On the Existence of Antiferromagnetism in Hubbard's Approach to the Hubbard Model

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We investigate the possibility of selfconsistent solutions for antiferromagnetism in the Hubbard model in the decoupling of the Greens functions introduced by Hubbard in his first paper. On the base of this approximation Arai has calculated the band splitting for antiferromagnetism, but, as will be shown in this paper, Hubbard's approach fails to yield antiferromagnetism for nearest neighbour hopping in the same way as it does not yield ferromagnetism, and no selfconsistent solutions of the problem beyond the well known paramagnetic solution do exist.

1. Introduction

In the same paper in which Hubbard introduced his Hamiltonian for electron interactions in narrow energy bands, which is now commonly denoted as the HUBBARD model [1], he gave a treatment of the correlation problem in terms of temperature dependent Greens functions [2] which is founded on two well-distinguished and independent suppositions. The first consists in a special decoupling of the hierarchy of Greens functions [3] and the second is the assumption that the expectation value of the number of electrons of a given spin direction will not depend on the lattice site, to which the electrons are attached. This homogeneity on the lattice is equivalent to the assumption of ferromagnetic ordering (because it leads to ferromagnetism for a different partition of the electrons on the two spin directions) and will therefore be denoted as ferromagnetic hypothesis.

Hubbard gets interesting results for the band splitting of the pseudo-particles, but the only self-consistent solution of his equations is the paramagnetic one, at least for a large class of reasonable single-centred densities of states for the free electrons. That means, there is no ferromagnetism in the Hubbard decoupling.

On the other hand, it has been established in the meanwhile both by the investigation of the ground state of the model [4] and by single particle theories [5-7] which are more refined than the usual Hartree-Fock approach that antiferromagnetic ordering is more likely than ferromagnetism for the nearly neutral model, i. e. if the number of electrons $N_e \cong$ the number of lattice sites N, at least for sufficiently small electron coupling.

Therefore, the question may be asked whether the Hubbard decoupling would lead to *antiferromagnetism* when the ferromagnetic hypothesis is given up in favour of a periodical variation of the expectation value of the number of electrons of a given spin on the lattice.

Recently this problem has been attacked by ARAI [3] for a general hopping interaction; Arai discussed the complicated effects of antiferromagnetism on band splitting, but he did not investigate the existence of selfconsistent solutions for this type of ordering.

This problem will be considered in the present paper, but we shall restrict ourselves from the begin to the case of nearest neighbour interaction in AB-lattices, where not only the density of the free electrons is well known [9] but also the general evaluation of the formulae is much more straightforward than in the case of general hopping distances.

The result of these investigations will mainly be a negative one, because we shall show that the Hubbard decoupling fails to yield antiferromagnetic solutions in the same way, as it fails to yield ferromagnetism.

2. Hubbard-Decoupling and AB-Hypothesis

To become concrete, we shall start from the Hamiltonian

$$H = -T \sum_{j,\Delta,\sigma} c^+_{j+\Delta,\sigma} c_{j\sigma} + \tfrac{1}{2} V_0 \sum_{j,\sigma} n_{j\sigma} n_{j,-\sigma}, \qquad (1)$$

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where $c_{j\sigma}^+$ generates an electron in a Wannier state localized at the lattice site j, $n_{j,\sigma} = c_{j\sigma}^+ c_{j\sigma}$, Δ comprehends all nearest neighbour vectors of a given lattice site, T is the hopping constant for nearest neighbour transitions and V_0 is the repulsive interaction, which electrons of opposite spin feel when they are brought together to the same lattice site.

Following Hubbard we consider the equation of motion of the quantum-statistical Greens functions

$$G_{jk}^\sigma (E) = \langle\langle c_{j\sigma} ; c_{k\sigma}^+ \rangle\rangle_E , \qquad (2)$$

which after performing of the Hubbard decoupling is given by

$$E \, G_{jk}^\sigma (E) = F_j^{-\sigma} \left\{ \frac{1}{2\pi} \delta_{jk} - T \sum_\Delta G_{j+\Delta,k}^\sigma \right\}, \qquad (3\,a)$$

with $F_j^{-\sigma}$ defined by

$$F_j^{-\sigma} = \left\{ \frac{E - V_0 (1 - \langle n_{j,-\sigma}\rangle)}{E - V_0} \right\}. \qquad (3\,b)$$

In fact this formula is identical with Eq. (51) of Hubbard's paper apart from the fact that due to the ferromagnetic hypothesis of this paper $\langle n_{j,-\sigma} \rangle$ is taken independent of j and therefore also $F_j^{-\sigma}$ does not depend on the lattice site [10].

