Fermi Surface of the 2D Hubbard Model at Weak Coupling

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Abstract

We calculate the interaction-induced deformation of the Fermi surface in the two-dimensional Hubbard model within second order perturbation theory. Close to half-filling, interactions enhance anisotropies of the Fermi surface, but they never modify the topology of the Fermi surface in the weak coupling regime.

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1 Introduction

Since the discovery of high-temperature superconductivity, the structure of low-lying single-particle excitations in two-dimensional interacting Fermi systems has attracted much interest. A key role is thereby played by the shape of the Fermi surface which determines the phase space for residual scattering processes and thus decay rates and Fermi liquid instabilities. In a recent Monte Carlo simulation of the two-dimensional Hubbard model Bulut, Scalapino and White have found that strong interactions may not only deform the Fermi surface of the non-interacting reference system, but may even lead to a different topology. While the Fermi surface of the non-interacting Hubbard model (with nearest-neighbor hopping) is always closed around the origin in k-space for densities n < 1, the strongly interacting system exhibited a Fermi surface centered around (π, π) for densities close to but below half-filling. This result raises the interesting question whether such a behavior occurs only in a strong coupling regime. Zlatić, Schotte and Schliecker have recently argued that the Fermi surface topology can be changed by arbitrarily weak interactions in the limit n → 1, since in that limit arbitrarily small deformations could lead to a topologically different shape.

In the following we will analyze the interaction-induced deformation of the Fermi surface in the two-dimensional Hubbard model within second order perturbation theory. We show that interactions enhance the anisotropy of the Fermi surface for densities close to half-filling, but they do not change the topology by deforming a (0,0)-centered surface into a (π,π)-centered one in the weak coupling regime.

The deformation of the Fermi surface in two-dimensional Hubbard models has been studied already earlier by Schönhammer and Gunnarsson and by Os-sadnik. The aim of the former authors was to show that Kohn-Sham Fermi surfaces are in general not exact. The behavior of deformations in the limit n → 1, however, has not been addressed in these earlier works.

2 Fermi Surface and Perturbation Expansion

The Hubbard model Hamiltonian is given by

\[ H = -t \sum_{\langle j,j' \rangle} c^{\dagger}_{j\sigma} c_{j'\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow} \]  

where t is the nearest-neighbor hopping amplitude and U the on-site Coulomb repulsion. The operators \( c_{j\sigma}^{\dagger} (c_{j\sigma}) \) create (annihilate) fermions with spin projection \( \sigma \) on lattice site \( j \) and \( n_{j\sigma} = c_{j\sigma}^{\dagger} c_{j\sigma} \).

The non-interacting band-structure for nearest-neighbor hopping on a square lattice is

\[ \epsilon_{k}^{0} = -2t (\cos k_{x} + \cos k_{y}) \]  

This leads to a strictly convex Fermi surface centered around \( k = (0,0) \) for densities \( n < 1 \), to a diamond shaped surface at half-filling \( n = 1 \), and a \((\pi,\pi)\)-centered Fermi surface for densities \( n > 1 \) (see Fig. 1).

The Fermi surface of the interacting system can be obtained from the one-particle Green function

\[ G(k,\omega) = \frac{1}{\omega - (\epsilon_{k}^{0} - \mu) - \Sigma(k,\omega)} \]
where $\Sigma(\mathbf{k}, \omega)$ is the self-energy. The chemical potential $\mu$ controls the average particle density $n$. The equation

$$\text{Re} \ G^{-1}(\mathbf{k}, \omega) = \xi_\mathbf{k} - (\epsilon^0_\mathbf{k} - \mu) - \text{Re} \ \Sigma(\mathbf{k}, \xi_\mathbf{k}) = 0$$  \hspace{1cm} (4)$$
determines the energy $\xi_\mathbf{k} \equiv \epsilon_\mathbf{k} - \mu$ of coherent single-particle excitations (quasi-particles) in the interacting system [3]. The Fermi surface is the set of those points in $\mathbf{k}$-space where the excitation energy vanishes, i.e. $\xi_{\mathbf{k}_F} = 0$, and thus determined by

$$\epsilon^0_{\mathbf{k}_F} - \mu + \text{Re} \ \Sigma_{\mathbf{k}_F, 0} = 0$$  \hspace{1cm} (5)$$
According to the Luttinger theorem [3], the volume enclosed by the Fermi surface is related to the particle density by

$$n = 2 \int \frac{d^2 \mathbf{k}_F}{(2\pi)^d} \Theta(\mu - \epsilon_\mathbf{k})$$  \hspace{1cm} (6)$$

We now calculate the interaction induced deformation of the Fermi surface to second order in the coupling strength $U$. The particle density is kept fixed by a suitable choice of an interaction-dependent chemical potential $\mu = \mu(n, U) = \mu_0 + \delta \mu$, where $\mu_0 = \mu_0(n)$ is the chemical potential corresponding to density $n$ at $U = 0$. We denote the Fermi wave vectors of the non-interacting system by $\mathbf{k}_F0$ and the deformation vectors by $\delta \mathbf{k}_F = \mathbf{k}_F - \mathbf{k}_F0$.

