Fermionic lattice models with internally competing symmetries: Nontrivial algebraic corrections in the Hartree-Fock ground-state energy

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We show that even for homogeneous ground states the Hartree-Fock (HF) energy of fermionic lattice models may contain nontrivial *algebraic* corrections in the interaction. Hence the standard HF result for the energy, i.e., the *linear* dependence on the interaction, is found to be nongeneric. Algebraic corrections will appear in the HF energy whenever the **k**-space symmetry of the interaction is different from that of the kinetic energy, this being the generic case. The ensuing symmetry conflict leads to a distortion of the noninteracting Fermi surface. The energy corrections are explicitly evaluated for a generalized, two-dimensional Hubbard model with nearest-neighbor hopping and interaction along the diagonal. Algebraic corrections in the HF ground-state energy due to spontaneously broken symmetries may only occur if $\epsilon_{\mathbf{k}}$, the dispersion of free particles, has a special form.

I. INTRODUCTION

Fermionic lattice models, such as the Hubbard model and its generalizations, are investigated to gain qualitative insight into the fundamental interaction and correlation effects in realistic condensed-matter systems. In view of the well-known technical problems involved in such investigations the application of approximations becomes inevitable. A standard approximation scheme for interacting electronic systems is the Hartree-Fock (HF) theory.[1] In this self-consistent one-particle theory true correlations (i.e. two-particle effects) are neglected. Hence HF becomes exact only in the limit of small particle density and/or weak interaction. HF theory has been extensively used in the investigation of *continuum* models. It also serves as a natural first step in the study of fermionic *lattice* models (e.g., the Hubbard model[2]) which have recently received particular attention in the context of high-T_c superconductivity.[3]

In contrast to the case of continuum models the existence of an underlying periodicity in lattice systems naturally opens the possibility for long-range positional order of particles, e.g., spin- or charge-density waves. This kind of ordering can already be described, although rather crudely, on the HF level. Using HF wave functions with a broken symmetry, i.e., containing one or more order parameters, correlation effects can thus be "mimicked" even within HF theory. This theory is therefore often used to obtain at least a rough description of the possible type of ordering in interacting systems.[4–6]

In the following we will consider Hubbard-type fermionic lattice models:

$$\hat{H}=\hat{H}_{\rm kin}+\hat{H}_I\ , \tag{1a}$$

with $\hat{H}_{\rm kin}$ and $\hat{H}_I$ as the kinetic and interaction energy operators, respectively:

$$\hat{H}_{\rm kin}=\sum_{\mathbf{ij}}\sum_{\alpha} t_{\mathbf{ij}}^{\alpha}\hat{c}_{i\alpha}^{+}\hat{c}_{\mathbf{j}\alpha}=\sum_{\mathbf{k}}\sum_{\alpha}\epsilon_{\mathbf{k}}^{\alpha}\hat{n}_{\mathbf{k}\alpha}\ , \tag{1b}$$

$$\hat{H}_I=\frac{\lambda}{2}\sum_{\mathbf{ij}}\sum_{\alpha,\beta}V_{\mathbf{ij}}^{\alpha\beta}\hat{n}_{\mathbf{i}\alpha}\hat{n}_{\mathbf{j}\beta}\equiv\lambda\hat{V}\ . \tag{1c}$$

Here **i** and **j** refer to lattice sites, while **k** is the wave vector with $\hat{c}_{\mathbf{i}\alpha}(\hat{c}_{\mathbf{i}\alpha}^{+})$ and $\hat{a}_{\mathbf{k}\alpha}(\hat{a}_{\mathbf{k}\alpha}^{+})$ as the corresponding annihilation (creation) operators and $\hat{n}_{\mathbf{i}\alpha}=\hat{c}_{\mathbf{i}\alpha}^{+}\hat{c}_{\mathbf{i}\alpha}$, $\hat{n}_{\mathbf{k}\alpha}=\hat{a}_{\mathbf{k}\alpha}^{+}\hat{a}_{\mathbf{k}\alpha}$. The indices α,β describe internal degrees of freedom, such as spin and/or band quantum numbers. The interaction is assumed to be translationally invariant, with $V_{\mathbf{ij}}^{\alpha\beta}=V_{\mathbf{ij}}^{\beta\alpha}=V^{\alpha\beta}(|\mathbf{i}-\mathbf{j}|)$. It may have a purely local part, in which case it is a Hubbard interaction, as well as nearest-neighbor and next-nearest-neighbor contributions, etc. The parameter λ in (1c) is a small coupling parameter which will help us to keep track of the order of perturbation theory in $\hat{H}_I$. In HF theory the interaction term is linearized (mean-field approximation), $\hat{H}_I\rightarrow\hat{H}_I^{\rm HF}$, where