Clearly the method of solving the system (3) by a simple Fourier-transformation used by Hubbard is restricted just to this case. In order to get a comparably simple solution for spatially varying $\langle n_{j\sigma} \rangle$ we now introduce an "AB hypothesis" by dividing the lattice into an A and a (mathematically equivalent) B lattice and defining

$$\langle n_{j\sigma} \rangle = \begin{cases} n_A^\sigma : & \text{for } j \text{ from the } A \text{ lattice,} \\ n_B^\sigma : & \text{for } j \text{ from the } B \text{ lattice;} \end{cases} \qquad (4)$$

in this way we get two different quantities $F_A^{-\sigma}$ and $F_B^{-\sigma}$.

In fact this definition is slightly more general than the assumption of antiferromagnetism, because it comprehends also the ferromagnetic hypothesis for $n_A^\sigma \equiv n_B^\sigma$. This will give rise to an useful check of our calculations, which must yield Hubbard's results under these circumstances.

The next thing to note is that we may label also the Greens functions according to the sublattices to which the vectors j and k belong, i. e. as $G_{jk}^{AA\sigma}$, $G_{jk}^{AB\sigma}$, $G_{jk}^{BA\sigma}$ and $G_{jk}^{BB\sigma}$, and that for j from the A lattice — say — all $j+\Delta$ occurring in Eq. (3 a) will be from the B lattice and vice versa. In order to decouple the equations for different sublattices we

may write down Eq. (3 a) for the functions $G_{j+\Delta,k}$, insert them into (3 a) and get the result

$$E \, G_{jk}^{AA\sigma} = F_A^{-\sigma} \frac{\delta_{jk}}{2\pi} + \frac{T^2}{E} F_A^{-\sigma} F_B^{-\sigma} \sum_{\Delta,\Delta'} G_{j+\Delta+\Delta',k}^{AA\sigma}, \qquad (5)$$

or interchanging A and B the analogous formula for $G_{jk}^{BB\sigma}$.

Now we may introduce the translation vector $l = j - k$ of the sublattice (where it is important that the A and B lattices are equivalent) and assume translation symmetry in the sublattices, such that (5) may be written as

$$E \, G^{AA\sigma} = F_A^{-\sigma} \frac{\delta_{l0}}{2\pi} + \frac{T^2}{E} F_A^{-\sigma} F_B^{-\sigma} \sum_{\Delta,\Delta} G_{l+\Delta+\Delta'}^{AA\sigma}. \qquad (6)$$

As this is a system of coupled linear equations for $G_l^{AA\sigma}$, it may be solved by a Fourier-transformation on the sublattice, which will be introduced in the next section.

3. The Sublattice Fourier-Transformation

When the periodicity volume of the lattice contains N lattice sites each sublattice will consist of $N/2$ sites. Therefore we introduce

$$G_q = \frac{2}{N} \sum_l G_l \exp\{-i\,q\,l\}, \qquad (7\,a)$$

where l runs over all sublattice vectors and get

$$G_l = \sum_q G_q \exp\{i\,q\,l\}, \qquad (7\,b)$$

where q now runs over the Brillouin zone of the sublattice [11].

When we multiply Eq. (6) by $(2/N) \exp\{-i\,k\,l\}$ and sum over all sublattice vectors l we find for the last summand of (6)

$$\begin{aligned} T^2 \frac{2}{N} \sum_{l,\Delta,\Delta'} & G_{l+\Delta+\Delta'} \exp\{-i\,k\,l\} \\ &= T^2 \frac{2}{N} \sum_{l',\Delta,\Delta'} G_{l'} \exp\{-i\,k(l' - (\Delta + \Delta'))\} \\ &= G_k T^2 \sum_{\Delta,\Delta'} \exp\{i\,k(\Delta + \Delta')\} \end{aligned} \qquad (8)$$

and introducing

$$T_k = T \sum_\Delta \exp\{i\,k\Delta\} \qquad (9)$$

this expression results in $G_k T_k^2$. What is important to note is that Δ is no sublattice vector and therefore T_k is not a sublattice-Fourier transformed.

