Electron Correlation in Narrow Energy Bands. I. The Two-Pole Approximation in a Narrow S Band

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An improved version of Hubbard's treatment of correlation in a nondegenerate narrow band is obtained by the use of a new Green's-function decoupling scheme. The resulting one-electron Green's function has two poles on the real axis corresponding to a splitting of the electron bands due to the strong correlations between electrons on the same site. This is the same result that Hubbard obtained, but in our case the poles are shifted and their positions agree with the results of Harris and Lange, who used a moment technique. The theory is applied to a simple cubic lattice with nearest-neighbor interaction, and the lattice is found to be ferromagnetic in the strongly correlated limit for a sufficiently large number of electrons per atom. An examination of the low-density limit shows that the two-pole approximation does not reduce to Kanamori's T-matrix result, a failing which it shares with Hubbard's theory. A method is outlined for improving the theory so as to give the correct low-density result. In addition, the possibility of obtaining a minimum principle for the theory is explored.

I. INTRODUCTION

We consider here the problem of correlation in a narrow band with the second-quantized Hamiltonian between Wannier states:

$$H=U\sum_i n_{i\uparrow}n_{i\downarrow}+\sum_{i,\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}. \quad (1)$$

This model, often called the Hubbard[1] Hamiltonian, contains in its simplest form the competition between the Coulomb interaction U between electrons on the same site, tending toward magnetic alignment, and the hopping term t_{ij}, which tends to destroy the single-site correlations. The correlation problem was considered by Hubbard,[1] Kanamori,[2] and Gutzwiller[3] in 1963; we follow most closely the work of Hubbard. In Hubbard I a Green's-function decoupling scheme was used, which most carefully treated the correlations on a single site and which resulted in a one-particle Green's function with two poles on the real axis. Hubbard's result for the case of $t_{ij}\ll U$ gave no ferromagnetism for a simply shaped density of states. Harris and Lange,[4] by looking at the moments of individual peaks in the spectral function, found that there should be an additional energy shift, which makes the ferromagnetic state more likely to stablize. This result was in line with the work of Nagaoka,[5] who showed that for certain nearest-neighbors models and for $U\rightarrow\infty$ the almost half-filled band was ferromagnetic. There were also spin-wave calculations by Roth[6] and by Edwards[7] which suported Nagaoka's conclusion.

In this paper, we apply to the problem a decoupling scheme which improves upon Hubbard's procedure. A preliminary account of this work has appeared.[8] The scheme is essentially identical to that proposed by Linderberg and Öhrn[9]; they showed that it gives the correct result for the two-site problem. There is also a strong relationship to the work of Rowe.[10] We obtain a result which has, as in Hubbard's calculations, two poles in the one-particle Green's function and which has the positions and moments of the poles given by expressions which, in the strongly correlated limit, reduce to those of Harris and Lange,[4] and of Esterling and Lange.[11] Hubbard and Linderberg[12] also obtained these expressions. We reduce the results to a form in which all expressions can be evaluated self-consistently; then we apply the theory to the simple cubic nearest-neighbor case in the strongly correlated limit.

A defect of the two-pole approximation is found: it does not reduce to the correct low-density result obtained by Kanamori.[2] We show that an approximation analogous to the "resonance broadening" correction obtained in Hubbard III[1] corrects the deficiency and so leads to an improved theory. In the second paper of this series, we shall apply the improved version to the case of one reversed spin in a fully aligned band.

In Sec. VII we discuss the possibility of obtaining a minimum principle related to our method. This would be a stronger statement than the stationary principle already obtained.[8]

II. PRELIMINARIES

We adopt the formalism of retarded and advanced Green's functions,[1] following, in the main, Zubarev.[13]

[1] J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963); **281**, 401 (1964). We shall refer to these as Hubbard I and III.
[2] J. Kanamori, Progr. Theoret. Phys. (Kyoto) **30**, 276 (1963).
[3] M. C. Gutzwiller, Phys. Rev. Letters **10**, 5 (1963); Phys. Rev. **137**, A1726 (1965).
[4] A. B. Harris and R. V. Lange, Phys. Rev. **157**, 295 (1967).
[5] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[6] L. M. Roth, Phys. Chem. Solids **28**, 1549 (1967); J. Appl. Phys. **39**, 474 (1968).
[7] D. M. Edwards, Proc. Roy. Soc. (London) **A300**, 373 (1963); J. Appl. Phys. **39**, 481 (1968).
[8] L. M. Roth, Phys. Rev. Letters **20**, 1431 (1968). Note that Eqs. (11) and (17) are in error. For the correct expressions see Eqs. (21) and (59) in this article.
[9] J. Linderberg and Y. Öhrn, Chem. Phys. Letters **1**, 295 (1967).
[10] D. Rowe, Rev. Mod. Phys. **40**, 153 (1968).
[11] D. M. Esterling and R. V. Lange, Rev. Mod. Phys. **40**, 796 (1968).
[12] J. Hubbard and J. Linderberg, Harwell Progress Report No. AERE-PR/TP 15 (1968).
[13] D. N. Zubarev. Usp. Fiz. Nauk **71**, 116 (1960) [English Transl.: Soviet Phys. Usp. **3**, 320 (1960)].

Since we shall be interested in the Fourier transform of the time-dependent Green's function, it is convenient to define this directly as

$$\langle\langle A;B\rangle\rangle_\omega=\frac{1}{2\pi i}\oint\left\langle\left[\frac{1}{z-H}A\frac{1}{\omega+z-H},B\right]_+\right\rangle dz, \quad (2)$$

where the contour encircles the real axis but excludes ω, which has a small positive (negative) imaginary part for the retarded (advanced) Green's function. This definition is equivalent to the usual one except for a factor $1/2\pi$, which we omit. The equation of motion is readily obtained from Eq. (2):

$$\omega\langle\langle A;B\rangle\rangle=\langle[A,B]_+\rangle+\langle\langle[A,H];B\rangle\rangle. \quad (3)$$

The thermal average $\langle BA\rangle$ is obtained now from the relation[13]

$$\langle BA\rangle=\mathfrak{F}_\omega\langle\langle A;B\rangle\rangle\equiv\frac{1}{2\pi i}\oint f(\omega)\langle\langle A,B\rangle\rangle_\omega d\omega, \quad (4)$$

where $f(\omega)$ is the Fermi function and the contour encircles the real axis. We use a notation due to Hamann.[14]

Let us now outline Hubbard's truncation procedure[1] for the Green's-function equations of motion. We need the commutators

$$[c_{i\sigma},H]=Un_{i-\sigma}c_{i\sigma}+\sum_j t_{ij}c_{j\sigma}, \quad (5)$$

$$[n_{-\sigma}c_{i\sigma},H]=Un_{i-\sigma}c_{i\sigma}+\sum_j t_{ij}(n_{i-\sigma}c_{j\sigma}+c_{i-\sigma}^\dagger c_{j-\sigma}c_{i\sigma}-c_{j-\sigma}^\dagger c_{i-\sigma}c_{i\sigma}). \quad (6)$$

