PHYSICAL REVIEW B VOLUME 37, NUMBER 6 15 FEBRUARY 1988-II

Difference between the quasiparticle and the Kohn-Sham-Fermi surfaces

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(Received 21 October 1987)

The question addressed is whether the Fermi surface calculated from the exact density-functional one-electron eigenvalues coincides with the "quasiparticle Fermi surface" calculated from the self-energy $\Sigma(\mathbf{k},\mu)$, where μ is the chemical potential. For the case of density-functional theory on a lattice this is shown *not* to be the case.

Density-functional theory[1,2] in the local (spin) density approximation [L(S)DA] is a very successful theory for the calculation of electronic properties of solids.[3] In density-functional theory (DFT) the density is used as the basic variable and the calculation of ground-state properties is formally exactly reduced to a problem of noninteracting electrons in an effective potential v_{eff}. The self-consistent solution of the Schrödinger equation for electrons in the potential v_{eff} yields as a by-product one-electron eigenvalues ε_i, which have no obvious meaning in the formalism. The ground-state density is given by the sum of densities of all one-electron states with $\varepsilon_i \leq \varepsilon_F$, where ε_F is the Fermi energy. For a crystalline metal this procedure leads to the "Kohn-Sham Fermi surface" (KS FS). Even for systems in which electronic correlations play an important role, the KS FS calculated in the LDA seems to agree quite well with results from de Haas–van Alphen experiments.[4] This naturally poses the question whether the remaining discrepancy is due to the LDA and whether the KS FS obtained from the *exact* v_{eff} would coincide with the "quasiparticle FS" (QP FS) obtained from the self-energy at the Fermi energy.[5] For the simplest case, i.e., the homogeneous electron gas (jellium), the two Fermi surfaces can *both* be *exactly* determined and they agree: The exact effective potential is constant and the KS FS is just the free-electron Fermi sphere. The same holds true for the QP FS due to Luttinger's theorem.[6] In the neighborhood of the FS the quasiparticle energies $E(p)=\varepsilon_F+(p-p_F)p_F/m^*$ and the KS eigenvalues $\varepsilon(p)=\varepsilon_F+(p-p_F)p_F/m$ *differ,* and the difference is described by the ratio of the effective mass m^* to the bare electron mass.[7] The agreement of the two FS's for jellium is, however, misleading, as the *shape* of FS is determined by *symmetry* and the volume is determined by Luttinger's theorem. Unfortunately, there exists no realistic electronic system which allows the exact determination of the two FS's.

We therefore study the question for the case of a *DFT on a lattice,* where the basic variables are the local occupation numbers n_i, where i refers to the ith lattice site.[8] The Hamiltonian H is of the form

$$H=T+\hat{U}+V_{\text{ext}} \ , \tag{1}$$

where the "kinetic energy" T is given by the hopping between sites (e.g., nearest-neighbor + next-nearest-neighbor hopping), $\hat{U}$ describes the "Coulomb" repulsion between the electrons and is in the following assumed to be of the on-site Hubbard form, and V_{ext} is an arbitrary external potential.

Because of the underlying lattice structure the shape of the Fermi surface is in this case nontrivial, even for $V_{\text{ext}}=0$. We therefore study this lattice DFT for $V_{\text{ext}}=0$, where we can determine the KS FS *exactly:* As the effective potential is constant on the lattice the Fermi surface is determined by the "kinetic-energy" term T and the number of electrons. The shape of the KS FS is therefore *independent* of the strength U of the Coulomb repulsion, and the two FS's could only be the same, if the shape of the QP FS is *independent of U.* This greatly simplifies the discussion of our problem. The determination of the exact QP FS still requires the exact solution of a nontrivial many-body problem corresponding to the Hamiltonian $H_0=T+\hat{U}$. As it is sufficient to prove the difference of the two FS's by showing a U dependence of the QP FS in an arbitrary parameter regime, we will prove the difference by showing a U dependence in the limit $U\rightarrow 0$. For that purpose it is sufficient to calculate the leading order frequency-dependent term of the self-energy, i.e., the self-energy to second order in U. The QP FS is determined by the equation

$$\varepsilon_{\mathbf{k}}+\Sigma(\mathbf{k},\mu)=\mu \ , \tag{2}$$

where the $\varepsilon_{\mathbf{k}}$ are the one-electron eigenvalues of the kinetic energy operator T, and the chemical potential $\mu(U)$ is determined by fixing the number of electrons to N, independently of U. The implicit equation (2) determines locally, e.g., the first component of the wave vector, in terms of the others, $k_1=f^{(\alpha)}(k_2,\ldots,k_d;U)$, where d is the spatial dimension and α labels different parts of the FS. The part of the self-energy proportional to U is k independent and does not change the FS. One therefore has an expansion of the type

$$k_1=f_0^{(\alpha)}(k_2,\ldots,k_d)+U^2f_2^{(\alpha)}(k_2,\ldots,k_d)+\cdots \ . \tag{3}$$

