fermi surface deformation in the local case comes from the diagram in fig. 2c) and
has been computed in the literature and found to be very small. The interaction $V$ contributes to the fermion self–energy at the one loop level through diagram in fig. 2b).

We compute numerically the contribution of diagram in fig. 2b) to the Fermi surface deformation in eq. (4) by solving self-consistently the equation

$$
\varepsilon(k) = \varepsilon_{\text{kin}}(k) + \varepsilon_{\text{exch}}(k) - \mu
$$

$$=-2t\cos k_x - 2t\cos k_y + 4t'\cos k_x\cos k_y - 2V\sum_{k_x',k_y'}[\cos(k_x-k_x') + \cos(k_y-k_y')]n(k') - \mu ,
$$

where $\mu$ is adjusted so that the total number of electrons remains constant and spin interactions are not taken into account.

Ferromagnetism is included by starting with two different Fermi surfaces for electrons with spin up and down and solving the equations

$$
\varepsilon_{\uparrow}(k) = \varepsilon_{\uparrow}^{0}(k) + \varepsilon_{\text{exch}}^{\uparrow}(k) + U\frac{n_{\uparrow}}{N} - \mu
$$

$$\varepsilon_{\downarrow}(k) = \varepsilon_{\downarrow}^{0}(k) + \varepsilon_{\text{exch}}^{\downarrow}(k) + U\frac{n_{\downarrow}}{N} - \mu ,
$$

where the total number of electrons $N = n_{\uparrow} + n_{\downarrow}$ remains constant.

From eqs. (6) and (7), it is clear that in the absence of ferromagnetism, i.e starting with two identical Fermi surfaces in (6), the interaction $U$ contributes to the total energy with a global constant that is absorbed in the chemical potential. The deformations induced by $V$ are in general similar to the ones obtained in the literature when computing diagram in fig. 2c) with a local $U$ interaction. The reason is that the electron susceptibility inserted in the loop acts as a $k$–dependent effective interaction. The global sign is also the same (attractive). In the second order perturbation theory because of the closed fermion loop in the diagram, and in $V$ due to the exchange. The present analysis has the relevance of acting already at the one loop level.

Our results can be summarized as follows. The deformation of the Fermi surface depends on the filling. The general effect of $V$ is to smoothen out anisotropies in the curvature of the Fermi surface. This has a number of interesting consequences. In particular for closed surfaces (electron–like), the inflection points present with a finite $t'$ which were related in (10) to pairing instabilities with an extended-s order parameter, disappear at a value of $V \sim 1$. In the context of ref. (4), the presence of $V$ favors a d-wave pairing. This result seems at odds with the claims in (8) which find spontaneous generation of $t'$ in a Monte Carlo analysis of the $t - J$ model. We think that this is due to the sign of the interaction. The effect of a positive $V$ is the reversed one: it reinforces the curvature of the Fermi surface leading to bigger values of $t'$.

The general agreement of our computation with other very different approaches (8) suggests that there will be a general tendency towards nesting in the $t - t'$–Hubbard model with an extended attractive interaction of any origin.

A related topic of experimental relevance (11) concerns the possible change in Fermi surface topology induced by interactions. The presence of a $t'$ parameter breaking the electron–hole symmetry of the Hubbard model is crucial in this analysis. We find no changes in the Fermi surface topology with $t'=0$ in agreement with (8). In the presence of finite $t'$ and $V$, the Fermi surface does undergo changes in topology from open (hole–like) to closed (electron–like) when the initial Fermi energy lies close to – and slightly over – the Van Hove filling. This effect can explain recent measurements of electron–like surfaces in BISCO (11, 12). The reversed change would be observed by reversing the sign of $V$.

It is interesting to note that the interacting Fermi surface lies at the level of the Van Hove singularities for a variety of initial fillings in the hole–like regime. The Van Hove filling is never reached if starting with an overdoped situation (closed Fermi surface). This last result is very insensitive to the value of $t'$ and mimics the result about the pinning of the Fermi surface obtained in (13).