Introducing this into Eq. (6) we get the result

$$\{E^2 - T_k^2 F_A^{-\sigma} F_B^{-\sigma}\} G_k^{AA\sigma} = \frac{1}{2\pi}\frac{2}{N} E F_A^{-\sigma}. \quad (10)$$

Now we insert Eq. (3 b) into this equation, and solving for $G_k^{AA\sigma}$, we find

$$G_k^{AA\sigma}(E) = \frac{1}{2\pi}\frac{2}{N}\frac{P_A^\sigma(E)}{Q_k^\sigma(E)}, \quad (11\,a)$$

where P_A^σ and Q_k^σ are the polynomials

$$P_A^\sigma(E) = E(E - V_0)(E - V_0(1 - n_A^{-\sigma})) \quad (11\,b)$$

and

$$Q_k^\sigma(E) = E^2(E - V_0)^2 \quad (11\,c)$$
$$- T_k^2(E - V_0(1 - n_A^{-\sigma}))(E - V_0(1 - n_B^{-\sigma}))$$

respectively; $G_k^{BB\sigma}(E)$ is given by the same formula with A interchanged with B. It is worth mentioning here that P does not depend on the momentum and that the denominator $Q_k^\sigma(E)$ is in common to $G_k^{AA\sigma}$ and $G_k^{BB\sigma}$.

4. Resolution of $G_k(E)$ into Partial Fractions

In order to apply the special representation of the Greens functions later on it will be convenient to resolve Eq. (11 a) into partial fractions. If all zeros $E_{k\lambda}^\sigma$ of $Q_k^\sigma(E)$ are simple and real we may write

$$G_k^{AA\sigma}(E) = \frac{1}{2\pi}\frac{2}{N}\sum_{\lambda=1}^{4}\frac{A_{k\lambda}^{A\sigma}}{E - E_{k\lambda}^\sigma} \quad (12\,a)$$

with the quantities $A_{k\lambda}^{A\sigma}$ given by

$$A_{k\lambda}^{A\sigma} = \frac{P_A^\sigma(E_{k\lambda}^\sigma)}{Q_k^{\sigma\prime}(E_{k\lambda}^\sigma)}, \quad (12\,b)$$

where

$$Q_k^{\sigma\prime}(E_{k\lambda}^\sigma) = \frac{dQ_k^\sigma}{dE}\Bigg|_{E=E_{k\lambda}^\sigma} \quad (13)$$

holds.

As we shall show later on it will not be necessary to know the zeros $E_{k\lambda}^\sigma$ explicitly, which would mean to solve an equation of fourth order. What we have to do is to assure that for one thing these zeros are real under all circumstances and for another thing they are separated from one another by boundaries which do not depend on the momentum k. The latter point means, as to the band splitting of $G_k(E)$, we do not have band overlap and all zeros are simple.

Let the zeros $E_{k\lambda}^\sigma$ be ordered by $E_{k\lambda}^\sigma < E_{k,\lambda+1}^\sigma$ and let — without loose of generality — be $n_A^{-\sigma} \leqq n_B^\sigma$ for fixed σ.

From the sketch given in Fig. 1 we see that the zeros $E_{k\lambda}^\sigma$ independently of k are separated from one another by the zeros of the nominators P_A and P_B, i. e.

$$E_{k1}^\sigma \leqq 0,$$
$$0 \leqq E_{k2}^\sigma \leqq V_0(1 - n_B^{-\sigma}),$$
$$V_0(1 - n_A^{-\sigma}) \leqq E_{k3}^\sigma \leqq V_0, \quad (14)$$
$$V_0 \leqq E_{k4}^\sigma$$

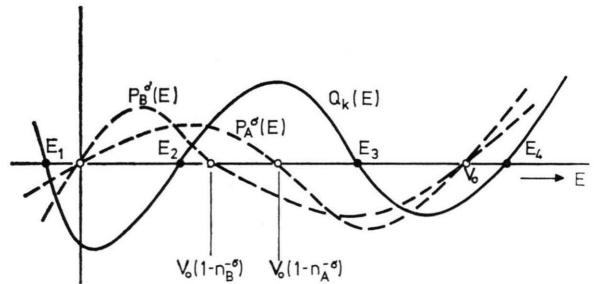holds; there are no zeros between $V_0(1 - n_B^{-\sigma})$ and $V_0(1 - n_A^{-\sigma})$.