The function $f_2^{(\alpha)}$ can be determined by inserting (3) into Eq. (2). Using $\mu=\mu_0+U\mu_1+U^2\mu_2+\cdots$ and $\Sigma=U\mu_1$

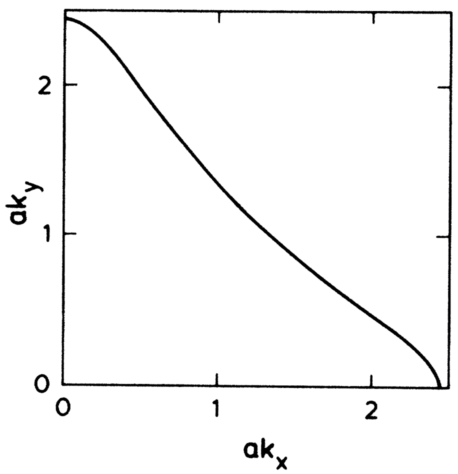

FIG. 1. The KS Fermi surface for $\frac{1}{4}$ of the Brillouin zone. The lattice parameter is a and the nearest-neighbor and second-nearest-neighbor hopping parameters are $t_1 = -1$ and $t_2 = 0.3$, respectively.

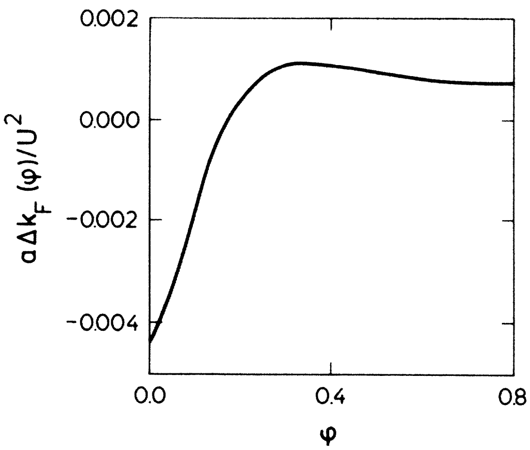

FIG. 2. The change $\Delta k_F(\phi)$ of the Fermi surface radius $k_F(\phi)$ as a function of ϕ for small values of U, where ϕ is the angle to the k_x axis. Because of the symmetry of the Fermi surface, results are only shown for $0 \leq \phi \leq \pi/4$. The same energy unit is used for U, t_1, and t_2.

$+U^2 g_2 + \cdots$ one obtains, comparing terms of order U^2,

$$f_2^{(a)}(k_2, \ldots, k_d) = \{\mu_2 - g_2[f_0^{(a)}(k_2, \ldots, k_d), k_2, \ldots, k_d]\}/(\partial\varepsilon/\partial k_1) \;, \tag{4}$$

where $\partial\varepsilon/\partial k_1$ is evaluated on the $U = 0$ FS. The FS for $U = 0$ can only remain unchanged if $f_2^{(a)} \equiv 0$. For this to happen the second-order self-energy $\Sigma_2(\mathbf{k},\mu)$ evaluated on the $U = 0$ FS has to be $\mathbf{k}$ independent. Unfortunately this cannot be checked without numerical calculations even if $\hat{U} = U\sum_i n_{i\sigma} n_{i-\sigma}$ is of the Hubbard type. One obtains

$$\Sigma_2(\mathbf{p},\omega) = (U/N)^2 \sum_{\mathbf{q},\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}})[1-f(\varepsilon_{\mathbf{q}})][1-f(\varepsilon_{\mathbf{p}+\mathbf{k}-\mathbf{q}})] - f(\varepsilon_{\mathbf{q}})f(\varepsilon_{\mathbf{p}+\mathbf{k}-\mathbf{q}})[1-f(\varepsilon_{\mathbf{k}})]}{\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{q}} - \varepsilon_{\mathbf{p}+\mathbf{k}-\mathbf{q}}} \;, \tag{5}$$

where the summations are over the first Brillouin zone. The numerical effort to calculate Σ_2 for the three-dimensional case is enormous. We have therefore performed calculations for $d = 2$. In connection with high-T_c superconductivity there have been speculations[9] recently that a two-dimensional Hubbard model is not a "normal Fermi system" near the half-filled band limit even for small repulsion U. Therefore a density 0.3 per spin has been chosen. To make the model "less symmetric" a next-nearest-neighbor hopping $t_2 = 0.3$ has been included in T in addition to a nearest-neighbor hopping $t_1 = -1$. The $U = 0$ FS is shown in Fig. 1. The numerical results for Σ_2 evaluated on this "free" FS show clearly a $\mathbf{k}$ dependence. *Therefore the KS FS and the QP FS differ for small values of U.* Figure 2 shows how the free FS is modified by U. It is sufficient to show $\frac{1}{8}$ of the first Brillouin zone.

This completes our proof that the two FS's are not necessarily the same by constructing a counterexample. Unfortunately our argument gives no hint how well the KS FS approximates the "true" QP FS in realistic systems.

This work was stimulated by discussions with C. O. Almbladh.

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