Through Eq. (3), the first of these equations relates $G_{ij\sigma}=\langle\langle c_{i\sigma};c_{j\sigma}^\dagger\rangle\rangle$ to $\Gamma_{ij\sigma}=\langle\langle n_{i-\sigma}c_{i\sigma};c_{j\sigma}^\dagger\rangle\rangle$, and the second relates Γ to itself plus some more complicated Green's functions. Hubbard approximates the last term in Eq. (6) by replacing the $-\sigma$ quantities by their average values, whereupon the last two terms in parentheses cancel and we have

$$[n_{i-\sigma}c_{i\sigma},H]\cong U_{n-\sigma}c_{i\sigma}+\langle n_{i-\sigma}\rangle\sum_j t_{ij}c_{j\sigma}. \quad (7)$$

Thus the equation-of-motion sequence for G and Γ terminates. Hubbard assumes that $\langle n_{i-\sigma}\rangle=n_\sigma$ is independent of i. Then the results can be recast in terms of Bloch functions, for which the operators are

$$c_{\mathbf{k}\sigma}=\frac{1}{\sqrt{N}}\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i}c_{i\sigma}, \quad (8)$$

and the Green's function is given by

$$\langle\langle c_{\mathbf{k}\sigma},c_{\mathbf{k}\sigma'}^\dagger\rangle\rangle=G_{\mathbf{k}\sigma}\delta_{\mathbf{k}\mathbf{k}'}=\frac{\delta_{\mathbf{k}\mathbf{k}'}}{F(\omega)-\epsilon_{\mathbf{k}}},$$
$$F^{-1}(\omega)=\frac{1-n_{-\sigma}}{\omega}+\frac{n_{-\sigma}}{\omega-U}(\text{Hubbard}). \quad (9)$$

Here $\epsilon_{\mathbf{k}}$ is the band energy,

$$\epsilon_{\mathbf{k}}=\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i}t_{i0}, \quad (10)$$

and we assume that t_{00} is zero so that the center of gravity of the band is the zero of energy. In the limit in which U is very large and when we look in the vicinity of $\omega=0$, we neglect the second term of F^{-1} and find that the pole of G is at $(1-n_{-\sigma})\epsilon_{\mathbf{k}}$, so that the presence of the $-\sigma$ spins effectively narrows the σ spin band, but does not change the center of gravity of the band.

As mentioned in the Introduction, Harris and Lange[4] showed that the center of gravity of the band should in fact be shifted,[15] and the author found this to be true for the special case of a fully aligned band.[6] Figure 1 shows how this shift can be encouraging for the occurrence of ferromagnetism for the fully aligned case.

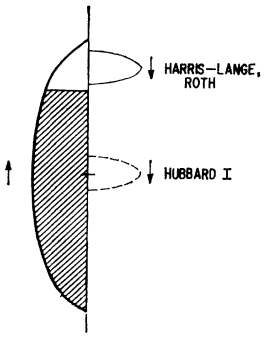

FIG. 1. For the fully aligned partly filled band, the Hubbard I result gives a down-spin band, presumed empty, which has its center of gravity at the center of the band; for the band shape shown, it is below the Fermi level, so the state is obviously not stable. The band shift found by Harris and Lange (Ref. 4) and the author (Ref. 6) can push the down-spin band up above the Fermi level, thus making it possible for the ferromagnetic state to be stable.

III. DECOUPLING PROCEDURE

We now review and present in more detail the application of our decoupling scheme[8–10,12] to this model. Basically, in any equation of motion[16] or Green's-function[17] decoupling scheme, we seek a set of (here) fermion annihilation operators for which the equation-of-motion sequence [e.g., Eqs. (5) and (6)] terminates

[14] D. Hamann, Phys. Rev. **158**, 570 (1967).

[15] R. A. Tahir-Kheli and H. S. Jarrett, Phys. Letters **27A**, 485 (1968), pointed out that this shift can be obtained approximately for $U\to\infty$ by neglecting the last term in the parentheses of Eq. (6), arguing that it involves double occupancy on one site, and truncating the second term, which gives the part of the shift corresponding to the first term of our Eq. (21).

[16] H. Suhl and N. R. Werthamer, Phys. Rev. **122**, 359 (1961).

[17] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).

in some approximation. Thus we seek a relationship of the from

$$[A_n,H]=\sum_m K_{nm}A_m, \tag{11}$$

where we have changed the notation slightly from the Ref. 8 to distinguish the indices from those of Wannier states. Rather than replace various operators on the left-hand side of this equation by their expectation values in order to terminate the sequence, we use the following prescription. We anticommute both sides of Eq. (11) with $A_p\dagger$, where A_p is a member of the set, and take either the expectation value in the ground state or the thermal average of both sides. Thus we write

$$\langle[[A_n,H],A_p{}^\dagger]_+\rangle=\sum_m K_{nm}\langle[A_m,A_p{}^\dagger]_+\rangle, \tag{12}$$

or, if we define the energy and normalization matrices as

$$E_{nm}=\langle[[A_n,H],A_m\dagger]_+\rangle, \tag{13}$$

$$N_{nm}=\langle[A_n,A_m\dagger]_+\rangle, \tag{14}$$

we have, in matrix notation,

$$E=KN. \tag{15}$$

Thus, provided that we can evaluate the matrices E_{nm} and N_{nm}, and provided N_{nm} is nonsingular, we can determine the matrix K_{nm} and can then decouple the equations of motion with the desired set of operators.

Since the eigenvalues of K correspond to the singularities in a Green's function, it is essential that they be real. It can be shown that E is Hermitian if the brackets are the expectation value in a true eigenstate of the system. N is readily shown to be Hermitian, and we further require that N be positive definite. Then the characteristic equation for K, if we transform the matrices so as to diagonalize N, is

$$\begin{aligned}0&=\det(E_{nm}N_m{}^{-1}-\omega\delta_{nm})\\&=\det[N_n{}^{1/2}(N_n{}^{-1/2}E_{nm}N_m{}^{-1/2}-\omega\delta_{nm})N_m{}^{-1/2})\\&=\det[N_n{}^{-1/2}E_{nm}N_m{}^{-1/2}-\omega\delta_{nm}],\end{aligned} \tag{16}$$

i.e., it is the same as that of a Hermitian matrix; thus the eigenvalues of K are real. An additional reason to require E to be Hermitian is that $E^\dagger$ is what would be used in truncating equations of motion for $A_m{}^\dagger$. In Eq. (26) below, $E^\dagger$ would appear if we had begun with the alternative Green's function equation of motion in which the last term of Eq. (3) is replaced by $\langle\langle A,[B,H]\rangle\rangle$.

However, if the matrix elements are not in an exact eigenstate of H, the Hermiticity of E is not guaranteed[18] and each case must be investigated on its merits. We remark here that Rowe[12] averages his equivalent of E with its Hermitian conjugate. In the present example, E is, in fact, Hermitian, so there is no problem. We also remark that Linderberg and Öhrn[9] choose their N matrix to be diagonal.

Now, to apply the result to our case, we first note that due to translational invariance E, N, and K will certainly be diagonal in $\mathbf{k}$, so we need not put $\mathbf{kk}'$ indices in. We are assuming only spatially uniform solutions at this point; thus we will not discuss antiferromagnetic states. If we choose for the A_n the Bloch states $c_\mathbf{k}$, our "matrices" are 1×1 for each spin, N is just 1, and

$$\begin{aligned}E_{\mathbf{k}\sigma}&=\langle[[c_{\mathbf{k}\sigma},H],c_{\mathbf{k}\sigma}\dagger]_+\rangle\\&=\epsilon_\mathbf{k}+n_{-\sigma}U\ \text{(Hartree Fock)},\end{aligned} \tag{17}$$

where $n_{-\sigma}=\langle n_{i-\sigma}\rangle$ is the average number of $-\sigma$ spins on a site. This is simply the Hartree-Fock result.