Fig. 1. Plot of $Q_k(E)$ (in solid line) and of $P_A^\sigma(E)$ and $P_B^\sigma(E)$ (in dashed lines). As is seen from the figure the zeros E_λ of $Q_k(E)$ are separated by the zeros of $P_A^\sigma(E)$ and $P_B^\sigma(E)$, respectively. Moreover the coefficients $A_{k\lambda}^{A\sigma}$ [see Eq. (12)] are positive for all values of k.

Moreover, we may take from Fig. 1 that all $A_{k\lambda}^{A\sigma}$ are positive and may be written as

$$A_{k\lambda}^{A\sigma} = |P_A^\sigma(E_{k\lambda}^\sigma)|/|Q_k^{\sigma\prime}(E_{k\lambda}^\sigma)|, \quad (15)$$

which will be important for later use.

5. Calculation of the Correlation Functions

In order to draw thermodynamical conclusions from the Greens functions we conveniently may use the spectral theorem, which for the case of $\langle n_j^C \rangle$, where $C = A$ or B, respectively, reads

$$n_C^\sigma = \langle c_{j(c)\,\sigma}^+ c_{j(c)\,\sigma} \rangle \quad (16)$$
$$= i \lim_{\varepsilon \to +0} \int_{-\infty}^{+\infty} dE\, \frac{G_{l=0}^{CC\sigma}(E + i\varepsilon) - G_{l=0}^{CC\sigma}(E - i\varepsilon)}{e^{\beta(E-\mu)} + 1}.$$

As

$$G_{l=0} = \sum_k G_k \quad (17)$$

holds due to (7 b), this may be written in the form

$$n_C^\sigma = \frac{i}{2\pi} \frac{2}{N} \sum_{k\lambda} A_{k\lambda}^{C\sigma}$$

$$\times \lim_{\varepsilon \to +0} \int_{-\infty}^{+\infty} \frac{dE}{e^{\beta(E-\mu)}+1} \left\{ \frac{1}{E+i\,\varepsilon-E_{k\lambda}^\sigma} - \frac{1}{E-i\,\varepsilon-E_{k\lambda}^\sigma} \right\}$$

$$= \frac{2}{N} \sum_{k} \int_{-\infty}^{+\infty} \frac{dE}{e^{\beta(E-\mu)}+1} \, J_k^{C\sigma}(E), \quad (18)$$

where due to Dirac's identity the spectral density in momentum space $J_k^{C\sigma}(E)$ is given by

$$J_k^{C\sigma}(E) = \sum_\lambda A_{k\lambda}^{C\sigma} \delta(E - E_{k\lambda}^\sigma). \quad (19)$$

According to Eq. (15) this may be written as

$$J_k^{C\sigma}(E) = \sum_\lambda \left| P_C^\sigma(E_{k\lambda}^\sigma) \right| \delta(E - E_{k\lambda}^\sigma) / \left| Q_k^{\sigma'}(E_{k\lambda}^\sigma) \right| \quad (20)$$

and because of Fig. 1 we further find

$$J_k^{C\sigma}(E) = \left| P_C^\sigma(E) \right| \delta \left(Q_k^\sigma(E) \right). \quad (21)$$

It is this formula which will be brought together with certain sums over the free electron states in the following. At first we note that due to Eq. (14) $\delta \left(Q_k^\sigma(E) \right) \equiv 0$ holds for

$$V_0(1 - n_B^{-\sigma}) < E < V_0(1 - n_A^{-\sigma}).$$

Outside this interval in consequence of (11 c) it is of the form

$$\delta(\alpha\beta - T_k^2 \gamma_1 \gamma_2)$$

and may be resolved into δ-functions, which are linear in T_k with the final result

$$J_k^{A\sigma}(E) = \frac{1}{2} \sqrt{\frac{E - V_0(1 - n_A^{-\sigma})}{E - V_0(1 - n_B^{-\sigma})}}$$

$$\times \left\{ \delta \left(T_k - \tau(E) \right) + \delta \left(T_k + \tau(E) \right) \right\}, \quad (22\,a)$$

where $\tau(E)$ is given by

$$\tau(E) = \frac{E(E - V_0)}{\sqrt{\left(E - V_0(1 - n_A^{-\sigma}) \right) \left(E - V_0(1 - n_B^{-\sigma}) \right)}}. \quad (22\,b)$$

