direct response of Cooper pairs. We have

$$j^{(1)}=-(e^2n/m)\tfrac{1}{4}7\zeta(3)\chi(\rho)(\Delta^2/\pi^2T_c^2)A+\sigma i\Omega A. \quad (7.15)$$

These results confirm again Eq. (2.5). Note that quite generally,

$$\sigma_{s0}=i(e^2n/m)2\chi(\rho)(T_c-T/T_c)(1/\Omega). \quad (7.16)$$

Consider now the case where $1/\tau_c$ is not negligible. One obtains a result which can be considered as an interpolation between the two limits, Eqs. (6.8) and (7.12). Let these expressions be $\tau_R^{(c)}$ and $\tau_R^{(i)}$, respectively. Then, this interpolation can approximately be represented by the relation

$$\frac{1}{\tau_R}=\frac{1}{\tau_R^{(c)}}+\frac{1}{\tau_R^{(i)}}. \quad (7.17)$$

It conclusion it can be said that the results of the microscopic calculation agree with the phenomenological analysis given in Sec. II. In addition, quantitative expressions have been derived for the relaxation time τ_R [Eqs. (7.17), (7.12), and (6.8)] which hold for temperature close to the transition temperature. The relaxation time will be determined mainly by inelastic electron-phonon collisions. One expects impurity scattering to influence noticeably the relaxation time only when the superconductor has such a low transition temperature that the number of excited electrons and phonons is small. However, if one considers the dependence on the temperature difference (T_c-T) of these two processes, one is tempted to assume that for low temperatures (which are outside the scope of the present considerations) impurity scattering may give rise to an effective relaxation mechanism in a superconductor of short mean free path and considerable supercurrent flow.

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Electron Correlation in Narrow Energy Bands. II. One Reversed Spin in an Otherwise Fully Aligned Narrow S Band

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In a previous paper, a new Green's-function decoupling scheme was applied to the Hubbard Hamiltonian, and an improved version of Hubbard's first approximation was obtained. That result did not reduce to the correct low-density limit as obtained by Kanamori. In the present article, the theory is improved for the special case of a single reversed spin in an otherwise fully aligned band, and the improved theory is correct in the low-density limit. Numerical results are presented for the simple cubic lattice. If we define an effective exchange-interaction parameter U_{eff} as the $k=0$ reversed-spin self-energy for $U\to\infty$, divided by the number $n_\uparrow$ of up-spin electrons per site, we find that the present result departs rather rapidly from the Kanamori result as $n_\uparrow$ is increased, and it is concluded that the Kanamori result overestimates the increase in U_{eff} with $n_\uparrow$, at least in the present case. For intermediate values of $n_\uparrow$, the two-pole approximation of the previous article and the present calculation give very similar results for this quantity.

INTRODUCTION

IN the first paper in this series,[1] a new Green's-function decoupling scheme[2,3] was applied to the Hubbard model of a narrow nondegenerate band governed by the Hamiltonian

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

where c_i annihilates an electron on the ith Wannier site. This model includes in its simplest form the competition between the intra-atomic Coulomb energy and the electron kinetic energy. This was solved in an improved version of Hubbard's first approximation[4] in which the one-particle Green's function is assumed to have two poles on the real axis.

In I, an improvement of the theory was suggested which would lead to the correct low-density limit for the electron self-energy. In the present article, we shall apply the improved version of the theory to the case of one reversed spin in an otherwise aligned nondegenerate band. The advantage of this special case is that in the fully aligned state, the electrons are noninteracting so that the wave function is known. An argument will be given to show that the approximation is good for finite densities in this particular case. There are two purposes

[1] L. M. Roth, Phys. Rev. **184**, 451 (1969). We shall refer to this as I.
[2] L. M. Roth, Phys. Rev. Letters **20**, 431 (1968).
[3] J. Linderberg and Y. Öhrn, Chem. Phys. Letters **1**, 295 (1967).
[4] J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963).

to this study. One is to examine the stability of the ferromagnetic state toward single-particle excitations. We have studied already the stability of the ferromagnetic state toward spin-wave formation.[5] The other purpose of the work is to compare the present approximation with the two pole approximation, and with Kanamori's[6] T-matrix result, which is believed to be a good approximation for Ni,[7] and which has been studied extensively by Calloway.[8]

For numerical calculations we use once more the simple-cubic nearest neighbors (scnn) case. The author hopes in the future to apply the calculation to Calloway's[8] face-centered-cubic second-nearest-neighbor model. It will be argued that the present results represent an extension of the T-matrix results to higher densities, and that for a middle range of particle densities, our 2-pole approximation is quite reasonable.