$$\hat{H}_I^{\rm HF}=\lambda\sum_{\mathbf{ij}}\sum_{\alpha\beta}V_{\mathbf{ij}}^{\alpha\beta}[\langle\hat{c}_{\mathbf{j}\beta}^{+}\hat{c}_{\mathbf{j}\beta}\rangle\hat{c}_{\mathbf{i}\alpha}^{+}\hat{c}_{\mathbf{i}\alpha}-\langle\hat{c}_{\mathbf{j}\beta}^{+}\hat{c}_{\mathbf{i}\alpha}\rangle\hat{c}_{\mathbf{i}\alpha}^{+}\hat{c}_{\mathbf{j}\beta}]-\tfrac{1}{2}\lambda\tilde{E} \tag{2a}$$

with the complex number

$$\tilde{E}=\sum_{\mathbf{ij}}\sum_{\alpha\beta}V_{\mathbf{ij}}^{\alpha\beta}[\langle\hat{c}_{\mathbf{j}\beta}^{+}\hat{c}_{\mathbf{j}\beta}\rangle\langle\hat{c}_{\mathbf{i}\alpha}^{+}\hat{c}_{\mathbf{i}\alpha}\rangle-\langle\hat{c}_{\mathbf{j}\beta}^{+}\hat{c}_{\mathbf{i}\alpha}\rangle\langle\hat{c}_{\mathbf{i}\alpha}^{+}\hat{c}_{\mathbf{j}\beta}\rangle]\ . \tag{2b}$$

The angular brackets stand for the ground-state expectation value at $T=0$.

Equation (2) stands for a self-consistency problem: finding the ground state $\Phi_{\rm HF}$ of $\hat{H}^{\rm HF}=\hat{H}_{\rm kin}+\hat{H}_I^{\rm HF}$, where $\hat{H}_I^{\rm HF}$ itself depends also on $\Phi_{\rm HF}$. This self-consistency problem is, in general, arbitrarily complicated because in the lattice problem under investigation the lattice translational symmetry of the ground state may be spontaneously broken in some sophisticated way. In this situation the state $\Phi_{\rm HF}$ and the HF potential will depend on a (in principle macroscopically large) number of order parameters. Hence, even though it is a single-particle problem there does not exist a systematic procedure to find the ground state of the HF Hamiltonian $\hat{H}^{\rm HF}$.

In the rest of the paper we shall use the term translational symmetry referring to the *discrete* translational

symmetry of the lattice. In this sense "homogeneous" means *discrete* translationally invariant if we refer to lattice models. Assuming such a homogeneous solution and particle conservation for each electron species α the self-consistency problem (2) is simplified considerably. It is still not trivial for general interactions as we will demonstrate in Sec. II. The HF Hamiltonian can be suitably expressed in $\mathbf{k}$ space

$$\hat{H}^{\mathrm{HF}}=\sum_{\mathbf{k}}\sum_{\alpha}[\epsilon_{\mathbf{k}}^{\alpha}+\lambda v_{\mathbf{k}}^{\alpha}]\hat{n}_{\mathbf{k}\alpha}-\tfrac{1}{2}\lambda\tilde{E}\ , \tag{3a}$$

where

$$v_{\mathbf{k}}^{\alpha}=\sum_{\mathbf{k}',\beta}[V_{\mathbf{k}=0}^{\alpha\beta}-V_{\mathbf{k}-\mathbf{k}'}^{\alpha\beta}\delta_{\alpha\beta}]\langle\hat{n}_{\mathbf{k}'\beta}\rangle \tag{3b}$$

is the HF potential with $V_{\mathbf{k}}^{\alpha\beta}$ as the Fourier transform of $V_{\mathbf{ij}}^{\alpha\beta}$. Note that for the Hubbard model, where the exchange term [second term on the right-hand side of (3b)] is absent, HF theory reduces to the Hartree approximation. The HF potential $v_{\mathbf{k}}^{\alpha}$ depends on the amplitudes

$$n_{\mathbf{k}\alpha}:=\langle\hat{n}_{\mathbf{k}\alpha}\rangle\ . \tag{4a}$$

This momentum distribution is given by

$$n_{\mathbf{k}\alpha}=\Theta\left[\epsilon_{\mathbf{k}}^{\alpha}+\frac{\lambda}{2}v_{\mathbf{k}}^{\alpha}[\{n_{\mathbf{k}\alpha}\}]-E_F\right]\ , \tag{4b}$$

where E_F is the Fermi energy. The factor $\frac{1}{2}$ accounts for $\tilde{E}$ as explained in Ref. 7. The self-consistency problem is now the following: One searches for a set $\{n_{\mathbf{k}\alpha}\}$ which fulfills (4b) self-consistently. This determines the Fermi surface.