Applying the formula

$$\delta(a - x) = \int_{-\infty}^{+\infty} dt \, \delta(a - t) \, \delta(t - x) \quad (23)$$

we may further transform

$$J_k^{A\sigma}(E) = \frac{1}{2} \sqrt{\frac{E - V_0(1 - n_A^{-\sigma})}{E - V_0(1 - n_B^{-\sigma})}} \quad (24\,a)$$

$$\times \int_{-\infty}^{+\infty} dt \{ \delta(t - T_k) + \delta(t + T_k) \} \, \delta \left(t - \tau(E) \right)$$

for $\quad E < V_0(1 - n_B^{-\sigma}) \quad$ or $\quad E > V_0(1 - n_A^{-\sigma})$

and $\quad J_k^{A\sigma}(E) \equiv 0 \quad (24\,b)$

for $\quad V_0(1 - n_B^{-\sigma}) \leq E \leq V_0(1 - n_A^{-\sigma})$,

and the same expression with A and B interchanged for $J_k^{B\sigma}(E)$. Now let us consider the sum

$$(2/N) \sum_k J_k^{A\sigma}(E)$$

occuring in Eq. (18) and denote it by $\varrho_A^\sigma(E)$. From Eq. (24) we find

$$\varrho_A^\sigma(E) = 0$$

for $\quad V_0(1 - n_B^{-\sigma}) \leq E \leq V_0(1 - n_A^{-\sigma}) \quad (25\,a)$

and $\quad \varrho_A^\sigma(E) = \sqrt{\dfrac{E - V_0(1 - n_A^{-\sigma})}{E - V_0(1 - n_B^{-\sigma})}} \quad (25\,b)$

$$\times \int_{-\infty}^{+\infty} dt \{ g^+(t) + g^-(t) \} \, \delta \left(t - \tau(E) \right)$$

$$= \sqrt{\frac{E - V_0(1 - n_A^{-\sigma})}{E - V_0(1 - n_B^{-\sigma})}} \left\{ g^+\left(\tau(E) \right) + g^-\left(\tau(E) \right) \right\}$$

otherwise, where we have used functions $g^\pm(t)$ defined by

$$g^\pm(t) = \frac{1}{N} \sum_k \delta(t \pm T_k). \quad (26)$$

Introducing $\varrho_A^\sigma(E)$ into Eq. (18) finally yields

$$n_A^\sigma = \int_{-\infty}^{-\infty} dE \, \frac{\varrho_A^{\sigma'}E)}{e^{\beta(E-\mu)}+1} \quad (27)$$

and identifies $\varrho_A^\sigma(E)$ as the effective density of states of the pseudo-particles in the splitted bands; in analogy n_B^σ is coupled to $\varrho_B^\sigma(E)$, which is defined by (25) when A and B are interchanged.

In order to evaluate Eq. (27) we must investigate the functions $g^\pm(t)$. As can be shown these functions are connected by

$$g^+(t) + g^-(t) = g(t); \quad (28)$$

$g(t)$ is the density of states function of the free electrons in the crystal lattice, which is defined by

$$g(t) = \frac{1}{N} \sum_k \delta(t - T_k), \quad (29)$$

where in this case k runs over the Brillouin zone of the original lattice and not over that of the sub-lattice only. This function is well known for the s.c. and the b.c.c. lattice [9]. We shall not reproduce the proof of Eq. (28) in this paper [12], but we shall see in the subsequent section that this result is very suggestive in the light of some simple limiting cases discussed there.