CALCULATION OF ONE-PARTICLE GREEN'S FUNCTION

We wish to calculate the Fourier transform of retarded and advanced Green's functions,[1,9] which can be defined 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 A and B are Fermion-type operators such as c_k and $c_k^\dagger$ in the one-particle Green's function $\langle\langle c_k;c_k^\dagger\rangle\rangle$. The expectation value is in the ground state, or is a thermal average, as we wish, and the contour integral encircles the real axis but excludes ω which is above (below) the real axis for the retarded (advanced) case. The equation of motion is given by

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

In our decoupling scheme, we truncate[1,2] the infinite set of equations of motion

$$[A_n,H]=\sum_m K_{nm}A_m \quad (4)$$

by choosing a restricted set of operators $\{A_n\}$, anticommuting both sides of Eq. (4) with $A_l^\dagger$, where A_l is in the set, and taking the expectation value of both sides. Then if we define the energy and normalization matrices

$$E_{nm}=\langle[[A_n,H],A_m^\dagger]_+\rangle, \quad (5)$$

$$N_{nm}=\langle[A_n,A_m^\dagger]_+\rangle, \quad (6)$$

we can solve for K,

$$E=KN, \quad (7)$$

provided that we choose the A_n so that N is nonsingular. Other conditions are discussed in I. We then use the K from Eq. (7) via Eq. (4), in the Green's-function equa- of motion, Eq. (3). We quote here the result for Green's functions in which $B^\dagger$ is a member of the set $\{A_m\}$:

$$G_{nm}=\langle\langle A_n,A_m^\dagger\rangle\rangle, \quad (8)$$

and the result is, for the matrix G,

$$G=(\omega-\epsilon-K)^{-1}N=N[N(\omega+\epsilon)-E]^{-1}N. \quad (9)$$

This is the only type of Green's function we shall need here.

In dealing with the case of one reversed spin in an otherwise aligned band, we construct Green's functions in which the expectation value in Eq. (1) is in the fully aligned state. The up-spin retarded Green's function is given by

$$\langle\langle c_{k\uparrow};c_{k'\uparrow}^\dagger\rangle\rangle=\delta_{kk'}G_{k\uparrow}=\delta_{kk'}/(\omega-\epsilon_k+i\epsilon), \quad (10)$$

where $c_{k\sigma}$ is the Bloch state operator:

$$c_{k\sigma}=N^{-1/2}\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i}c_{i\sigma}. \quad (11)$$

In calculating the down-spin Green's function, we begin with the single fermion operator $c_{k\downarrow}$. Commuting this past H we find

$$[c_{k\downarrow},H]=\epsilon_k c_{k\downarrow}+UN^{-1}\sum_{k'q} c_{k'\uparrow}^\dagger c_{q\uparrow}c_{k+k'-q\downarrow}. \quad (12)$$

In the two-pole approximation, we used the coefficient of U as a second operator in the set

$$d_{k\downarrow}=N^{-1/2}\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i}n_{i\uparrow}c_{i\downarrow}, \quad (13)$$

and then truncated with c_k and d_k. If we regard the three-fermion operators as annihilation operators for intermediate state particles, then in the two-pole approximation both the up-spin $\mathbf{k}'$ and electron $\mathbf{q}$ are localized at the down-spin site. This results in their kinetic energies being replaced by average values. In I it was argued that in the low-density limit it was permissible to average the hole energy as this is essentially the band edge energy. This is accomplished by keeping the sum over $\mathbf{k}'$ in the second term of Eq. (12). Then we use the operator

$$A_{kq}=N^{-1}\sum_{k',(k'\neq q)} c_{k'\uparrow}^\dagger c_{q\uparrow}c_{k+k'-q\downarrow}. \quad (14)$$

Here we exclude the $\mathbf{k}'=\mathbf{q}$ term to make this term independent of c_k. In the omitted term, we have $n_{q\uparrow}c_{k\downarrow}$ and except for terms lower in order by $1/N$, we can[10] replace n_q by its average value $\langle n_q\rangle$. We use this fact to rewrite A_{kq} in the alternate form

$$A_{kq}=N^{-1}\sum_{ij} e^{i\mathbf{k}\cdot\mathbf{R}_i+i\mathbf{q}\cdot\mathbf{R}_{ji}}(c_{i\uparrow}^\dagger c_{j\uparrow}-\langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle)c_{i\downarrow}. \quad (15)$$

[5] L. M. Roth, J. Phys. Chem. Solids **28**, 1549 (1966).
[6] J. Kanamori, Progr. Theoret. Phys. (Kyoto) **30**, 276 (1963).
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[8] J. Calloway, Phys. Rev. **170**, 576 (1968); **140**, A618 (1965); J. Calloway and R. K. M. Chow, *ibid.* **145**, 412 (1966).
[9] D. N. Zubarev, Usp. Fiz. Nauk SSSR **71**, 116 (1959) [English transl.: Soviet Phys.—Usp. **3**, 320 (1960)].
[10] H. Suhl and N. R. Werthamer, Phys. Rev. **122**, 359 (1961).

We see that here we have tied the hole to the reversed-spin electron, but we are allowing the up-spin electron to wander.