On a diagrammatic level the HF approximation sums a certain class of diagrams which include diagrams of *all* orders in the interaction.[8] One may therefore ask whether or not the weak-coupling expansion of the HF ground-state energy in terms of the interaction leads to arbitrary powers in this interaction. On the other hand, it is common knowledge that for a homogeneous ground state the HF ground-state energy of continuum models, and even the Hubbard model, only acquires a *linear* shift by the interaction, while the existence of long-range order in the ground state (e.g., a spin-density wave in the case of the Hubbard model) only produces a *nonanalytically* small lowering of the energy[2] on top of the linear shift. In fact, the term "HF energy" is often used synonymously for an energy with a linear shift due to the interaction. (Here we only address the *ground state;* at finite temperatures algebraic corrections can be expected to enter anyway). The question is then whether this is the only possible outcome even for more general models than the Hubbard model. In other words: is it possible that the HF ground-state energy ever contains *algebraic* corrections in the interaction parameters ($\sim V^{\alpha},\alpha>1$, where V is a typical interaction constant)? Such corrections are usually associated with genuine (two-particle) correlation effects in which case they appear in standard perturbation theory.[9]

We will show below that the answer to the latter question is *yes:* even for homogeneous solutions the ground-state energy may contain algebraic corrections in the interaction parameters, provided that the symmetry in $\mathbf{k}$ space of different parts of the Hamiltonian is different. This competition of internal symmetries expresses itself in a distortion of the Fermi surface, which then leads to the above algebraic corrections *even within* HF. Of course the Fermi surface will always be distorted by genuine (two-particle) *correlation* effects [see, for example, Fig. 1(a) for a typical second-order correlation contribution to the self-energy].[10–12] Within perturbation theory these correlations give $\mathbf{k}$ states a finite lifetime; so the term "Fermi surface" refers to quasiparticles in this case.

Algebraic corrections in the HF ground state may even appear in the case of ground states with *spontaneously broken symmetries* (which generally only leads to nonanalytically small correction). However, this is only possible for very special dispersion relations $\epsilon_{\mathbf{k}}$. In Sec. II we will discuss the situation for a homogeneous ground state, and in Sec. III the case of spontaneously broken symmetries. In Sec. IV a discussion will end the presentation.

II. HOMOGENEOUS GROUND STATE

Most fermionic lattice models used to study correlation effects have a rather simple structure. For example, the kinetic energy usually involves only nearest neighbors and the interaction is reduced to on-site and/or nearest-neighbor coupling. Indeed the models *have* to be simple to allow for investigations at all, since even the simplest of these models defines a highly complicated quantum-mechanical many-body problem, which typically cannot be solved even in $d=1$ dimension. Their simplicity usually makes them highly *symmetric,* i.e., the Fermi surface corresponding to $\epsilon_{\mathbf{k}}^{\alpha}+(\lambda/2)V_{\mathbf{k}}^{\alpha}$ in (4b) has the *same* shape as that of the noninteracting case. (This is, for example, the case of the Hubbard model; see below). In this situation the noninteracting ground state Φ_0, reflecting the $\epsilon_{\mathbf{k}}$ relation, is a self-consistent solution of the HF equations, too. Consequently, the HF ground-state energy is found to depend only *linearly* on the coupling constant λ,

$$E_{\mathrm{HF}}=E_0+\lambda\langle\Phi_0|\hat{V}|\Phi_0\rangle\ , \tag{5}$$

where E_0 is the energy of the free system. It is this well-known, rather uninteresting result which is found by strictly applying a $T=0$ perturbation formalism.[13] Such a formalism is captured in the symmetry class defined by the free case and the corresponding ground state. This shortcoming of the general $T=0$ formalism was first

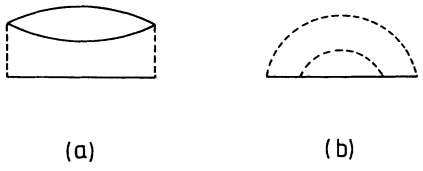

FIG. 1. Diagrammatic second-order contributions to the self-energy: (a) genuine two-particle correlation; (b) pure exchange contribution within Hartree Fock (anomalous diagram).

pointed out by Kohn and Luttinger[14] and Luttinger and Ward.[15] They showed that the problem can be solved by using a finite-T formalism in the limit $T\to 0$.[16] In this way the so-called "anomalous" diagrams, which do not contribute in the $T=0$ formalism,[13–15] are properly included. The scheme can also be applied to the HF diagrams only [see, for example, Fig. 1(b) for a typical Fock contribution to second order in the interaction]. One can easily convince oneself that *all HF diagrams beyond first order are anomalous.* In effect this amounts to the result expressed by Eq. (5).

Nevertheless, even when the anomalous diagrams are properly taken care of by the above-mentioned scheme, it turns out that they give zero contribution unless the interaction term in the Hamiltonian has a *different symmetry* than that of the kinetic energy. As already stated this means that the Fermi surface corresponding to $\epsilon_{\mathbf{k}}^{\alpha}+(\lambda/2)v_{\mathbf{k}}^{\alpha}$ in (4b) must have a different shape than that corresponding to $\epsilon_{\mathbf{k}}^{\alpha}$.

