Absence of magnetization in a nondegenerate half-filled band of electrons: Weak coupling

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We examine the conditions of coexistence of ferromagnetism, antiferromagnetism, and charge order in a one-dimensional system of weakly interacting electrons. The extended Hubbard Hamiltonian with one electron per atom is decoupled in a Hartree-Fock approximation and self-consistent equations for the three order parameters are obtained, including ferromagnetic band splitting. These equations are solved numerically at 0°K. We find no solution with a net magnetic moment. This result is consistent with Hubbard's result that there is no ferromagnetic solution for small enough interaction. Since we allow the ferromagnetic order paramater to be coupled to the charge order or to the antiferromagnetic order our proof is more general than Hubbard's, even though it is not the more general one.

I. INTRODUCTION

In a recent paper[1] we investigated the extended Hubbard model within the Hartree-Fock approximation. We restricted our attention to solutions with no net spin ($m=0$), allowing nonzero sublattice spin ($s\neq 0$) and charge-density ordering (described by a quantity $c\neq 0$). Although there is no obvious motivation in the extended Hubbard model for ferromagnetism, it seemed possible that some intricate effects, such as a partial mixture of m, s, and c, could be overlooked in so subtle a problem. The purpose of this note is to investigate solutions in which, *a priori*, m, s, and c are simultaneously allowed to be nonzero. Our result is that $m=0$. We note that the weakly interacting electron gas is generally believed[2,3] to be unstable with respect to charge- and spin-density waves and not to a ferromagnetic state. The result of this paper agrees with this belief. It also agrees with Hubbard's result[4] that at sufficiently small coupling one does not get a ferromagnetic solution. Hubbard did not allow for the possibility of coexistence of m and s and therefore our proof is more general than his, although not the most general one (even within Hartree-Fock); a more complex wave function, perhaps with a larger unit cell, might lower the energy still further.

II. ORDER PARAMETERS AND ENERGY LEVELS

We follow the notation of Ref. 1. The Hamiltonian is

$$H=-t\sum_{i\sigma}(c_{i\sigma}^{\dagger}c_{i+1,\sigma}+c_{i+1,\sigma}^{\dagger}c_{i\sigma}) + U\sum_i n_{i\uparrow}n_{i\downarrow}+V\sum_i n_i n_{i+1}\,. \tag{2.1}$$

Equation (2.1) is written in the Wannier-function basis of a nondegenerate band; $c_{i\sigma}$, $c_{i\sigma}^{\dagger}$, and $n_{i\sigma}$ are the destruction, creation, and number operators, respectively, in this basis; σ is the spin index, $\uparrow$ or $\downarrow$; $n_i=n_{i\uparrow}+n_{i\downarrow}$.

Next we attempt standing-wave solutions as follows:

$$\langle n_{i\uparrow}\rangle=A_\uparrow+2n_\uparrow\cos q_\uparrow R_i\,, \tag{2.2}$$

$$\langle n_{i\downarrow}\rangle=A_\downarrow+2n_\downarrow\cos q_\downarrow R_i\,. \tag{2.3}$$

$\langle\cdots\rangle$ denotes thermal average, R_i denotes the position of atom i, $A_{\uparrow,\downarrow}$, and $q_{\uparrow,\downarrow}$ are parameters which satisfy the following equation:

$$\sum_i\langle n_{i\sigma}\rangle=NA_\sigma\,, \tag{2.4}$$

NA_σ is the average number of electrons with spin σ(N is the total number of atoms).

$$q_\sigma=2k_{F\bar\sigma}\quad(\bar\sigma=-\sigma)\,, \tag{2.5}$$

where $k_{F\bar\sigma}$ is the Fermi momentum of the one-particle energy band with spin σ. Since we allow for the existence of a net moment, we assume $A_\uparrow\neq A_\downarrow$, $k_{F\uparrow}\neq k_{F\downarrow}$ and we define the average magnetization per atom as

$$m=A_\uparrow-A_\downarrow\,. \tag{2.6}$$

Furthermore, from the definition of Fermi momentum

$$k_{F\sigma}=(\pi/a)A_\sigma\,, \tag{2.7}$$

where a is the lattice constant.