To first order in $U$, the self-energy is a real constant: $\Sigma_1(\mathbf{k}, \omega) = Un/2$. To keep the density fixed, the chemical potential has to be shifted accordingly by $\delta \mu_1 = Un/2$, which cancels $\Sigma_1$ completely in $G$.

To second order in $U$, two Feynman diagrams contribute to the self-energy of the Hubbard model (see Fig. 2). The second one is a real constant which is completely cancelled by a corresponding shift of the chemical potential.

The first diagram, however, leads to a $\mathbf{k}$-dependent contribution and generates a Fermi surface deformation. Expanding Eqs. (3) and (4) with $\mathbf{k}_F = \mathbf{k}_F0 + \delta \mathbf{k}_F$ and $\mu = \mu_0 + \delta \mu$ in powers of $U$ and comparing the second order terms, one obtains the relation

$$\nabla \epsilon^0_{\mathbf{k}_F0} \cdot \delta \mathbf{k}_F = \delta \mu_2 - \Sigma_2(\mathbf{k}_F0, 0)$$  \hspace{1cm} (7)$$
for the deformation of the Fermi surface to second order in $U$, where the chemical potential shift is given by the Fermi surface average

$$\delta \mu_2 = \frac{\int d^2 k \ \delta(\epsilon^0_{\mathbf{k}} - \mu) \Sigma_2(\mathbf{k}, 0)}{\int d^2 k \ \delta(\epsilon^0_{\mathbf{k}} - \mu)}$$  \hspace{1cm} (8)$$
Note that $\Sigma_2$ is real at zero frequency. Of course there are many ways to define a map $\mathbf{k}_F0 \rightarrow \mathbf{k}_F$ between non-interacting and interacting Fermi surfaces. A natural choice is $\delta \mathbf{k}_F = \delta \mathbf{k}_F \mathbf{n}_{\mathbf{k}_F0}$, where $\mathbf{n}_{\mathbf{k}_F0}$ is a unit vector normal to the non-interacting Fermi surface in $\mathbf{k}_F0$. Eq. (8) then determines the modulus of the shift as

$$\delta \mathbf{k}_{F2} = \delta \mathbf{k}_{F2}(\mathbf{k}_{F0}) = \frac{\delta \mu_2 - \Sigma_2(\mathbf{k}_{F0}, 0)}{\epsilon^0_{\mathbf{k}_{F0}}}$$  \hspace{1cm} (9)$$
where $\epsilon^0_{\mathbf{k}_{F0}} = |\nabla \epsilon^0_{\mathbf{k}_{F0}}|$ is the Fermi velocity of the non-interacting system. (See also the equivalent expression (4) in [3])

The second order self-energy has not yet been evaluated by purely analytical means. Using the spectral representation of the non-interacting propagator $G_0$, one can write the imaginary part of the self-energy contribution associated with the first Feynman diagram in Fig. 2 as

$$\text{Im} \Sigma_{2a}(\mathbf{k}, \omega) = -\frac{\text{sgn}(\omega)}{\pi} U^2 \int \frac{d^2 q}{(2\pi)^2} \int_0^\infty d\nu \text{Im} \Pi_0(q, \nu) \text{Im} G_0(k - q, \omega - \nu)$$  \hspace{1cm} (10)$$

We note that this diagram is "anomalous" in the sense of Kohn and Luttinger [4], i.e. it vanishes if the thermodynamic limit is taken strictly at $T = 0$, while it yields a finite contribution if the zero temperature limit is taken after the thermodynamic limit.
where the imaginary part of the non-interacting polarisation bubble is given by

$$\text{Im} \Pi_0(q, \nu) = \frac{\text{sgn}(\nu)}{\pi} \int \frac{d^2 p}{(2\pi)^2} \int_0^\omega d\omega' \text{Im} G_0(p, \omega') \text{Im} G_0(p + q, \omega' + \nu)$$

and $$\text{Im} G_0(k, \omega) = -\pi \text{sgn}(\omega) \delta \left[ \omega - (\epsilon_k^0 - \mu_0) \right].$$ Performing the integrals over $$\omega', p_x$$ and $$q_x$$ in (10) and (11) analytically (eliminating thus three $$\delta$$-functions), one obtains the expression

$$\text{Im} \Sigma_{2a}(k, \omega) = -\text{sgn}(\omega) \frac{U^2}{64\pi^3 t^2} \int dq_y \int dp_y \int_0^\omega d\nu \sum_{q_x^0, q_y^0} \left[ \frac{\Theta(\mu_0 - \epsilon_p^0) - \Theta(\mu_0 - \epsilon_{p+q}^0)}{\sqrt{(1 - f^2)(4\sin^2(q_x^0/2) - g^2)}} \right]$$