To elucidate this point and its implications for the ground-state energy one may take the Hubbard model as an example (in this case $\alpha\equiv\sigma=\uparrow$ or $\downarrow$, $\lambda=U$, $V_{\mathrm{ij}}^{\sigma\sigma'}=\delta_{\mathrm{ij}}\delta_{\sigma,-\sigma'}$, $t_{ij}^{\sigma}\equiv -t$ for nearest-neighbor hopping only). The Fock term in (3) vanishes then and $\lambda v_{\mathbf{k}}^{\sigma}=Un_{-\sigma}$ is a constant. Hence, the Fermi surfaces corresponding to $\epsilon_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}}+\frac{1}{2}Un_{-\sigma}$, respectively, have the same shape. This also shows that pure Hartree contributions cannot change the Fermi surface and that, if at all, it will be the exchange contributions, i.e., the Fock term in (3), that leads to a distortion. Nevertheless, a generalization of the interaction to a nearest-neighbor interaction, giving rise to an exchange term, will still not distort the Fermi surface because its Fourier transform is proportional to $\epsilon_{\mathbf{k}}$. If the kinetic energy connects only nearest neighbors this shows that a Fermi-surface distortion requires interaction *beyond* nearest neighbors, e.g., along a diagonal on a hypercubic lattice.

A. Second-order contributions to the Hartree-Fock ground-state energy

To obtain quantitative insight into the distortion of the Fermi surface within HF theory and hence of the change in the HF ground energy, we now calculate the second-order contribution to the HF ground-state energy, $E_{\mathrm{HF}}^{(2)}$. Expanding the self-consistency equation (4b) to second order in λ one obtains, omitting the factor λ^2,

$$E_{\mathrm{HF}}^{(2)}=-\tfrac{1}{2}LN(E_F^0)\overline{(v_{\mathbf{k}}^{\alpha}-\bar{v}_{\mathbf{k}}^{\alpha})^2}\ , \tag{6}$$

where L is the number of lattice sites, E_F^0 is the Fermi energy for $\lambda=0$, $N(E)$ is the density of states, and a bar indicates the average over the noninteracting Fermi surface at $\lambda=0$,

$$\bar{v}_{\mathbf{k}}^{\alpha}=[LN(E_F^0)]^{-1}\sum_{\mathbf{k},\alpha}\delta(\epsilon_{\mathbf{k}}^{\alpha}-E_F^0)v_{\mathbf{k}}^{\alpha}|_{\lambda=0}\ . \tag{7}$$

Note, that (6) can also be obtained using the approach of Kohn and Luttinger[14,15] (see, Ref. 13) for HF diagrams. $E_{\mathrm{HF}}^{(2)}$ is proportional to the fluctuation of the HF potential at the Fermi surface. We will now apply the above results to a two-dimensional, generalized Hubbard model on a square lattice

$$\hat{H}=-t\sum_{\langle \mathrm{ij}\rangle,\sigma}\hat{c}_{i\sigma}^{+}\hat{c}_{j\sigma}+U\sum_{i}\hat{n}_{\mathrm{i}\uparrow}\hat{n}_{\mathrm{i}\downarrow}+\sum_{\sigma\sigma'}\left[V\sum_{\langle ij\rangle}\hat{n}_{\mathrm{i}\sigma}\hat{n}_{\mathrm{j}\sigma'}+U_D\sum_{[\mathrm{ij}]}\hat{n}_{i\sigma}\hat{n}_{j\sigma'}\right]\ , \tag{8}$$

which includes interactions between nearest neighbors (summation index $\langle \mathrm{ij}\rangle$) and next-nearest neighbors, i.e., along the diagonal (summation index $[\mathrm{ij}]$), respectively. As argued above only the latter interaction, proportional to U_D, contributes to $E_{\mathrm{HF}}^{(2)}$. The result is shown in Fig. 2 as a function of the particle density n. For small n one has

$$E_{\mathrm{HF}}^{(2)}=-\left[\frac{\pi^{11}}{2^7}\right]^{1/2}n^{13/2}\left[1-\frac{3\pi}{2}n+\mathcal{O}(n^2)\right]U_D^2\ , \tag{9}$$

where the hopping element t has been set to unity and the energy is given per site. On the other hand, near half-filling, logarithmic terms appear and the curve asymptotically acquires a parabolic shape. Parametrizing n and $E_{\mathrm{HF}}^{(2)}$ by the chemical potential μ yields

$$E_{\mathrm{HF}}^{(2)}=-\left[\frac{\sqrt{2}}{\pi}\right]^{3}\mu^2(\ln|\mu|+1-4\ln 2)^2U_D^2+\text{higher terms}\ , \tag{10a}$$

$$n=1+\frac{\mu}{\pi^2}(\ln|\mu|-1-4\ln 2)+\text{higher terms}\ . \tag{10b}$$

The fact that $E_{\mathrm{HF}}^{(2)}$ vanishes at half filling ($n=1$) is not accidental. For $n=1$ the diamond-shaped Fermi surface implies that the HF potential $v_{\mathbf{k}}^{\sigma}$ has the perfect-nesting-like property $v_{\mathbf{k}}^{\sigma}+v_{\mathbf{k}+\mathbf{Q}}^{\sigma}=\text{const}$ for all $\mathbf{k}$, where $\mathbf{Q}=(\pi,\pi)$. This fact in turn implies that for $n=1$ $v_{\mathbf{k}}^{\sigma}$ is constant at the diamond-shaped Fermi surface. Hence, according to (6), no quadratic corrections will appear.