If we now use the Hubbard choice of operators, we have $A_{1\mathbf{k}\sigma}=c_{\mathbf{k}\sigma}$ [Eq. (8)] and

$$A_{2\mathbf{k}\sigma}=d_{\mathbf{k}\sigma}=\frac{1}{N}\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i}n_{i-\sigma}c_{i\sigma}. \tag{18}$$

We now have 2×2 matrices for each spin for both $E_{\mathbf{k}\sigma}$ and $N_{\mathbf{k}\sigma}$. We calculate the double commutators in Eqs. (14) and (15); these are given by

$$E_{\mathbf{k}\sigma}=\begin{bmatrix}\epsilon_\mathbf{k}+Un_{-\sigma} & (U+\epsilon_\mathbf{k})n_{-\sigma}\\(U+\epsilon_\mathbf{k})n_{-\sigma} & Un_{-\sigma}+\epsilon_\mathbf{k}n_{-\sigma}{}^2+n_{-\sigma}(1-n_{-\sigma})W_{\mathbf{k}-\sigma}\end{bmatrix}, \tag{19}$$

$$N_{\mathbf{k}\sigma}=\begin{bmatrix}1 & n_{-\sigma}\\n_{-\sigma} & n_{-\sigma}\end{bmatrix}, \tag{20}$$

where

$$\begin{aligned}n_\sigma(1-n_\sigma)W_{\mathbf{k}\sigma}=&-\sum_{j\neq0}t_{0j}\langle c_{0\sigma}{}^\dagger c_{j\sigma}(1-n_{0-\sigma}-n_{j-\sigma})\rangle\\&+\sum_{j\neq0}t_{0j}e^{i\mathbf{k}\cdot\mathbf{R}_j}\{(\langle n_{j\sigma}{}^\dagger n_{0\sigma}\rangle-n_\sigma{}^2)\\&+\langle c_{j\sigma}{}^\dagger c_{j-\sigma}c_{0-\sigma}{}^\dagger c_{0\sigma}\rangle-\langle c_{j\sigma}{}^\dagger c_{j-\sigma}{}^\dagger c_{0-\sigma}c_{0\sigma}\rangle\}.\end{aligned} \tag{21}$$

We now wish to construct the Green's functions. If we substitute Eq. (11) into Eq. (3), in general we have

$$\omega\langle\langle A_n;B\rangle\rangle=\langle[A_n,B]_+\rangle+\sum_m K_{nm}\langle\langle A_m;B\rangle\rangle, \tag{22}$$

or, inverting,

$$\langle\langle A_n;B\rangle\rangle=\sum_m \tilde{G}_{nm}\langle[A_m,B]_+\rangle, \tag{23}$$

where

$$\tilde{G}=(\omega+i\epsilon-K)^{-1}=N[N(\omega+i\epsilon)-E]^{-1}. \tag{24}$$

In particular, if $B=A_m\dagger$ with A_m a member of the set, we can define a Green's-function matrix G such that

$$\langle\langle A_n;A_m\dagger\rangle\rangle=G_{nm}. \tag{25}$$

[18] As an example, consider the exact $\{A_n\}$ set $\{|n\rangle\langle0|\}$, where $|0\rangle$ is the N-particle ground state and $|n\rangle$ is an $(N-1)$-particle excited state. Then we know that the K matrix is $(\epsilon_0-\epsilon_n)\delta_{nm}$. However, if the expectation value is not in an eigenstate, N_{nm} need not be diagonal and, therefore $E_{nm}=(\epsilon_0-\epsilon_n)N_{nm}$ need not be Hermitian.

Then, from Eqs. (23) and (24), we have

$$G=N[N(\omega+i\epsilon)-E]^{-1}N. \tag{26}$$

We can use Eqs. (19) and (20) to obtain the matrices $\tilde{G}$ and G for our case:

$$\tilde{G}_\sigma=\frac{1}{D_\sigma}\begin{bmatrix}\omega-U-W_{\mathbf{k}-\sigma} & U\\ n_{-\sigma}(\epsilon_{\mathbf{k}}-W_{\mathbf{k}-\sigma}) & \omega-\epsilon_{\mathbf{k}}\end{bmatrix}, \tag{27}$$

$$D_\sigma=(\omega-\epsilon_{\mathbf{k}})(\omega-U-W_{\mathbf{k}-\sigma})-Un_{-\sigma}(\epsilon_{\mathbf{k}}-W_{\mathbf{k}}), \tag{28}$$

$$G_\sigma=D_\sigma^{-1}\times\begin{bmatrix}\omega-U(1-n_{-\sigma})-W_{\mathbf{k}-\sigma} & n_{-\sigma}(\omega-W_{\mathbf{k}-\sigma})\\ n_{-\sigma}(\omega-W_{\mathbf{k}-\sigma}) & n_{-\sigma}[\omega-\epsilon_{\mathbf{k}}(1-n_{-\sigma})-n_{-\sigma}/W_{-\sigma}]\end{bmatrix}, \tag{29}$$

with G_{11} giving the one-particle Green's function. Also, Hubbard's $\Gamma_{\mathbf{k}}$ is given by G_{21}.

It is interesting to point out that, in Hubbard III the improved Green's function [Eqs. (58) and (59)] has the same functional form as our G_{11}, but with $W_{\mathbf{k}-\sigma}$ replaced by Ω_σ. We shall return to Hubbard III later, noting here that W and Ω_σ are quite different quantities.

To complete the definition of the Green's functions in our scheme, we must now evaluate the averages in Eqs. (19) and (20), namely, n_σ and $W_{\mathbf{k}\sigma}$. We can readily obtain n_σ from the one-particle Green's function by the use of Eq. (4):

$$n_\sigma=\frac{1}{N}\sum_{\mathbf{k}}\mathfrak{F}_\omega G_{11\sigma}(\mathbf{k}). \tag{30}$$

Similarly, in evaluating the first term of Eq. (21) for $n_\sigma(1-n_\sigma)W_{\mathbf{k}\sigma}$, we find that it can be expressed in terms of G_{11} and G_{12}:

$$-\sum_{j\neq 0}t_{0j}\langle c_{j\sigma}^\dagger c_{0\sigma}(1-2n_{0-\sigma})\rangle=-\frac{1}{N}\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}[\mathfrak{F}_\omega G_{11\sigma}(\mathbf{k})-2\mathfrak{F}_\omega G_{21\sigma}(\mathbf{k})], \tag{31}$$

where, on the left-hand side, we assume the angular brackets to be real and we assume inversion symmetry so that n_0 and n_j can be interchanged.