6. Discussion and Specialization for Antiferromagnetism

In this paper we are mainly interested in the temperature $T = 0$ properties of the Hubbard model. We therefore may simplify the formula (27) to

$$n_C^\sigma = \int_{-\infty}^{\mu} dE\, \varrho_C^\sigma\,(E) \qquad (30)$$

(where C is A or B) and the final result for $\varrho_A^\sigma(E)$ following from (25) and (28) is

$$\varrho_A^\sigma(E) = \begin{cases} 0: & V_0(1-n_B^{-\sigma}) \leqq E \leqq V_0(1-n_A^{-\sigma}) \\[2mm] \sqrt{\dfrac{E - V_0(1-n_A^{-\sigma})}{E - V_0(1-n_B^{-\sigma})}} \\[2mm] g\left(\dfrac{E(E-V_0)}{\sqrt{(E-V_0(1-n_A^{-\sigma}))\,(E-V_0(1-n_B^{-\sigma}))}}\right) \\[2mm] \text{otherwise;} \end{cases} \qquad (31)$$

$\varrho_B^\sigma(E)$ is given by interchanging A and B in Equation (31).

Therefore Eqs. (30) and (31) are a system of coupled nonlinear equations, the solutions of which yield selfconsistent values for the densities of the spin up and down electrons in the different sublattices.

Before we turn to the case of antiferromagnetic ordering we shall consider two simple limiting cases, which will help to clarify the meaning of these equations.

At first let us investigate the limit of vanishing Coulomb repulsion $V_0 = 0$, which clearly must give the results for the non-interacting model.

Introducing this limit into Eq. (31) and observing the fact, that $g(t)$ is a symmetric function of its argument, we immediately get

$$\varrho_C^\sigma(E) = g(E). \qquad (32)$$

This is in fact the density of states of non-interacting electrons, which is independent of their spin orientation and of the sublattice and, therefore, leads to no magnetic ordering. Here we have a simple check of Eq. (28) because the function $\tau(E)$ introduced in Eq. (22 c) reduces to $|E|$ and therefore (32) is true iff (28) holds.

For the second limiting case we assume ferromagnetic ordering by postulating

$$n_A^\sigma = n_B^\sigma = n^\sigma. \qquad (33)$$

In fact, as we have clarified in Section 2, the AB-hypothesis of this paper comprehends Hubbard's ferromagnetic hypothesis and, therefore, (33) is a legitimate postulate.

With it the difference of the two sublattices vanishes and we get

$$\varrho^\sigma(E) = g\left(\frac{E(E-V_0)}{E - V_0(1-n^{-\sigma})}\right). \qquad (34)$$

This expression is exactly the density of states of the pseudo-particles, which Hubbard finds in his paper [Eqs. (62) and (63) of [1]], as it must be under the special assumption of Equation (33). Again (34) is true if and only if Eq. (28) holds.

Also in the strong coupling limit $T \to 0$ we find the correct result for the spectral density, as is seen most conveniently from Equation (20).

Now let us contemplate the case of antiferromagnetism with the aim of investigating whether the Eqs. (30) and (31) have selfconsistent solutions for antiferromagnetic ordering, which is the main goal of the present paper. That means, is the Hubbard approximation together with the AB-hypothesis sensitive enough to reproduce the antiferromagnetic groundstate, which according to [4] is found for a suitable range of electron concentrations (mainly $N_e \approx N$) and coupling constants V_0.

For antiferromagnetism the total electron density has the full translation symmetry, i. e.

$$n_A^\uparrow + n_A^\downarrow = n_B^\uparrow + n_B^\downarrow = n_e = N_e/N \qquad (35)$$

and the local magnetization alternates, i. e.

$$n_A^\uparrow - n_A^\downarrow = 2\,s_A^Z = -2\,s_B^Z = -n_B^\uparrow + n_B^\downarrow \qquad (36)$$

holds. Therefore we have the relation

$$n_A^\sigma = n_B^{-\sigma}. \qquad (37)$$

This assumption is consistent with Eqs. (30) and (31) because the symmetry of Eq. (37) is reflected also in the density of states by

$$\varrho_B^\sigma = \varrho_A^{-\sigma} = \varrho^{-\sigma}, \qquad (38)$$

and therefore we may confine our further attention to the A-sublattice — say.

If we introduce m for the difference in the occupation of the two spin directions

$$m = 2\,s_A^Z = n_A^\uparrow - n_A^\downarrow \qquad (39)$$

the transcendental Eqs. (30) and (31) may be written as

$$\binom{n_e}{m} = \int_{-\infty}^{\mu} dE\{\varrho^\uparrow\,(n_e, m, E) \pm \varrho^\downarrow\,(n_e, m, E)\} \qquad (40)$$

where the plus-sign refers to n_e and the minus-sign to m.