B. Higher-order corrections

Next we will investigate the implications of a *vanishing* $E_{\mathrm{HF}}^{(2)}$. To this end we state, and then prove, the following theorem.

Theorem: If $E_{\mathrm{HF}}^{(2)}$ defined in (6) vanishes, the ground

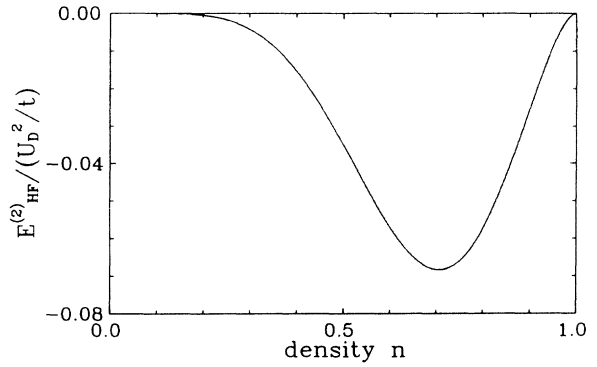

FIG. 2. Second-order Hartree-Fock ground-state energy correction $E_{\mathrm{HF}}^{(2)}$, Eq. (6), in units of U_D^2/t per site, vs particle density n.

state of the noninteracting system is the self-consistent, homogeneous solution of the HF problem within a certain interval $[\lambda_-,\lambda_+]$ of the coupling constant λ.

Here a "homogeneous" solution is one without a broken symmetry. If the precondition (homogeneous solution and $\lambda\epsilon[\lambda_-,\lambda_+]$) are met, one is thus led back to (5) for the ground-state energy, i.e., there is only a linear dependence on λ. If they are not fulfilled higher corrections in λ will typically occur. For the proof of the theorem we consider the linearized Hamiltonian[7]

$$\hat{H}^{\mathrm{HF}}_{\mathrm{hom}}=\sum_{\mathbf{k},\alpha}\left[\epsilon^{\alpha}_{\mathbf{k}}+\frac{\lambda}{2}v^{\alpha}_{\mathbf{k}}\right]\hat{n}_{\mathbf{k}\alpha}\ , \tag{11}$$

where $v^{\alpha}_{\mathbf{k}}$ is the HF potential defined in (3b).

The ground-state energy of $\hat{H}^{\mathrm{HF}}_{\mathrm{hom}}$ has to be minimized. This amounts up to occupying the lowest N $\mathbf{k}$ states with respect to the effective dispersion $\epsilon^{\alpha}_{k}+(\lambda/2)v^{\alpha}_{\mathbf{k}}$. The resulting Fermi body can be, but need not be, identical to the free one since the precondition requires $v^{\alpha}_{\mathbf{k}}$ to be constant at the Fermi surface, i.e. the noninteracting Fermi surface is an equipotential surface for the HF potential, too. Let μ_+ be the value of $v^{\alpha}_{\mathbf{k}}$ at the Fermi surface. The noninteracting Fermi body contains the lowest-lying states for the effective dispersion if λ lies in the interval $[\lambda_-,\lambda_+]$ where

$$\lambda_+=\inf\left[2\frac{\mu-\epsilon^{\alpha}_{\mathbf{k}}}{v^{\alpha}_{\mathbf{k}}-\mu_+}\ \middle|\ (\mu-\epsilon^{\alpha}_{\mathbf{k}})(v^{\alpha}_{\mathbf{k}}-\mu_+)>0,\mathbf{k}\in\mathrm{BZ}\right]\ , \tag{12a}$$

$$\lambda_-=\sup\left[2\frac{\mu-\epsilon^{\alpha}_{\mathbf{k}}}{v^{\alpha}_{\mathbf{k}}-\mu_+}\ \middle|\ (\mu-\epsilon^{\alpha}_{\mathbf{k}})(v^{\alpha}_{\mathbf{k}}-\mu_+)<0,\mathbf{k}\in\mathrm{BZ}\right]\ . \tag{12b}$$

BZ stands for the Brillouin zone.