Since we restrict ourselves to the half-filled band, we have

$$\frac{1}{N}\sum_{i\sigma}\langle n_{i\sigma}\rangle=A_\uparrow+A_\downarrow=1\,. \tag{2.8}$$

From Eqs. (2.6)–(2.8) we have

$$k_{F\uparrow}=(\pi/2a)(1+m)\,, \tag{2.9}$$

$$k_{F\downarrow}=(\pi/2a)(1-m)\,. \tag{2.10}$$

Our order parameters are then $n_\uparrow, n_\downarrow$, and m, which we will use in the Hamiltonian after pulling out averages in the Hartree-Fock decoupling. It is also instructive to relate $n_\uparrow$ and $n_\downarrow$ to the antiferromagnetic (s) and charge (c) order parameters at $m=0$. We have

$$\tfrac{1}{2}s=n_\uparrow-n_\downarrow\,, \tag{2.11}$$

$$\tfrac{1}{2}c=n_\uparrow+n_\uparrow\,. \tag{2.12}$$

In a previous paper[1] we showed that the lowest-energy self-consistent solution with $m=0$ has either $s\neq 0$ or $c\neq 0$ depending upon whether $U>2V$ or $U<2V$ but not both s and $c\neq 0$. Therefore we will look for self-consistent solutions with $m\neq 0$ and either $n_\uparrow+n_\downarrow$ or $n_\uparrow-n_\downarrow$ equal to zero. For the time being we carry through the general case. Substituting

$$n_{i\uparrow}n_{i\downarrow}\cong n_{i\uparrow}\langle n_{i\downarrow}\rangle+n_{i\downarrow}\langle n_{i\uparrow}\rangle\,, \tag{2.13}$$

$$n_i n_{i+1}\cong n_i\langle n_{i+1}\rangle+n_{i+1}\langle n_i\rangle \tag{2.14}$$

in Eq. (2.1) and using Eqs. (2.2)–(2.10), we get, after some algebraic manipulations:

$$H=-t\sum_{i\sigma}(c^\dagger_{i\sigma}c_{i+1,\sigma}+c^\dagger_{i+1,\sigma}c_{i\sigma})-\frac{U}{2}m\sum_i(n_{i\uparrow}-n_{i\downarrow})+2U\sum_{\substack{j=1\\ \sigma}}^{N/2}n_{-\sigma}\{\cos(2\pi jm)n_{2j\sigma}-\cos[\pi(2j+1)m]\,n_{2j+1,\sigma}\}$$

$$-4V\cos(\pi m)(n_\uparrow+n_\downarrow)\sum_{j=1}^{N/2}\{\cos(2\pi jm)n_{2j}-\cos[\pi(2j+1)m]\,n_{2j+1}\}\,. \tag{2.15}$$

To diagonalize Eq. (2.15) one needs to rewrite H in the Bloch basis using the identity

$$\sum_{j=\text{even or odd}}\cos(\pi jm)n_j=\frac{1}{4}\sum_k(c^\dagger_k c_{k-(\pi/a)m}\pm c^\dagger_{k-(\pi/a)(m\pm1)}+c^\dagger_k c_{k+(\pi/a)m}\pm c^\dagger_k c_{k+(\pi/a)(m\pm1)})\,, \tag{2.16}$$

where the minus signs in the terms in parentheses refer to the case j odd. The plus or minus signs in the wave vector labels

$$k-(\pi/a)(m\pm1),\quad k+(\pi/a)(m\pm1)$$

in Eq. (2.16) have to be chosen appropriately as explained below.

With $\epsilon_k=+2t\cos ka$ and (2.16) in (2.15) we have

$$H=-\sum_{k\sigma}\epsilon_k n_{k\sigma}-\frac{Um}{2}\sum_k(n_{k\uparrow}-n_{k\downarrow})+U\sum_{k\sigma}n_{-\sigma}(c^\dagger_{k\sigma}c_{k-(\pi/a)(m\pm1),\sigma}+c^\dagger_{k\sigma}c_{k+(\pi/a)(m\pm1),\sigma})$$

$$-2V\cos(\pi m)(n_\uparrow+n_\downarrow)\sum_{k\sigma}(c^\dagger_{k\sigma}c_{k-(\pi/a)(m\pm1),\sigma}+c^\dagger_{k\sigma}c_{k+(\pi/a)(m\pm1),\sigma})\,. \tag{2.17}$$

To make the problem tractable we now make a simplification which we believe does not affect the important effects of the interaction.