(12)

with the functions

$$f = (\nu - \omega - \mu_0)/2t - \cos(k_y - q_y)$$
$$g = \nu/2t + \cos(p_y + q_y) - \cos(p_y)$$

(13)

The summation variables $$q_x^0$$ and $$p_y^0$$ in (12) are the roots of the set of equations

$$\cos(k_x - q_x) = f$$
$$2\sin(p_x + q_x/2)\sin(q_x/2) = g$$

(14)

The remaining three-fold integral is easily computed numerically (e.g. via a standard Monte-Carlo routine on a work-station). Note that the representation in (12) is particularly suitable for a high resolution of the low-energy limit $$\omega \to 0$$, since the integration region shrinks with $$\omega$$. The full self-energy function can be reconstructed from its imaginary part $$\text{Im} \Sigma_{2a}$$ by a simple Hilbert transform

$$\Sigma_{2a}(k, \omega) = -\frac{\text{sgn}(\nu)}{\pi} \int_0^\omega d\omega' \left| \frac{\text{Im} \Sigma_{2a}(k, \omega')}{\omega' - \omega + i0^+ \text{sgn}(\omega')} \right|$$

(15)

The constant contribution $$\Sigma_{2b}$$ from the second diagram in Fig. 2 need not be calculated since it is completely cancelled by a corresponding shift $$\delta \mu_{2b}$$ of the chemical potential. Our numerical results for the second order self-energy agree with those published recently by Zlatić et al. [5], who computed $$\Sigma_{2a}$$ via a sequence of fast Fourier transforms. They also agree with earlier results by Schweitzer and Czycholl [11] and by Ossadnik [6].

3 Results for the Fermi Surface Deformation

To discuss explicit results for the Fermi surface deformation we introduce polar coordinates in $$k$$-space. Points on the Fermi surface of the non-interacting system are thus specified by an angle $$\phi$$. Due to the discrete symmetries of the square lattice it is sufficient to consider angles between 0 and 45 degrees. In Fig. 3 we show results for $$\delta k_{F2}/U^2$$ as a function of $$\phi$$ for various densities $$n$$. Here and in the following we set the hopping amplitude $$t = 1$$. At low densities $$n < 0.6$$ weak interactions tend to compensate anisotropies of the non-interacting Fermi surface while at densities $$0.7 < n < 1$$ anisotropies are further enhanced by interactions, as observed already earlier in unpublished work by Ossadnik [6]. The diamond shaped Fermi surface at half-filling is of course not affected at all by interactions, as a consequence of the particle-hole symmetry of the Hubbard model [11]. More generally, particle-hole symmetry maps the Fermi surface at density $$n$$ onto the surface for density $$2 - n$$ by a simple $$(\pi, \pi)$$-shift in $$k$$-space (the diamond at half-filling is thereby mapped onto itself).

Let us now clarify whether weak interactions can modify the Fermi surface topology at densities close to half-filling. The first Fermi point that may reach the Brillouin zone boundary (and thus introduce a different topology) upon increasing $$U$$ is obviously the one at $$\phi = 0$$, since it is closer to the zone boundary than any other Fermi point already in the non-interacting system and in addition $$\delta k_F(\phi)$$ is maximal for $$\phi = 0$$ (if $$n > 0.7$$). Quantitative information on the Fermi surface deformation in the "critical" regime $$n \to 1$$ and $$\phi \to 0$$ is provided in Fig. 4 where we have plotted $$\delta k_{F2}/U^2$$ as a function of density for various small angles $$\phi$$. Within numerical accuracy, $$\delta k_{F2}(\phi)$$ tends to 0 for $$n \to 1$$ for all $$\phi$$, as expected from particle-hole symmetry and continuity. Finally, in Fig. 4 we...
we show the critical coupling strength $U_c(n)$ that is required to make $k_F = k_{F0} + \delta k_F$ reach the Brillouin zone boundary (at the point $(\pi, 0)$). Close to half-filling, $U_c(n)$ behaves linearly as a function of density and extrapolates to a rather big finite value in the limit $n \to 1$. Hence, interactions do not modify the Fermi surface topology of the two-dimensional Hubbard model within the perturbatively controlled weak coupling regime at any density.

Zlatić et al. have calculated the critical coupling strength from second order perturbation theory for $n = 0.97$ (only), where they obtained a smaller $U_c$ (by a factor of about 2) than we did, although our results for the self-energy agree. The discrepancy arises because these authors have determined the new Fermi surface by directly solving Eq. (5) with the second order self-energy, while we have expanded $\delta k_F$ to second order in $U$, which is the order we really control. In the small $U$ limit both procedures yield the same shift to order $U^2$, but quantitative differences arise for finite $U$. The qualitative result that $U_c(n)$ remains finite in the limit $n \to 1$ is thereby not affected.

In summary, we have calculated the interaction-induced deformation of the Fermi surface in the two-dimensional Hubbard model within second order perturbation theory. Close to half-filling, interactions enhance anisotropies of the Fermi surface, but they never modify the topology of the Fermi surface in the weak coupling regime.

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