We have searched for Pomeranchuck instabilities by investigating the response of the system to very small perturbations of the free Fermi surface. The result is extremely sensitive to the value of the chemical potential of the final system. The effect of the interactions is, in general, to restore the lattice symmetry for generic values of the final $\mu$. Even in the case of very strong initial perturbation (of the order of a 4 per cent), the final Fermi surface is four-fold symmetric. The exception arises when the chemical potential of the interacting system coincides with the Van Hove singularity. We have checked that, in the absence of ferromagnetism, the Van Hove filling is unstable towards Pomeranchuck deformations. This result agrees with the general considerations exposed in (14) that the Fermi level of electron systems tend to avoid peaks in the density of states.

Fig. 3 shows the deformation caused by $V = 2$ in a paramagnetic situation when a point is removed by hand in the initial Fermi surface of a $61 \times 61$ lattice (corresponding to an anisotropy of less than $10^{-3}$).
FIG. 3. Deformation of the Fermi surface induced by \( V \) and by a small anisotropy in the free band. Solid line: free FS; dotted line: final FS in the absence of anisotropies; dashed line: deformed FS.

The solid line represents the free Fermi surface, the dotted line is the interacting Fermi surface in the absence of the perturbation, and the dashed line shows the final Fermi surface obtained after perturbing the free Fermi surface. Similar results are obtained with different values of \( V(n) \). This result is independent of \( t' \) and occurs also at \( t' = 0 \). It is nevertheless extremely sensitive to the value of the final chemical potential which has to be fine tuned by selecting the initial number of particles.

Magnetic interactions do substantially change the former picture. We have centered our attention on the effect of ferromagnetism as the predominant competing interaction in the forward channel \[16\]. Our results show that ferromagnetism is enhanced by \( U \) and \( t' \) as expected, but it is disfavored by \( V \). This can be understood on the light of our previous analysis showing that \( V \) renormalizes the \( t' \) parameter downwards. For small to moderate values of \( U \), the free ferromagnetic system evolves to an interacting paramagnetic state. There is, however, a critical value of \( U(V) \) where the final state corresponds to a fully polarized ferromagnetic system. This supression of ferromagnetism by exchange interactions might explain the absence of ferromagnetic phases in real systems which are otherwise well described by the \( t - t' \)–Hubbard model as the one in \[16\].

The Pomeranchuck instabilities described above compete with ferromagnetism. A schematic phase diagram showing the evolution of the ferromagnetic behavior of the system as a function of \( U \) and \( V \) is depicted in fig. 4.

FIG. 4. Schematic evolution of ferromagnetism with the interactions. PM: paramagnetic phase, FM\( \uparrow \) (FM\( \downarrow \)): magnetic polarization of the interacting system smaller (bigger) than that of the free system; FM: fully polarized final state.

Pomeranchuck instabilities are found systematically under the appropriate conditions in the paramagnetic zone of the phase diagram. By increasing \( U \) and keeping \( V \) constant, they enter into the phase denoted by FM\( \downarrow \) in fig. 4, changing it into a paramagnetic phase. Finally there is a critical value of \( U \) for which ferromagnetism prevails and the deformation dissapears.
In conclusion we have shown that exchange interactions renormalize \( t' \) to smaller values. An immediate consequence of this is that, in our search for microscopic models of the cuprates, one should start the computations with a bigger value of \( t' \) to account for a phenomenologically fitted value of \( t' \). The effect is doping-dependent and should be stronger in the underdoped situation where screening is less effective. In this regime it will increase the nesting of the Fermi surface and enhance antiferromagnetic instabilities. The renormalization of the \( t' \) parameter may also explain the absence of ferromagnetic phases in some real systems described by the \( t-t' \)-Hubbard model, and recent measurements of electron-like Fermi surfaces in some cuprates.

Pomeranchuck instabilities are found as the response of the system to small impurities when the Fermi surface lies at the Van Hove filling and can be regarded as an instability of the Van Hove level. They compete with ferromagnetism and dissipate at a critical value \( U(V) \).

Although the results presented in this paper are mean field results, we believe that the main features will survive the test with more accurate methods and that exchange interactions should be included – or checked to be negligible – in Hubbard related studies.

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