However, in evaluating the second part of Eq. (21), we encounter averages of the form $A_n^\dagger A_m^\dagger A_p A_q$, where A_n, etc., are members of our set. The first two terms in the square brackets are density and spin-correlation functions on two sites and the third is a "double-hop" correlation function. Rather than assuming that the averages factor, we shall make use of Green's functions whose right-hand members are of the form $A_n^\dagger A_m^\dagger A_p$. We write

$$\langle BA_n\rangle=\mathfrak{F}_\omega\sum_m\tilde{G}_{nm}\langle[A_m,B]\rangle \tag{32}$$

and then introduce four B functions:

$$B_1=N^{-1/2}\sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i}n_{i+j\sigma}c_{i\sigma}^\dagger, \tag{33}$$

$$B_2=N^{-1/2}\sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i}n_{i+j-\sigma}c_{i\sigma}^\dagger, \tag{34}$$

$$B_3=N^{-1/2}\sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i}c_{i+j\sigma}^\dagger c_{i+j-\sigma}^\dagger c_{i-\sigma}, \tag{35}$$

$$B_4=N^{-1/2}\sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i}c_{i+j\sigma}^\dagger c_{i+j-\sigma}^\dagger c_{i-\sigma}. \tag{36}$$

These should have labels $\mathbf{k}$, σ, j, which we suppress. B_1 and B_2 are needed (see below) to evaluate $\langle n_{j\sigma}n_{0\sigma}\rangle-n_\sigma^2$ and B_3 and B_4 for the remaining terms in the expression in Eq. (21). Firstly, we have

$$\langle n_{j\sigma}n_{0\sigma}\rangle=\frac{1}{N}\sum_{\mathbf{k}}\langle B_1c_{\mathbf{k}\sigma}\rangle. \tag{37}$$

For any of the B's we, can write

$$\frac{1}{N}\sum_{\mathbf{k}}\langle B_sc_{\mathbf{k}\sigma}\rangle=\frac{1}{N}\sum_{\mathbf{k}}\mathfrak{F}_\omega\tilde{G}_{11\sigma}\langle[c_{\mathbf{k}\sigma},B_s]_+\rangle+\frac{1}{N}\sum_{\mathbf{k}}\mathfrak{F}_\omega\tilde{G}_{12\sigma}\langle[d_{\mathbf{k}\sigma},B_s]_+\rangle. \tag{38}$$

For $s=1$ we have

$$[c_{\mathbf{k}\sigma},B_1]_+=n_\sigma-e^{i\mathbf{k}\cdot\mathbf{R}_j}\langle c_{0\sigma}^\dagger c_{j\sigma}\rangle, \tag{39}$$

$$[d_{\mathbf{k}\sigma},B_1]_+=\langle n_{0-\sigma}n_{j\sigma}\rangle-e^{i\mathbf{k}\cdot\mathbf{R}_j}\langle c_{0\sigma}^\dagger n_{j-\sigma}c_{j\sigma}\rangle. \tag{40}$$

Introducing the notation

$$n_{j\sigma}=\langle c_{0\sigma}^\dagger c_{j\sigma}\rangle=\frac{1}{N}\sum_{\mathbf{k}}\mathfrak{F}_\omega G_{11\sigma}e^{i\mathbf{k}\cdot\mathbf{R}_j}, \tag{41}$$

$$m_{j\sigma}=\langle c_{0\sigma}^\dagger n_{j-\sigma}c_{j\sigma}\rangle=\frac{1}{N}\sum_{\mathbf{k}}\mathfrak{F}_\omega G_{12\sigma}e^{i\mathbf{k}\cdot\mathbf{R}_j}, \tag{42}$$

where we assume the brackets to be real, and unchanged when the indices 0 and j are interchanged, and further defining

$$\alpha_{j\sigma}=\frac{1}{N}\sum_{\mathbf{k}}\mathfrak{F}_\omega\tilde{G}_{11\sigma}e^{i\mathbf{k}\cdot\mathbf{R}_j}, \tag{43}$$

$$\beta_{j\sigma}=\frac{1}{N}\sum_{\mathbf{k}}\mathfrak{F}_\omega\tilde{G}_{12\sigma}e^{i\mathbf{k}\cdot\mathbf{R}_j}, \tag{44}$$

we have

$$\langle n_{j\sigma}n_{0\sigma}\rangle=\alpha_\sigma n_\sigma-\alpha_{j\sigma}n_{j\sigma}+\beta_\sigma\langle n_{0-\sigma}n_{j\sigma}\rangle-\beta_{j\sigma}m_{j\sigma}, \tag{45}$$

where we write $n_{0\sigma}=n_\sigma$, etc. We see that we now need to evaluate a correlation function for opposite spins, for which we use B_2 in Eq. (38) with Eqs. (43)–(44) and

$$[c_{\mathbf{k}\sigma},B_2]_+=n_{-\sigma}, \tag{46}$$

$$[d_{\mathbf{k}\sigma},B_2]=\langle n_{0-\sigma}n_{j-\sigma}\rangle, \tag{47}$$

to obtain

$$\langle n_{j-\sigma}n_{0\sigma}\rangle=\frac{1}{N}\sum_{\mathbf{k}}\langle B_2 c_{\mathbf{k}\sigma}\rangle=\alpha_\sigma n_{-\sigma}+\beta_\sigma\langle n_{0-\sigma}n_{j-\sigma}\rangle. \quad (48)$$

Letting $\sigma\rightarrow-\sigma$ in this equation, substituting into Eq. (45), and solving for $\langle n_{j\sigma}n_{0\sigma}\rangle$, we have

$$\langle n_{j\sigma}n_{0\sigma}\rangle=\frac{\alpha_\sigma n_\sigma-\alpha_{j\sigma}n_{j\sigma}+\beta_\sigma\alpha_{-\sigma}n_\sigma-\beta_{j\sigma}m_{j\sigma}}{1-\beta_\sigma\beta_{-\sigma}}. \quad (49)$$

Let us now evaluate α and β. We can solve for $\tilde{G}$ in terms of G to give

$$\tilde{G}_{11}=(G_{11}-G_{12})/(1-n_{-\sigma}), \quad (50)$$

$$\tilde{G}_{12}=(G_{12}/n_{-\sigma}-G_{11})/(1-n_{-\sigma}), \quad (51)$$

so that we have

$$\alpha_{j\sigma}=(n_{j\sigma}-m_{j\sigma})/(1-n_{-\sigma}), \quad (52)$$

$$\beta_{j\sigma}=(m_{j\sigma}/n_{-\sigma}-n_{j\sigma})/(1-n_{-\sigma}). \quad (53)$$

We can use these results to write Eq. (49) as

$$\langle n_{j\sigma}n_{0\sigma}\rangle-n_\sigma{}^2=-\frac{\alpha_{j\sigma}n_{j\sigma}+\beta_{j\sigma}m_{j\sigma}}{1-\beta_\sigma\beta_{-\sigma}}. \quad (54)$$

Now for the spin-correlation term, from entirely similar considerations, except that we need only B_3 for this case, we have

$$\langle c_{j\sigma}{}^\dagger c_{j-\sigma}c_{0-\sigma}{}^\dagger c_{0\sigma}\rangle=\langle S_j{}^+S_0{}^-\rangle=-\frac{\alpha_{j\sigma}n_{j-\sigma}+\beta_{j\sigma}m_{j-\sigma}}{1+\beta_\sigma}. \quad (55)$$