As n_e and V_0 are given parameters, the two equations involved in (40) are to be used for a determination of the chemical potential μ as well as of the magnetization m.

The first thing we note is that $m = 0$, i. e. $n^\uparrow = n^\downarrow$, is a solution of (40) independent of n_e and V_0.

This solution is characterized by the absence of magnetic ordering and is identical with the unmagnetic solution, which is the only existing one under Hubbard's ferromagnetic hypothesis.

Moreover the symmetry of the Hamiltonian against reflections of all spin-directions has its counterpart in the property of (40) that for (μ, m) being a solution also $(\mu, -m)$ solves the equations. Therefore we may restrict our further attention to the case $m \geqq 0$, i. e. $n_A^{\uparrow} \geqq n_A^{\downarrow}$.

The formulae (40) may be simplified with the following result:

$$n_e = \int_{-\infty}^{\mu} dE \left| 2 E - V_0 (2 - n_e) \right| \varrho_{\text{eff}}(E), \quad (41 \text{ a})$$

$$m \left\{ 1 + V_0 \int_{-\infty}^{\mu} dE \, \varLambda(E) \, \varrho_{\text{eff}}(E) \right\} = 0, \quad (41 \text{ b})$$

where we have introduced an effective density of states

$$\varrho_{\text{eff}}(E) = \begin{cases} 0 : \frac{1}{2} V_0 (2 - n_e - m) \leqq E \leqq \frac{1}{2} V_0 (2 - n_e + m) \\ [[E - \frac{1}{2} V_0 (2 - n)]^2 - (\frac{1}{2} V_0)^2 m^2]^{-1/2} \\ g \left(\frac{E (E - V_0)}{[[E - \frac{1}{2} V_0 (2 - n)]^2 - (\frac{1}{2} V_0)^2 m^2]^{1/2}} \right) \\ \qquad : \text{ otherwise} \end{cases} \quad (42)$$

and $\varLambda(E)$ is a sign-function, given by

$$\varLambda(E) = \begin{cases} -1 : & E < \frac{1}{2} V_0 (2 - n - m), \\ +1 : & E > \frac{1}{2} V_0 (2 - n + m), \end{cases} \quad (43)$$

i. e. -1 in the lower and $+1$ in the upper of the two splitted bands of the pseudo-particles.

From Eq. (41 b) we see again that $m = 0$ is a permanent solution of the problem; for an antiferromagnetic solution with $m > 0$, however, the part of (41 b) written in brackets must vanish.

It is the crucial question of this paper whether this condition may be fulfilled together with Eq. (41 a) at least for a certain range of values for n_e and V_0. This will be discussed by a mixture of computational and analytical arguments in the following.

7. Investigation for Antiferromagnetic Solutions

Let us begin the discussion of these equations for the case of the neutral model with $n_e = 1$, which due to the results of NAGAOKA [4] is most likely to yield antiferromagnetic order in the ground state.

It has been proven as a rigorous result which also holds for the approximation of Eq. (41) that for the neutral model the chemical potential is given by

$$\mu = V_0/2. \quad (44)$$

This means, exactly the lower one of the two splitted band is completely filled up with pseudo-particles and the condition for antiferromagnetism derives from Eq. (41 b) as

$$1 = V_0 \int_{-\infty}^{\frac{1}{2} V_0 (1 - m)} dE \left[(E - \frac{1}{2} V_0)^2 - (\frac{1}{2} V_0 m)^2 \right]^{1/2}$$
$$g \left(\frac{E (E - V_0)}{[(E - \frac{1}{2} V_0)^2 - (\frac{1}{2} V_0 m)^2]^{1/2}} \right); \quad (45)$$

$\frac{1}{2} V_0 (1 - m)$ is just the upper bound of the lower pseudo-particle band.