This results from the following argument. The new chemical potential in the interacting case is $\mu+(\lambda/2)\mu_+$. If $(\mu-\epsilon^{\alpha}_{\mathbf{k}})(v^{\alpha}_{\mathbf{k}}-\mu_+)>0$, then

$$2\frac{\mu-\epsilon^{\alpha}_{k}}{v^{\alpha}_{\mathbf{k}}-\mu_+}\geq\lambda_+\geq\lambda\Longleftrightarrow\mathrm{sgn}(\mu-\epsilon^{\alpha}_{\mathbf{k}})=\mathrm{sgn}\left[\mu+\frac{\lambda}{2}\mu_+-\left[\epsilon^{\alpha}_{\mathbf{k}}+\frac{\lambda}{2}v^{\alpha}_{\mathbf{k}}\right]\right]\ . \tag{13a}$$

If $(\mu-\epsilon^{\alpha}_{\mathbf{k}})(v^{\alpha}_{\mathbf{k}}-\mu_+)<0$, then

$$2\frac{\mu-\epsilon^{\alpha}_{\mathbf{k}}}{v^{\alpha}_{\mathbf{k}}-\mu_+}\leq\lambda_-\leq\lambda\Longleftrightarrow\mathrm{sgn}(\mu-\epsilon^{\alpha}_{\mathbf{k}})=\mathrm{sgn}\left[\mu+\frac{\lambda}{2}\mu_+-\left[\epsilon^{\alpha}_{\mathbf{k}}+\frac{\lambda}{2}v^{\alpha}_{\mathbf{k}}\right]\right]\ . \tag{13b}$$

This concludes the derivation. Of course $\lambda=0$ will always be an element of the interval $[\lambda_-,\lambda_+]$. It may happen that one of the limits is zero, e.g., if the gradient of the free dispersion relation is zero on the Fermi surface while the gradient of the HF potential remains finite. This indicates that the free ground state is instable against a perturbation of the form of $v^{\alpha}_{\mathbf{k}}$. There are even cases conceivable where the interval $[\lambda_-,\lambda_+]$ only encloses zero.

III. GROUND STATES WITH SPONTANEOUSLY BROKEN SYMMETRY

In the last section a quadratic interaction term was shown to appear in the HF ground-state energy if the Fock potential had a different $\mathbf{k}$ space symmetry than the kinetic energy. This symmetry conflict is therefore a *necessary consequence* of the built-in symmetries of different parts of the Hamiltonian. In particular, it is not a *dynamic* effect such as the occurrence of a spontaneously broken symmetry of the ground state.

We will now discuss ground states with spontaneously broken symmetries and how, within HF theory, breaking of a symmetry may lower the ground-state energy with respect to the homogeneous solution. We focus in the following on the *difference* between homogeneous and nonhomogeneous solutions. Let us take a Hamiltonian of the form (11),

$$\hat{H}_{\mathrm{hom}}=\hat{H}_{\mathrm{kin}}+\lambda\hat{W}\ , \tag{14}$$

where $\hat{W}[\Phi,\Phi]$ is a one-particle operator which has been obtained by linearizing a two-particle operator using the state Φ. More generally, using different bra and ket states Φ_1 and Φ_2, one may define an operator-valued function $\hat{W}[\Phi_1,\Phi_2]$ which depends antilinearly on Φ_1 and Φ_2.

Suppose we had found a homogeneous self-consistent solution Φ_0 of (14) which defines $\hat{W}_0:=\hat{W}[\Phi_0,\Phi_0]$. Φ_0 may depend on λ if an internal symmetry competition requires this (see Sec. II). Thus the corresponding energy and $\hat{W}_0$ may also be λ dependent. Now we want to investigate the dependence of a symmetry-breaking order parameter $b(\lambda)$ on λ for $\lambda\rightarrow 0$, which parametrizes the deviation from W_0,

$$\hat{W}=\hat{W}_0+b\hat{W}_1+\cdots\ . \tag{15}$$

Since we are only interested in the weak-coupling behavior we neglect higher orders in b and set $\hat{W}_1$ constant. The additional term $\lambda b\hat{W}_1$ in the Hamiltonian produces some correction to the ground state,

$$\Phi=\Phi_0+A(\lambda b)\Phi_1+\cdots\ . \tag{16}$$

Again we neglect higher-order terms, setting Φ_1 constant. Due to norm conservation of Φ and the free choice of phase we may assume

$$\langle\Phi_0|\Phi_1\rangle=0\ . \tag{17}$$

$A(x)$ is a real-valued function which expresses how strongly the system will respond to the perturbation. Normally ordinary perturbation theory tells us that $A(x)=x$, i.e., the response of the system will be of the same order as the perturbation. Deviation from this behavior will be discussed a little later in some detail. So far, Φ_1 is determined by $\hat{W}_1$. As the HF procedure is self-consistent the converse is also true:

$$\hat{W}=\hat{W}[\Phi,\Phi]$$
$$=\hat{W}[\Phi_0,\Phi_0]+A(\lambda b)(\hat{W}[\Phi_0,\Phi_1]+\hat{W}[\Phi_1,\Phi_0])$$
$$+\cdots . \tag{18}$$