Similarly, using B_4, we have

$$\langle c_{j\sigma}{}^\dagger c_{j-\sigma}{}^\dagger c_{0-\sigma}c_{0\sigma}\rangle=\frac{\alpha_{j\sigma}n_{j-\sigma}+\beta_{j\sigma}(n_{j-\sigma}-m_{j-\sigma})}{1-\beta_\sigma}. \quad (56)$$

In the last two correlation functions the left-hand side is unchanged if we let $\sigma\rightarrow-\sigma$. Therefore the right-hand side should give equivalent results for the two spins. This symmetry is not evident, and this points up an ambiguity in our method of evaluating the four operator averages $\langle A_n{}^\dagger A_m{}^\dagger A_p A_q\rangle$, namely, that the division into the A and B of Eq. (32) is not unique. In the limits $U\rightarrow\infty$ and $U\rightarrow 0$, the two spin directions do give equivalent results. For intermediate values it would seem best to average them. The problem of the nonuniqueness of the four operator averages needs further study. Summarizing, we substitute Eqs. (30) and (54)–(56) into Eq. (21) to obtain

$$n_\sigma(1-n_\sigma)W_{\mathbf{k}\sigma}=-\sum_{j\neq0}t_{0j}(n_{j\sigma}-2m_{j\sigma})-\sum_{j\neq0}e^{i\mathbf{k}\cdot\mathbf{R}_j}t_{0j}$$
$$\times\left\{\frac{\alpha_{j\sigma}n_{j\sigma}+\beta_{j\sigma}m_{j\sigma}}{1-\beta_\sigma\beta_{-\sigma}}+\frac{\alpha_{j\sigma}n_{j-\sigma}+\beta_{j\sigma}m_{j-\sigma}}{1+\beta_\sigma}\right.$$
$$\left.+\frac{\alpha_{j\sigma}n_{j-\sigma}+\beta_{j\sigma}(n_{j-\sigma}-m_{j-\sigma})}{1-\beta_\sigma}\right\}, \quad (57)$$

where α and β are given by Eqs. (52) and (53), and n and m by Eqs. (41) and (42). This, together with n_σ from Eq. (41) or (32), determines the parameters in the Green's function [Eq. (29)].

IV. STRONGLY CORRELATED LIMIT

In the limit $U\gg t_{ij}$, the one-particle Green's function $G_{\mathbf{k}\sigma}=G_{11\sigma}(\mathbf{k})$ becomes

$$G_{\mathbf{k}\sigma}\cong\frac{1-n_{-\sigma}}{\omega-\epsilon_{\mathbf{k}}(1-n_{-\sigma})-n_{-\sigma}W_{\mathbf{k}-\sigma}}$$
$$+\frac{n_{-\sigma}}{\omega-U-\epsilon_{\mathbf{k}}n_{-\sigma}-W_{\mathbf{k}-\sigma}(1-n_{-\sigma})}. \quad (58)$$

Assuming that $n_\uparrow+n_\downarrow<1$, only the band of energies corresponding to the lower pole is occupied. In fact, the $U\rightarrow\infty$ limit corresponds to the replacement of the interaction by an exclusion of double occupancy of the sites. Evaluating the contour integral in Eq. (4), we have for $n_{j\sigma}$

$$n_{j\sigma}=\frac{1}{N}\sum_{\mathbf{k}}f(\epsilon_{\mathbf{k}}{}^a)e^{i\mathbf{k}\cdot\mathbf{R}_j}(1-n_{-\sigma}), \quad (59)$$

where $\epsilon_{\mathbf{k}}{}^a$ is the position of the lower pole:

$$\epsilon_{\mathbf{k}}{}^a=\epsilon_{\mathbf{k}}(1-n_{-\sigma})+n_{-\sigma}W_{\mathbf{k}-\sigma}. \quad (60)$$

As discussed in the Ref. 8, the band has become both narrowed and shifted by the interaction. Equation (59) for $j=0$ gives n_σ. We also have $m_{j\sigma}=0$ since G_{12} involves only the upper pole; thus

$$n_\sigma(1-n_\sigma)W_{\mathbf{k}\sigma}\,|_{\,U\rightarrow\infty}=-\sum_j t_{0j}n_{j\sigma}$$
$$-\sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j}t_{0j}\frac{\{n_j{}^2(1-n_\sigma)+n_{j\sigma}n_{j-\sigma}\}}{(1-n_\sigma-n_{-\sigma})}. \quad (61)$$

The two terms in the curly brackets are the density and spin-correlation functions. The double-hop correlation function vanishes in this limit both exactly and in our approximation [Eq. (56)]. The spin-correlation function in this limit is, as stated above, symmetrical between the two spin directions.

The result is simplified if we consider a nearest-neighbor model with $t_{0j}=t$ for the z neighbors. Then we need only one value of $n_{j\sigma}$, which we call $n_{1\sigma}$, in addition to n_σ:

$$n_\sigma(1-n_\sigma)W_{k\sigma}=-tzn_{1\sigma}-\epsilon_{\mathbf{k}}\frac{n_{1\sigma}(1-n_\sigma)+n_{1\sigma}n_{1-\sigma}}{1-n_\sigma-n_{-\sigma}}, \quad (62)$$

$$n_\sigma=\frac{1}{N}\sum_{\mathbf{k}}f(\epsilon_{\mathbf{k}}{}^a)(1-n_{-\sigma}), \quad (63)$$

$$n_{1\sigma}=\frac{1}{N}\sum_{\mathbf{k}}f(\epsilon_{\mathbf{k}}{}^a)\frac{\epsilon_{\mathbf{k}}}{tz}(1-n_{-\sigma}). \quad (64)$$

The Fermi surface for each band has just the shape of the unperturbed Fermi surface for each band, and so is related to the unperturbed Fermi energy Z_σ. Let

$$N_\sigma=\frac{1}{N}\sum_{\mathbf{k},\epsilon_\mathbf{k}<Z_\sigma}=\int_{\epsilon_b}^{Z_\sigma}\rho(\epsilon)d\epsilon, \tag{65}$$

$$Y_\sigma=-\frac{1}{N}\sum_{\mathbf{k},\epsilon_\mathbf{k}<Z_\sigma}\epsilon_\mathbf{k}=-\int_{\epsilon_b}^{Z_\sigma}\rho(\epsilon)\epsilon d\epsilon, \tag{66}$$

where $\rho(\epsilon)$ is the density of states for the noninteracting band and ϵ_b is the band-edge energy. Then we have

$$n_\sigma=N_\sigma(1-n_{-\sigma}). \tag{67}$$

Reversing σ and then solving the two equations for n_σ, we find

$$n_\sigma=N_\sigma(1-N_{-\sigma})/(1-N_\sigma N_{-\sigma}). \tag{68}$$

From Eqs. (64), (66), and (68), we can also write $n_{1\sigma}$:

$$n_{1\sigma}=Y_\sigma(1-N_{-\sigma})/tz(1-N_\sigma N_{-\sigma}). \tag{69}$$

Combining the last two equations, for $n_\sigma W_\sigma$ we have

$$n_\sigma W_\sigma=\frac{Y_\sigma(1-N_{-\sigma})}{1-N_\sigma}\times\left[1-\frac{\epsilon_\mathbf{k}}{(tz)^2}\left(\frac{Y_\sigma}{1-N_\sigma N_{-\sigma}}+\frac{Y_{-\sigma}}{1-N_{-\sigma}}\right)\right]. \tag{70}$$

We see that, given the unperturbed Fermi levels together with a knowledge of the density of states, we can evaluate N and Y and so determine the parameters n and W. We can then solve for the perturbed Fermi levels

$$\zeta_\sigma=Z_\sigma(1-n_{-\sigma})+n_{-\sigma}W_{-\sigma}. \tag{71}$$

In order for the solution to be self-consistent, the perturbed Fermi levels must match for the two spins. For the paramagnetic state ($Z_\uparrow=Z_\downarrow$) this is automatically the case. To seek magnetic solutions, we fix $Z_\uparrow$ and vary $Z_\downarrow$ until the perturbed Fermi levels match.