Let us consider the up and down bands separately. For the up band we have the situation shown in Fig. 1. We translate the k states as in the figure so that the new Brillouin zone extends from $-k_{F\uparrow}$ to $k_{F\uparrow}$, with a lower (l) and an upper (u) band.

For $-\pi/2<k<-\pi m/a$ we retain only those terms of Eq. (2.17) of the form $c^\dagger_{k\uparrow}c_{k+(\pi/a)(m+1),\uparrow}$ (choosing the plus sign in the momentum label). For $\pi m/a<k<\pi/a$ we retain the terms $c^\dagger_k c_{k-(\pi/a)(m+1)}$. We neglect the other terms because they couple pairs of Bloch states of much different energies. The states with $-\pi m/a<k<\pi m/a$ are left unchanged. In Eq. (2.17) we have therefore

$$Un_\downarrow\sum_k(c^\dagger_{k\uparrow}c_{k-(\pi/a)(m+1),\uparrow}+c^\dagger_{k\uparrow}c_{k+(\pi/a)(m+1),\uparrow})\cong Un_\downarrow\left(\sum_{k=-k_F}^{-\pi m/a}(c^{l\dagger}_{k\uparrow}c^u_{k\uparrow}+c^{u\dagger}_{k\uparrow}c^l_{k\uparrow})+\sum_{k=\pi m/a}^{k_{F\uparrow}}(c^{l\dagger}_{k\uparrow}c^u_{k\uparrow}+c^{u\dagger}_{k\uparrow}c^l_{k\uparrow})\right) \tag{2.18}$$

and similarly for the V term. l and u are the new band indices for "lower" and "upper." We have, for example, in the new notation,

$$c^l_{k\uparrow}=c_{k\uparrow}\,, \tag{2.19}$$

$$c^u_{k\uparrow}=c_{k+(\pi/a)(m+1)\uparrow}\quad\text{if } -k_{F\uparrow}<k<-\pi m/a\,, \tag{2.20}$$

etc.

We apply a similar procedure to the down band as shown in Fig. 2. Here $k_{F\downarrow}=(\pi/2a)(1-m)$ and therefore we choose the minus sign in the k labels in Eq. (2.17). After performing the translation as in Fig. 2 we again neglect the terms of Eq. (2.17) which couple k with $k+(\pi/a)(1-m)$ for $0<k<k_{F\downarrow}$ and those which couple k with $k-(\pi/a)(1-m)$ for

$-k_{F\downarrow}<k<0$. We entirely neglect the highest energy states for $-\pi m/a<k<\pi m/a$. In weak coupling these are states of high energy. We now proceed to diagonalize the approximate Hamiltonian by defining new fermion operators

$$a_{k\sigma}=\cos\theta_{k\sigma}c^{l}_{k\sigma}+\sin\theta_{k\sigma}c^{u}_{k\sigma}\,, \tag{2.21}$$

$$b_{k\sigma}=-\sin\theta_{k\sigma}c^{l}_{k\sigma}+\cos\theta_{k\sigma}c^{u}_{k\sigma}\,, \tag{2.22}$$

and their Hermitian conjugates.

The real parameters $\theta_{k\sigma}$ are found using the condition that the terms of the Hamiltonian proportional to $(a^\dagger_{k\sigma}b_{k\sigma}+b^\dagger_{k\sigma}a_{k\sigma})$ must vanish. These are the only nondiagonal terms which appear.

After some algebraic steps we arrive at the final form for the Hamiltonian

$$H=\sum_{k\sigma}(E^a_{k\sigma}a^\dagger_{k\sigma}a_{k\sigma}+E^b_{k\sigma}b^\dagger_{k\sigma}b_{k\sigma}) \tag{2.23}$$

with

$$E^a_{k\uparrow}=\begin{cases}-\tfrac12 Um-t\pi m\sin ka-[(\epsilon_k-t\pi m\sin ka)^2+\Delta^2_\uparrow]^{1/2} & \text{for } -k_{F\uparrow}<k<-\pi m/a\,,\\ -\tfrac12 Um-|\epsilon_k|\,, & \text{for } -\pi m/a<k<\pi m/a\,,\\ -\tfrac12 Um+t\pi m\sin ka-[(\epsilon_k+t\pi m\sin ka)^2+\Delta^2_\uparrow]^{1/2} & \text{for } \pi m/a<k<k_{F\uparrow}\,,\end{cases}$$