This implies $\hat{W}_1=(\hat{W}[\Phi_0,\Phi_1]+\hat{W}[\Phi_1,\Phi_0])$ and hence

$$b(\lambda)=A[\lambda b(\lambda)] . \tag{19}$$

This is the essential equation. Before we enter in its discussion we add the expansion of the HF ground-state energy,

$$E=\langle\Phi|\hat{H}_{\rm kin}+\lambda\hat{W}|\Phi\rangle$$
$$=E_0+A(\langle\Phi_1|\hat{H}_{\rm kin}+\lambda\hat{W}|\Phi_0\rangle+\text{h.c.})+\cdots , \tag{20a}$$
$$E=E_0(\lambda)-\lambda b(\langle\Phi_1|\hat{W}_0|\Phi_0\rangle+\text{h.c.})$$
$$+b^2\lambda(\langle\Phi_1|\hat{W}_1|\Phi_0\rangle+\text{h.c.})+\cdots , \tag{20b}$$

where we made use of (19) and of the fact that Φ_0 is an eigenstate of $\hat{H}_{\rm kin}$. In addition, the first term in (20b) usually vanishes, e.g., when Φ_0 is a product of momentum eigenstates and $\hat{W}_0$ is diagonal in **k** space. Equations (20) tell us how the energy lowering *due to spontaneous symmetry breaking* depends on the behavior of the order parameter b.

The simplest consequence of (19) is the following: If in (19) $A(x)$ is proportional to x for small arguments as in ordinary perturbation theory, *no* spontaneous symmetry breaking is possible at $\lambda=0$. Of course, the symmetry might break spontaneously at *finite* λ. This question cannot be answered within the present framework. It is sufficient that $|A(x)|<cx$ for some $c>0$ to exclude spontaneous symmetry breaking at $\lambda=0$. Thus $A(x)$ has to vanish slower than linearly to enable spontaneous symmetry breaking. To make this point clear we pass to the derivative $A'(x)$ which can be viewed as a measure of the susceptibility of the free system toward the perturbation $\hat{W}_1$. For $A(x)$ to have a sublinear behavior $A'(x)$ has to diverge for $x\to 0$. This is the physically well-known fact that the susceptibility diverges at a phase transition.

Assume, for example, a logarithmic divergence of $A'(x)$. Then $A(x)$ behaves as $-x\ln(x)$. Inserting this into (19) we find

$$b(\lambda)=(1/\lambda)\exp(-1/\lambda) , \tag{21}$$

i.e., the order parameter emerges nonalgebraically, i.e., very slowly.

Assuming a power law divergence $A'(x)\sim 1/(x^\gamma), 1>\gamma>0$ leads to $A(x)\sim(x^{(1-\gamma)})/(1-\gamma)$ and to

$$b(\lambda)\sim\lambda^{(1-\gamma)/\gamma} . \tag{22}$$

It can be seen from the last equation that in principle b can have any power-law behavior. If $A'(x)$ diverges more strongly than $1/x$ there is no $A(x)$ with $A(0)=0$. This is not physically reasonable since it would mean that the assumed free ground state is not stable, even without any interaction.

Since $b(\lambda)$ can have any power-law dependence we are led to the result that in principle the energy correction due to spontaneous symmetry breaking can have any power-law dependence greater than linear [see (20b)]. The question arises, however, as to which divergence of the susceptibility is physically likely to appear. The following qualitative argument shows that the logarithmic divergence of the susceptibility is the most common.

To calculate the susceptibility, first-order perturbation theory is used where simple energy denominators are involved. The susceptibility diverges only if the perturbation of a certain number of states displays vanishing energy denominators. These states have to be near the Fermi surface, otherwise their change shows no effect. At best, a finite part of the Fermi surface is concerned. If the Fermi body is d dimensional, this part is $(d-1)$ dimensional and will contribute to the susceptibility as

$$A'(x)\sim\int_{|k_F-k|\geq x}\frac{dk}{E_F-\epsilon_k}\sim\ln x \tag{23}$$

if the energy denominators vanish linearly on approaching the Fermi surface. Using the order of magnitude of the applied perturbation as cutoff in (23) we obtain the logarithmic divergent susceptibility $A'(x)$. Hence the order parameter—and thus the additional energy lowering [see (20)]—will be nonalgebraically small at $\lambda=0$ as shown in (21). As an example one may take the one- or three-dimensional Hubbard model with perfect nesting. The two-dimensional Hubbard model with perfect nesting displays an additional feature due to the singular corners of the diamond-shaped Fermi surface. Its susceptibility diverges like $[\ln(x)]^2$ (see, for example, Ref. 17).