The density of states for the simple cubic nearest-neighbor case is known from the work of Wolfram and Calloway.[19] A plot of $\rho(\epsilon)$ appears in an article of Penn's.[20] We have carried out the above self-consistent procedure for this case. The result is given in Ref. 8, and we reproduce the figure here as Fig. 2. We see that there is no ferromagnetic state for small n, but that for $n>0.36$ the paramagnetic state becomes unstable. At $n=0.63$, the ferromagnetism becomes saturated. It is interesting to compare our results with the spin-wave result for this case in the strongly correlated limit,[6] which showed that the saturated ferromagnetic state becomes unstable toward the formation of long-wavelength spin waves when n approaches 0.5 from above.

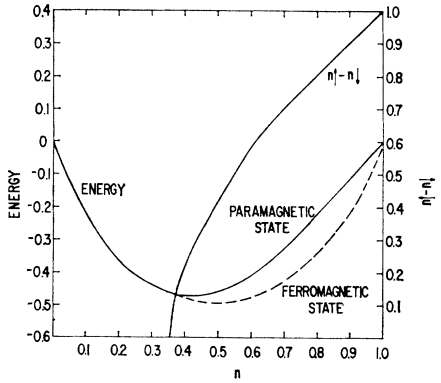

FIG. 2. Magnetization ($n_\uparrow-n_\downarrow$) and total energy per site versus the number of electrons per site, for a simple cubic lattice with nearest-neighbor interaction and $U\to\infty$. We have included the energy of the paramagnetic state. The units of energy are such that the band width is 6.

The present result gives a more restricted region for the stability of the saturated ferromagnetic state.

The energy in the figure is obtained from the relation[21]

$$E_T=\sum_{\mathbf{k},\sigma}\mathfrak{F}_{\omega\frac{1}{2}}(\omega+\epsilon_\mathbf{k})G_{\mathbf{k}\sigma}=\sum_{\mathbf{k}\sigma}\tfrac{1}{2}(\epsilon_\mathbf{k}{}^a+\epsilon_\mathbf{k})f(\epsilon_\mathbf{k}{}^a)(1-n_{-\sigma}). \tag{72}$$

We calculate it for both paramagnetic and ferromagnetic phases. We remark that if we calculated the energy for the fully aligned ferromagnetic state, it would be approximately the result of reflecting the dashed curve about $n=0.5$. It is interesting to note that this lies only slightly above the paramagnetic state energy.

In Fig. 3 we plot the calculated Fermi level and the limits of the up- and down-spin bands. We notice that the down-spin band becomes very narrow as $n\to 1$. Let us point out, however, that the inclusion of a level width will drastically change this result. In the next article in this series, we shall see that the broadening of the down-spin band becomes very severe in this region.

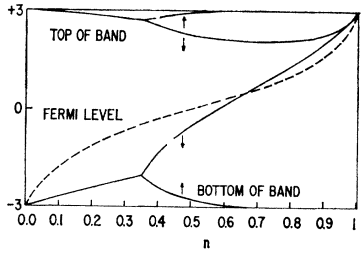

FIG. 3. Upper and lower limits of the resultant bands for the case of Fig. 2, plotted versus the number of electrons per site. The Fermi level is also shown. Note that the down-spin band is considerably narrowed.

[19] T. Wolfram and J. Calloway, Phys. Rev. **130**, 2207 (1963).
[20] D. R. Penn, Phys. Rev. **142**, 350 (1966).
[21] This result is the retarded Green's-function analog of Eq. (3.69) in Ref. 17.

V. LOW-DENSITY LIMIT

In the limit of low densities, Kanamori[2] has shown that the correlation problem can be solved exactly and that the Coulomb interaction is replaced by a T matrix exactly describing the scattering of two electrons. Let us examine our theory in this limit. It is convenient to express the one-particle Green's function in the form

$$G_{\mathbf{k}\sigma}=\{\omega-\epsilon_{\mathbf{k}}-\Sigma_\sigma(\mathbf{k},\omega)\}^{-1}, \tag{73}$$

where

$$\Sigma_\sigma(\mathbf{k},\omega)=n_{-\sigma}U\frac{\omega-W_{\mathbf{k}-\sigma}}{\omega-U(1-n_{-\sigma})-W_{\mathbf{k}-\sigma}} \tag{74}$$

is the self-energy. We wish to evaluate Σ to first order in $n_{-\sigma}$, so that we need $W_{\mathbf{k}\sigma}$ to zero order in n. In Eq. (57) the lowest-order term on the right-hand side is the part of the first term involving $n_{j\sigma}$, and all other terms are of higher order in the density. Assuming that the occupied region of the zone is near $\mathbf{k}=0$, we see from Eq. (42) that for low density $n_{j\sigma}\sim n_\sigma$, so that

$$W_{\mathbf{k}\sigma}\sim-\sum_j t_{0j}=-\epsilon_b, \tag{75}$$

where ϵ_b is the band-edge energy. Also in Σ we have $\omega\sim\epsilon_b$, so that

$$\Sigma_\sigma(\mathbf{k}\omega)\sim n_{-\sigma}\frac{U}{1+U/2|\epsilon_b|}. \tag{76}$$

We can compare this with the Kanamori result, which is exact in the low-density limit:

$$\Sigma_\sigma(\mathbf{k}\omega)=n_{-\sigma}U\left[1+U\sum_{\mathbf{q}}\frac{1}{2(\epsilon_{\mathbf{q}}-\epsilon_b)}\right]^{-1}. \tag{77}$$

We see that the results are not equal. Our "two-pole approximation" is in fact, equivalent to replacing $\epsilon_{\mathbf{q}}$ by its average value in Eq. (77).

The results for $U\to\infty$ are compared in Table I for the simple cubic lattice with nearest-neighbor interaction, and we have included some of Hubbard's work. It appears that our theory gives a worse result in this limit than Hubbard's first approximation and shares this distinction with Hubbard's improved theories.