In Fig. 2 we have plotted the result of computations of the right hand side of this formula for the s.c. lattice as a function of m for three values the parameter V_0. As is seen from the figure, no solution of (45) exists for these V_0.
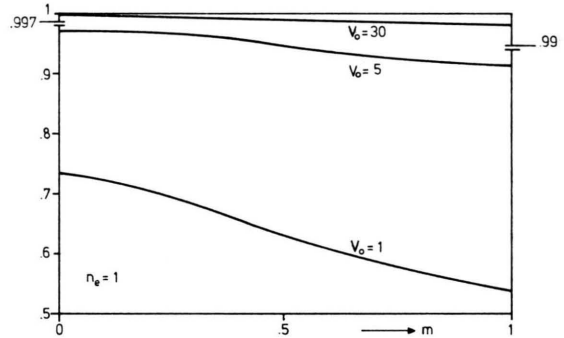

Fig. 2. Plot of the right hand side of Eq. (45) for the neutral model ($n_e = 1$) and $V_0 = 1$, 5, and 30, the latter one in a modified scale. As is seen these functions are less 1 everywhere thus excluding a solution of Equation (45).

Moreover, let us inspect formula (45) for the cases of $m = 0$ and $m = 1$, respectively. In these cases we may substitute for the argument of the single particle density g and get for the right hand side of Eq. (45)

$$\frac{1}{2} V_0 \int_{-\infty}^{+\infty} d\varepsilon \, \frac{g(\varepsilon)}{\sqrt{\varepsilon^2 + (\frac{1}{2} V_0)^2}} \quad (46 \text{ a})$$

for $m = 1$ and

$$V_0 \int_{-\infty}^{+\infty} d\varepsilon \, \frac{g(\varepsilon)}{\sqrt{\varepsilon^2 + V_0^2}} \quad (46 \text{ b})$$

for $m = 0$, respectively.

Integrals of this type are well known from [7] and have been discussed in length in this paper. What we may take from this discussion is that both integrals are less one and tend to 1 just in the limit of $V_0 \to \infty$.

Therefore we may conclude that Eq. (45) does not possess a solution for finite V_0. This means, apart from the strong coupling limit $V_0 \to \infty$, in which a large number of magnetic structures are degenerated, the Hubbard decoupling does not lead to antiferromagnetism for a neutral nearest neighbour Hubbard model in the s.c. lattice (but the arguments given above hold also for the b.c.c. lattice).

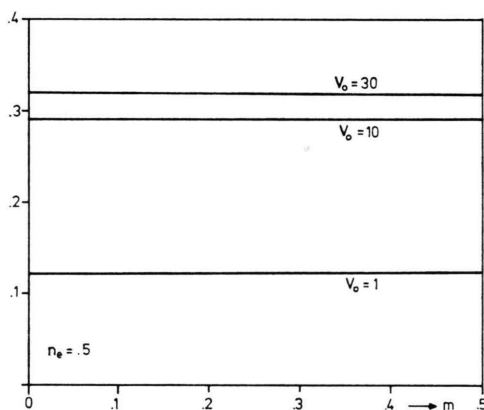In Fig. 3 the results of computations of the in-

Fig. 3. Plot of $-V_0 \times$ *the integral* in Eq. (41 b) with μ computed from Eq. (41 a); $n_e = 0.5$ and $V_0 = 1$, 10, and 30. As the curves are less 1 everywhere there exist no solutions of Eq. (41 b) apart from the trivial ($m = 0$) one.

tegral in Eq. (41 b) are plotted for the case of $n_e = 1/2$. Here the results miss the condition for antiferromagnetic ordering still more than in the neutral model. Therefore, together with the arguments of NAGAOKA [4] we are led to conject that the Hubbard decoupling of the nearest neighbour model (at least in cubic AB-lattices) does not lead to an antiferromagnetic ordering in the same way, as it does not lead to ferromagnetism under the ferromagnetic hypothesis.

Therefore the investigation of the band splitting by such an ordering is purely academic, because it is not based on selfconsistent calculations.

The only selfconsistent solution resulting from Hubbard's decoupling both with respect to ferromagnetism and to antiferromagnetism is the paramagnetic one. As we have shown in a preceeding paper [13] this solution leads to an approximation of the groundstate energy which for the neutral model is not so good than that one resulting from antiferromagnetic single particle theories, but is interesting for the fact that apparently part of the effects of magnetic order is simulated by the correlations in the paramagnetic state, which are involved in Hubbard's approach.

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[12] The simplest way of proving Eq. (28) is to show that the zone of the lattice is twice the zone of the sublattice. Moreover for each k out of the zone of the sublattice $T_k \geqq 0$, and there is a vector k' in the zone of the lattice for which $T_k = -T_k$ holds.
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