We think that the above argument describes the actual physical situation. Yet it is not possible to exclude stronger divergences completely. If, for example, the energy dispersion relation is such that

$$|\epsilon_k-E_F|\sim|k-k_F|^\alpha , \quad 1<\alpha , \tag{24}$$

as shown in Fig. 3, the susceptibility will diverge like

$$A'(x)\sim\int_{|k_F-k|^\alpha\geq x}\frac{1}{k^\alpha}dk\sim x^{(1-\alpha)/\alpha} . \tag{25}$$

Note that $(1-\alpha)/\alpha>-1$. This situation produces algebraic corrections to the ground state and the ground-state

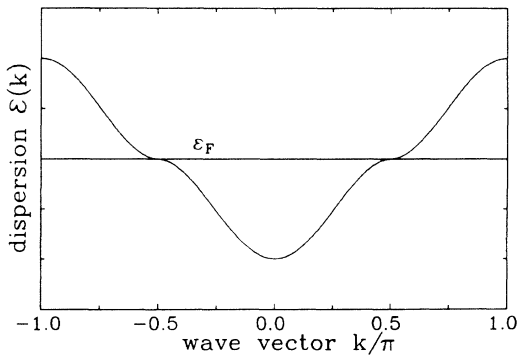

FIG. 3. Example of an energy dispersion of noninteracting particles for which algebraic corrections in the Hartree-Fock ground-state energy may appear due to a spontaneously broken symmetry of the ground state.

energy which are due to the spontaneous symmetry breaking. But the behavior of the dispersion relation at the Fermi energy necessary for that is somehow artificial.

Note that the susceptibility often does not diverge even though the energy denominators vanish, because the measure of the respective points at the Fermi surface is zero. This is the generic case for the Hubbard model in any but two dimensions *without perfect nesting,* see also Ref. 17.

IV. DISCUSSION

In this paper we investigated the interaction dependence of the HF ground-state energy for fermionic lattice models in the weak coupling limit. For homogeneous ground states, i.e., those without a broken symmetry, we found that the standard HF result, namely the *linear* dependence of the HF energy on the interaction, is actually *not* the generic case. We show that a purely linear shift is only obtained if the interaction, i.e., the HF potential, does not change the shape of the Fermi surface of the noninteracting particles. In this situation the noninteracting ground state is *also* the lowest-energy solution of the HF problem. Indeed, for the majority of fermionic lattice models, where the kinetic energy only involves nearest-neighbor hopping and the interaction acts only on-site and/or between nearest neighbors, this is the case. However, the compatibility of the interaction with the noninteracting Fermi surface in models is only accidental, being a consequence of the self-chosen simplicity of the model which makes it highly symmetric. For any somewhat more structured interaction, e.g., along a diagonal on a hypercubic lattice, the **k**-space symmetry of the Fock contribution will compete with that of $\epsilon_{\mathbf{k}}$, causing a *distortion* of the noninteracting Fermi surface. This distortion in turn will lead to additional *algebraic* interaction terms in the HF ground-state energy which are usually expected to enter only through pure two-particle correlation effects. This is the generic case. We explicitly calculated the second-order contribution to the HF energy for a generalized two-dimensional Hubbard model with interaction along the diagonal.

It should be noted that the above algebraic corrections are only nontrivial if in the model under consideration the particle number in a given band or for a given spin direction is a conserved quantity. If the particle numbers are not constant, as for example in the two-band periodic Anderson model where conduction and f electrons hybridize, such terms automatically appear irrespective of the type of the interaction.

In the case of ground states with spontaneously broken symmetry, we find that corrections to the HF energy of a homogeneous ground state generically are nonanalytically small. Our argument holds also if the homogeneous solution is already λ dependent. Algebraic corrections due to spontaneously broken symmetry may only arise if the dispersion of free electrons has rather special features.

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[7]Note that the following identity holds:

$$\langle \hat{H}_I^{\mathrm{HF}} \rangle = \frac{\lambda}{2} \sum_{\mathrm{ij}} \sum_{\alpha\beta} V_{\mathrm{ij}}^{\alpha\beta} [\langle \hat{c}_{\mathrm{j}\beta}^{+} \hat{c}_{\mathrm{j}\beta} \rangle \langle \hat{c}_{\mathrm{i}\alpha}^{+} \hat{c}_{\mathrm{i}\alpha} \rangle - \langle \hat{c}_{\mathrm{j}\beta}^{+} \hat{c}_{\mathrm{i}\alpha} \rangle \langle \hat{c}_{\mathrm{i}\alpha}^{+} \hat{c}_{\mathrm{j}\beta} \rangle] = \frac{\lambda}{2} \tilde{E} ,$$

with $\hat{H}_I^{\mathrm{HF}}$ given by (2a). For *homogeneous* ground states, where the form of the one-particle states is *a priori* known, we may therefore use the Hamiltonain

$$\hat{H}_{\mathrm{hom}}^{\mathrm{HF}} = \sum_{\mathbf{k}} \sum_{\alpha} \left[\epsilon_{\mathbf{k}}^{\alpha} + \frac{\lambda}{2} v_{\mathbf{k}}^{\alpha} \right] \hat{n}_{\mathbf{k}\alpha}$$

to calculate the shape of the Fermi surface.

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