$$E^b_{k\uparrow}=\begin{cases}-\tfrac12 Um-t\pi m\sin ka+[(\epsilon_k-t\pi m\sin ka)^2+\Delta^2_\uparrow]^{1/2} & \text{for } -k_{F\uparrow}<k<-\pi m/a\,,\\ -\tfrac12 Um+t\pi m\sin ka+[(\epsilon_k+t\pi m\sin ka)^2+\Delta^2_\uparrow]^{1/2} & \text{for } \pi m/a<k<k_{F\uparrow}\,,\end{cases} \tag{2.24}$$

$$E^a_{k\downarrow}=\begin{cases}\tfrac12 Um+t\pi m\sin ka-[(\epsilon_k-t\pi m\sin ka)^2+\Delta^2_\downarrow]^{1/2} & \text{for } -k_{F\downarrow}<k<0\,,\\ \tfrac12 Um-t\pi m\sin ka-[(\epsilon_k+t\pi m\sin ka)^2+\Delta^2_\downarrow]^{1/2} & \text{for } 0<k<k_{F\downarrow}\,,\end{cases}$$

$$E^b_{k\downarrow}=\begin{cases}\tfrac12 Um+t\pi m\sin kka+[(\epsilon_k+t\pi m\sin ka)^2+\Delta^2_\downarrow]^{1/2} & \text{for } -k_{F\downarrow}<k<0\,,\\ \tfrac12 Um-t\pi m\sin ka+[(\epsilon_k-t\pi m\sin ka)^2+\Delta^2_\downarrow]^{1/2} & \text{for } 0<k<k_{F\downarrow}\,.\end{cases}$$

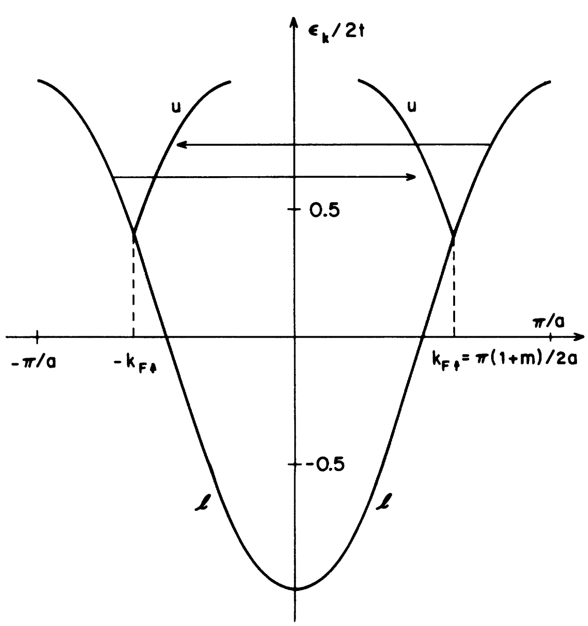

FIG. 1. Folding the Brillouin zone of the up band: $k_{F\uparrow}=(\pi/2a)\,(1+m)$.

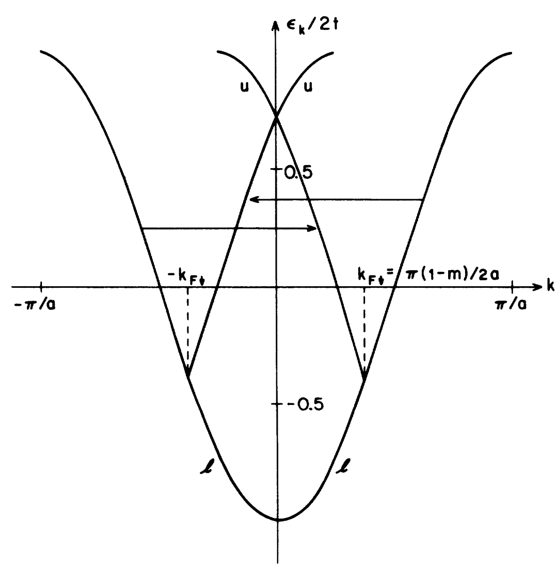

FIG. 2. Folding the Brillouin zone of the down band: $k_{F\downarrow}=(\pi/2a)\,(1-m)$.