We now wish to show how our theory can be improved so as to give the correct result in the low-density limit. Let us first use our method to obtain the exact low-density limit. We rewrite Eq. (5) in terms of Bloch-state operators:

$$[c_{\mathbf{k}\sigma},H]=\epsilon_{\mathbf{k}}c_{\mathbf{k}\sigma}+\frac{U}{N}\sum_{\mathbf{k}',q(\mathbf{k}'\neq q)}c_{\mathbf{k}'-\sigma}{}^\dagger c_{\mathbf{q}-\sigma}c_{\mathbf{k}'-\mathbf{q}+\mathbf{k}\sigma}+\frac{U}{N}\sum_{\mathbf{k}'}n_{\mathbf{k}'-\sigma}c_{\mathbf{k}\sigma}. \tag{78}$$

Here we have separated out the $\mathbf{k}'=\mathbf{q}$ term, which is the only three-fermion operator which is not "orthogonal" to c_k in the sense of having a zero matrix element of the normalization matrix Eq. (14). We then include in our set $\{A_n\}$, $A_1\,c_k$, and

$$A_{\mathbf{k}'\mathbf{q}\sigma}=c_{\mathbf{k}'-\sigma}{}^\dagger c_{\mathbf{q}-\sigma}c_{\mathbf{k}'-\mathbf{q}+\mathbf{k}\sigma} \tag{79}$$

with $\mathbf{k}'\neq\mathbf{q}$. Commuting the latter through H, we have

$$\begin{aligned}[c_{\mathbf{k}'-\sigma}{}^\dagger c_{\mathbf{q}-\sigma}c_{\mathbf{k}'-\mathbf{q}+\mathbf{k}\sigma},H]&=(\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k}'-\mathbf{q}+\mathbf{k}}-\epsilon_{\mathbf{k}'})c_{\mathbf{k}'-\sigma}{}^\dagger c_{\mathbf{q}-\sigma}c_{\mathbf{k}'-\mathbf{q}+\mathbf{k}\sigma}\\&+\frac{U}{N}\sum_{\mathbf{q}'\neq\mathbf{k}'}c_{\mathbf{k}'-\sigma}{}^\dagger c_{\mathbf{q}-\sigma}c_{\mathbf{k}'-\mathbf{q}'+\mathbf{k}\sigma}+\frac{U}{N}n_{\mathbf{k}'-\sigma}c_{\mathbf{k}\sigma}\\&+(\text{terms of form } c^\dagger c^\dagger ccc).\end{aligned} \tag{80}$$

The terms written out explicitly will give the low-density limit; the remaining terms are of higher order in the density and we shall neglect them. We can now calculate anticommutors and so evaluate the matrices E and N, going only to first order in the density, i.e., ignoring all averages of the form $\langle c^\dagger c^\dagger cc\rangle$. We note that here, as in the previous result, both E and N are diagonal in $\mathbf{k}$; thus we can suppress the $\mathbf{k}$ indices. We have

$$\begin{aligned}N_{11\sigma}&=1,\\N_{1\mathbf{k}'\mathbf{q}\sigma}&=0,\\N_{\mathbf{k}'\mathbf{q},\mathbf{k}''\mathbf{q}'\sigma}&=\langle n_{\mathbf{k}'-\sigma}\rangle\delta_{\mathbf{k}'\mathbf{k}''}\delta_{\mathbf{q}\mathbf{q}'},\end{aligned} \tag{81}$$

$$\begin{aligned}E_{11\sigma}&=\epsilon_{\mathbf{k}}+Un_{-\sigma},\\E_{1,\mathbf{k}'\mathbf{q}\sigma}&=E_{\mathbf{k}'\mathbf{q},1\sigma}=(U/N)\langle n_{\mathbf{k}'-\sigma}\rangle,\\E_{\mathbf{k}'\mathbf{q},\mathbf{k}''\mathbf{q}'\sigma}&=\delta_{\mathbf{k}'\mathbf{k}''}n_{\mathbf{k}'-\sigma}\times[(\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k}'-\mathbf{q}+\mathbf{k}}-\epsilon_{\mathbf{k}'})\delta_{\mathbf{k}\mathbf{k}'}+U/N],\end{aligned} \tag{82}$$

and we notice that $\mathbf{k}'$ should be restricted to occupied states. The one-electron Green's function is the 11 matrix element of the matrix Green's function of Eq. (26); in order to evaluate it we must take the inverse of $N\omega-E$. The result is Eq. (73), with the self-energy now given by

$$\Sigma_\sigma=\frac{1}{N}\sum_{\mathbf{k}'}\langle n_{\mathbf{k}'-\sigma}\rangle U\times\left(1+\frac{U}{N}\sum_{\mathbf{q}}\frac{1}{\epsilon_{\mathbf{q}}+\epsilon_{\mathbf{k}'-\mathbf{q}+\mathbf{k}}-\epsilon_{\mathbf{k}'}-\omega}\right)^{-1}. \tag{83}$$

TABLE I. Self-energy Σ_∞ in the low-density limit for $U\to\infty$, evaluated for the simple cubic nearest-neighbor (scnn) case. ϵ_b is the band-edge energy and $2|\epsilon_b|$ is the bandwidth.

Theory	Σ_∞	scnn
Hubbard I[a]	$-\epsilon_b$	$\lvert\epsilon_b\rvert$
Hubbard II[a]	$\epsilon_b+2N/\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}}-\epsilon_b)^{-1}$	$0.319\lvert\epsilon_b\rvert$[c]
Roth	$-2\epsilon_b$	$2\lvert\epsilon_b\rvert$
Kanamori[b]	$2N/\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}}-\epsilon_b)^{-1}$	$1.319\lvert\epsilon_b\rvert$[c]

[a] Reference 1.
[b] Reference 2.
[c] P. D. Loly and S. Doniach, Phys. Rev. **144**, 319 (1966).

In this case our method is essentially equivalent to the Suhl-Werthamer[16] and Martin-Schwinger[17] decoupling procedures.

Now, if we set $\mathbf{k}$ and $\mathbf{k}'$ equal to zero and ω equal to ϵ_b. this reduces to Eq. (77). In our three-fermion operator, we have an excited electron and hole, with wave vectors $\mathbf{q}$ and $\mathbf{k}'$, respectively. We see that in the low-density limit we can neglect the energy variation of the hole, but not of the electron, as the latter goes over all unoccupied states. On the other hand, in the two-pole approximation, we sum the three-fermion operator in Eq. (79) over both electron and hole states ($\mathbf{q}'$ and $\mathbf{k}'$), which results in the neglect of the energy variation of the electron. This suggests that a better approximation would be to sum Eq. (79) only over the hole states $\mathbf{k}'$.

Thus we use c_k and

$$A_q=\frac{1}{N}\sum_{k'} c_{k'-\sigma}^{\dagger}c_{q-\sigma}c_{k'-q+k\sigma}. \tag{84}$$

To obtain the new E and N we simply sum Eqs. (81) and (82) over $\mathbf{k}'$, giving

$$N_{qq'\sigma}=n_{-\sigma}\delta_{qq'},$$
$$E_{1q\sigma}=(U/N)n_{-\sigma},$$
$$E_{qq'\sigma}=\frac{1}{N}\sum_{k'} n_{k'-\sigma}(\epsilon_q+\epsilon_{k'-q+k}-\epsilon_{k'})\delta_{qq'}+\frac{U}{N}n_{-\sigma}, \tag{85}$$

with the remaining quantities unchanged. The result for Σ in this case is

$$\Sigma_\sigma=n_{-\sigma}U\left(1+\frac{U}{N}\sum_q \frac{n_{-\sigma}U}{(1/N)\sum_{k'}\langle n_{k'\sigma}\rangle(\epsilon_q+\epsilon_{k'-q+k}-\epsilon_{k'}-\omega)}\right)^{-1}. \tag{86}$$

Thus we see that the denominator is averaged over hole states. If we take $\mathbf{k}'\sim 0, \omega\sim\epsilon_b$, we again obtain Eq. (77).