In these expressions we have approximated $\sin\pi m$ by πm since we are interested in the weak-coupling regime, where the order parameter m is a small quantity with respect to unity. We have

$$\Delta_\uparrow = Un_\downarrow - 2V(n_\uparrow + n_\downarrow) , \tag{2.25}$$

$$\Delta_\downarrow = Uv_\uparrow - 2V(n_\uparrow + n_\downarrow) . \tag{2.26}$$

III. SELF-CONSISTENT EQUATIONS

As we explained above, we take it that $n_\uparrow = \pm n_\downarrow = n$; This reduces the order parameters to two, m and n; [from Eqs. (2.25) and (2.26)] in either case

$$\Delta_\uparrow = \Delta_\downarrow = \Delta = \begin{cases} (U-4V)n & \text{if } n_\uparrow = n_\downarrow , \\ -Un & \text{if } n_\uparrow = -n_\downarrow . \end{cases} \tag{3.1}$$

Let us suppose that $n_\uparrow = -n_\downarrow$ (all the calculations are the same if $n_\uparrow = n_\downarrow$). To find the self-consistent equations for the order parameters at 0 °K we Fourier transform Eqs. (2.2) and (2.3) and use the inverse transformations of Eqs. (2.21) and (2.22):

$$n_\uparrow = \frac{1}{N} \sum_{k=-k_{F\uparrow}}^{k_{F\uparrow}} \sin(2\theta_{k\uparrow}) \langle a_{k\uparrow}^\dagger a_{k\uparrow} - b_{k\uparrow}^\dagger b_{k\uparrow} \rangle , \tag{3.2}$$

$$n_{k\uparrow} = \frac{1}{N} \sum_{k=-k_{F\downarrow}}^{k_{F\downarrow}} \sin(2\theta_{k\downarrow}) \langle a_{k\downarrow}^\dagger a_{k\downarrow} - b_{k\downarrow}^\dagger b_{k\downarrow} \rangle . \tag{3.3}$$

Of course $\theta_{k\sigma}$ are functions of m and n and of the parameters of the Hamiltonian; the condition $n_\uparrow = -n_\downarrow = n$ gives [from Eqs. (3.2) and (3.3)] two self-consistent equations for the two parameters m and n:

$$1 = \frac{2U}{N} \sum_{k=0}^{(\pi/2)(1-m)} [(\epsilon_k + t\pi m \sin ka)^2 + U^2 n^2]^{-1/2} , \tag{3.4}$$

$$1 = \frac{2U}{N} \sum_{\pi m}^{(\pi/2)(1+m)} [(\epsilon_k - t\pi m \sin ka)^2 + U^2 n^2]^{-1/2} . \tag{3.5}$$

Equations (3.4) and (3.5) require justification. They are obtained by completely filling the $a_\uparrow$ and $a_\downarrow$ bands so as to favor m as much as possible. To be able to do this the b bands must be higher than the a bands and this imposes a restriction on the relative magnitude of m and n.

In fact, if we write the following quantities (retaining only terms of order m):

$$E^a_{k_{F\uparrow}} = t\pi m - |\Delta| - \tfrac{1}{2} Um , \tag{3.6}$$

$$E^a_{k_{F\downarrow}} = - t\pi m - |\Delta| + \tfrac{1}{2} Um , \tag{3.7}$$

$$E^b_{k_{F\uparrow}} = t\pi m + |\Delta| - \tfrac{1}{2} Um , \tag{3.8}$$

$$E^b_{k_{F\downarrow}} = - t\pi m + |\Delta| + \tfrac{1}{2} Um , \tag{3.9}$$

we see that $E^b_{k_{F\uparrow}} > E^b_{k_{F\downarrow}}$ and $E^a_{k_{F\uparrow}} > E^a_{k_{F\downarrow}}$ because in the weak-coupling regime $t\pi m$ is certainly $\gg |\Delta|$ and Um. Furthermore, to fill completely the two a bands, and thereby attain the maximum m, $E^b_{k_{F\downarrow}}$ must be $> E^a_{k_{F\uparrow}}$ and this means

$$m < Un/t\pi \ll 1 \tag{3.10}$$

(neglecting $\frac{1}{2}U$ as compared to $2\pi t$).

We solve numerically Eqs. (3.4) and (3.5) and we find that besides the solution $m = 0$, there is a solution with $m \neq 0$ which does not satisfy Eq. (3.10) (i.e., it is not self-consistent). The only self-consistent solution is $m = 0$.

This is the final result. We find that in the Hartree-Fock approximation a half-filled band of weakly interacting electrons is spin ordered, or charge ordered, but there is no ferromagnetic component (in the context of the particular types of solutions that we assume).

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