We can now envision using the set c_k, $A_q(\mathbf{k})$ for a more general density. The advantage it has over the use of *all* three fermion operators is that A_q depends on only one wave vector rather than two. Let us examine what the A_q operators are in terms of Wannier operators. We can readily see that

$$A_q(\mathbf{k})=-n_q c_k+N^{-1/2}\sum_{ij} e^{iq\cdot R_j+ik\cdot R_i}c_{i-\sigma}^{\dagger}c_{j-\sigma}c_{i\sigma}. \tag{87}$$

The first term is for orthogonalization and the second term has the hole tied to the same site as the initial electron, while the excited electron can wander. This is in contrast to the two-pole approximation, in which both electron and hole are tied to the site of the initial electron.

In order to give a reasonable result when both n and U are large, we should add to A another set

$$B_q=-c_q^{\dagger}d_q c_k+N^{-1/2}\sum_{i,j} e^{iq\cdot R_j+ik\cdot R_i}c_{i-\sigma}^{\dagger}n_{j\sigma}c_{j-\sigma}c_{i\sigma}. \tag{88}$$

A_q and B_q represent some of the terms retained by Hubbard in his "resonance-broadening" corrections. However, the results we expect are by no means equivalent, as evidenced by Table I.

We shall apply the improved theory to the case of a single down spin in an otherwise fully aligned band in the next paper in this series.

VI. POSSIBILITY OF A MINIMUM PRINCIPLE

As we discussed in the Ref. 8, our decoupling scheme is related to a stationary principle for the eigenvalues of K. As we also pointed out, a minimum principle would be more desirable. We suggest here a direction along which we could move to obtain such a minimum principle, although we have not succeeded in proving anything conclusive.

Let us first recall that if the two-body interaction is multiplied by a dimensionless coupling constant λ, we have

$$\frac{d}{d\lambda}\lambda H=\sum_{k\sigma} c_{k\sigma}^{\dagger}[c_{k\sigma},H]. \tag{89}$$

Let us take the expectation value of this equation in the N-particle ground state and apply Feynman's theorem[22]:

$$\frac{d}{d\lambda}\lambda\langle 0|H|0\rangle=\sum_{k\sigma}\langle 0|c_{k\sigma}^{\dagger}[c_{k\sigma},H]|0\rangle$$
$$=-\sum_n |\langle n|c_{k\sigma}|0\rangle|^2[E_n{}^{N-1}-E_0{}^N]. \tag{90}$$

Let us also recall that $E_0{}^{N-1}-E_0{}^N$ is just the negative of the chemical potential μ, so that

$$\frac{d}{d\lambda}\lambda\langle 0|H|0\rangle=\mu N$$
$$+\sum_n |\langle n|c_{k0}|0\rangle|^2(E_0{}^{N-1}-E_n{}^{N-1}). \tag{91}$$

Clearly, in the second summation, all the terms are negative. The quantity μN is just a constant, and we can modify H by replacing it by $H-\mu N=H'$.

Now, as pointed out in Ref. 8, in the exact solution to our problem, the A are of the form $|n\rangle\langle 0|$, with $|n\rangle$

[22] See, e.g., C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), p. 107.

a $(N-1)$-particle excited state. Thus the sum is

$$\frac{d}{d\lambda}\langle 0|H-\mu N|0\rangle = \sum_n |\langle 0|[A_n, c_k^\dagger]_+|0\rangle|^2 (K_n-\mu) f(K_n), \quad (92)$$

with K_n-U negative, K_{nm} diagonal, and N_{nm} a unit matrix.

We can now introduce a particular variation of the A_n, namely, omitting some of them. The sum clearly increases, and, integrating over λ, the result is an increase in the total energy. Thus we see that, for certain variations of the set A from the exact results, the energy increases. A possible generalization of this equation is

$$\frac{d}{d\lambda}\langle 0|H-\mu N|0\rangle = \sum_k \mathfrak{F}_\omega(\omega-\mu) \times \sum_{mn} \langle [c_k, A_n^\dagger]_+\rangle (N\omega - E)_{nm}^{-1} \langle [c_k^\dagger, A_m]_+\rangle. \quad (93)$$

This should also equal the following expression in terms of the one-particle Green's function:

$$\sum_k \mathfrak{F}_\omega(\omega-\mu) G_k(\omega). \quad (94)$$

If one of the set A_n is c_k and the rest are "orthogonal," we have exactly Eq. (94).

Again, consider a particular type of variation. Let us suppose that N is a unit matrix and that E is diagonal, but that the A_n are not the exact set. Then, if we add another A_n, such that N is also a unit matrix (of one more dimension) and suppose that $E=K$ remains diagonal, the expression in the right side of Eq. (93) decreases.

The catch here is that, in general, E will no longer be diagonal, so we must prove something more complicated, something which has thus far eluded this author. It must also be remembered that we are approximating the averages self-consistently rather than in the exact ground state. There are still some problems in showing that increasing the set will lower the right-hand side of Eq. (93). We conjecture that such a result can be proved, which would then, upon integration, yield a minimum principle for the energy.

We should remark that, in the low-density limit, our result for the self-energy is higher than the exact result, for if we let $x=\epsilon_k-\epsilon_b>0$, we have the following equality:

$$\left\langle x\left(\frac{1}{x}-\left\langle\frac{1}{x}\right\rangle\right)^2\right\rangle = \langle x\rangle\left\langle\frac{1}{x}\right\rangle\left(\left\langle\frac{1}{x}\right\rangle-\frac{1}{\langle x\rangle}\right). \quad (95)$$

Here the average is over the Brillouin zone. The left-hand side is positive, so this shows that $\langle 1/x\rangle > 1/\langle x\rangle$, which is true for averages of any positive quantity. Thus Eq. (76) is greater than Eq. (77). This is in contrast to the result of Hubbard I given in Table I, which is below the exact result.

VII. DISCUSSION

We have presented here an improved version of Hubbard's[1] two-pole approximation in a narrow nondegenerate band. We find that, contrary to Hubbard's result, a relatively simple band shape gives a ferromagnetic state in the strongly correlated limit for a sufficiently large concentration of carriers. The improved theory includes a band shift which is most important in the case of a nearly-half-filled band. We expect that further improvements will restrict further the region of ferromagnetism.

We have found that the two-pole approximation gives an incorrect result in the low-density limit,[2] and we indicate how the theory can be improved on this score. The same problem arises with some of Hubbard's improvements and with the results of Harris and Lange[4] and Esterling and Lange,[11] which are essentially equivalent to ours in the strongly correlated limit. In the work of Esterling and Lange, the claim is made that their result is exact in the strongly correlated limit. In view of the failure of the result at low densities, we must disagree with their claim.

While we have been approaching this problem from Hubbard's viewpoint, the improvements called for in the low-density limit suggest another way of looking at it. The T-matrix approach is useful for short-range interactions in the low-density limit, but in many systems the density is by no means low. Hence our aim is to use our methods to extend the T-matrix results to a finite density for the Hubbard Hamiltonian, which is a lattice gas with short-range interactions.

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