Another way of looking at our choice of fermion operators is that we restrict ourselves to one- and three-fermion operators, look at the limit of large U, and see which operators commute past the Coulomb part of the Hamiltonian without contributing a term of order U. Clearly, $(1-n_{i-\sigma})c_{i\sigma}$ will do this, and is the basis of our previous choice of $c_{k\sigma}$ and $d_{k\sigma}$. But in Eq. (15), $c_{j\uparrow}{}^{\dagger}c_{i\downarrow}$ will also commute past the Coulomb term for $i\neq j$, and then $c_{j\uparrow}$ does so also for our special case of the fully aligned band. Therefore, in $c_{\mathbf{k}}$ and $A_{\mathbf{kq}}$ we are using the most general one- and three-fermion operators which are allowed for $U\rightarrow\infty$, and we find a larger set for our special case of one reversed spin.

It is now a straightforward matter to calculate the matrices N and E, making use of the fact that the expectation values are in the all-up state, so that

$$c_{\mathbf{k}\downarrow}|0\rangle=A_{\mathbf{kq}}|0\rangle=0. \tag{16}$$

We can anticipate that N and E are diagonal in $\mathbf{k}$, and so replace, e.g., $N_{\mathbf{kk}'}$ by $N_{11}(\mathbf{k})\delta_{\mathbf{kk}'}$. We then have $N_{11}(\mathbf{k})=1$, and

$$N_{1\mathbf{q}}=\langle[A_{\mathbf{kq}},c_{\mathbf{k}\downarrow}{}^{\dagger}]\rangle=0, \tag{17}$$

which follows from the omission of the $\mathbf{q}=\mathbf{k}'$ term in Eq. (14). Next we have

$$N_{\mathbf{qq}'}=\langle A_{k\mathbf{q}}A_{k\mathbf{q}'}{}^{\dagger}\rangle$$
$$=N^{-1}\sum_{\mathbf{k}'}\langle c_{\mathbf{k}'\uparrow}{}^{\dagger}c_{\mathbf{q}\uparrow}[c_{\mathbf{k}+\mathbf{k}'-\mathbf{q}\downarrow},c_{\mathbf{k}+\mathbf{k}''-\mathbf{q}\downarrow}{}^{\dagger}]_{+}c_{\mathbf{q}'\uparrow}{}^{\dagger}c_{\mathbf{k}''\uparrow}\rangle, \tag{18}$$

where we have made use of Eq. (16). We can now factor the expectation value of four-fermion operators into products of 2 two-fermion expectation values for the noninteracting ground state. This gives

$$N_{\mathbf{qq}'}=N^{-1}\delta_{\mathbf{qq}'}\sum_{\mathbf{k}'}n_{\mathbf{k}'\uparrow}(1-n_{\mathbf{q}\uparrow}). \tag{19}$$

Here we write $n_{\mathbf{k}}$ for $\langle c_{\mathbf{k}\uparrow}{}^{\dagger}c_{\mathbf{k}\uparrow}\rangle$.

To evaluate E, we commute $A_{\mathbf{kq}}$ through H

$$[A_{\mathbf{kq}},H]=N^{-1}\sum_{\mathbf{k}'(\mathbf{k}'\neq\mathbf{q})}[(\epsilon_{\mathbf{k}+\mathbf{k}'-\mathbf{q}}+\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k}'})c_{\mathbf{k}'\uparrow}{}^{\dagger}c_{\mathbf{q}\uparrow}c_{\mathbf{k}+\mathbf{k}'-\mathbf{q}\downarrow}$$
$$+U(c_{\mathbf{k}'\uparrow}{}^{\dagger}c_{\mathbf{q}\uparrow}d_{\mathbf{k}+\mathbf{k}'-\mathbf{q}\downarrow}+c_{\mathbf{k}'\uparrow}{}^{\dagger}d_{\mathbf{q}\uparrow}c_{\mathbf{k}+\mathbf{k}'-\mathbf{q}\downarrow}$$
$$-d_{\mathbf{k}'\uparrow}{}^{\dagger}c_{\mathbf{q}\uparrow}c_{\mathbf{k}+\mathbf{k}'-\mathbf{q}\downarrow})], \tag{20}$$

where $d_{k\sigma}$ is given by Eq. (13). In the coefficient of U here we can drop terms involving $d_{\mathbf{k}'\uparrow}$ and $d_{\mathbf{q}\uparrow}$ as these will have two down-spin operators, only one of which will be removed by commuting with $c_{\mathbf{k}\downarrow}$ or $A_{\mathbf{kq}}$. To obtain $E_{\mathbf{q}1}$, we anticommute with $c_{\mathbf{k}}$, and using

$$[d_{\mathbf{k}+\mathbf{k}'\downarrow},c_{\mathbf{k}\downarrow}]_{+}=N^{-1}\sum_{\mathbf{k}''}c_{\mathbf{k}''\uparrow}{}^{\dagger}c_{\mathbf{k}'+\mathbf{k}''\uparrow}, \tag{21}$$

we find

$$E_{\mathbf{q}1}=\langle[[A_{\mathbf{kq}},H],c_{\mathbf{k}}{}^{\dagger}]_{+}\rangle=$$
$$=UN^{-3/2}\sum_{\mathbf{k}'(\mathbf{k}'\neq\mathbf{q})\mathbf{k}''}\langle c_{\mathbf{k}'\uparrow}c_{\mathbf{q}\uparrow}c_{\mathbf{k}''\uparrow}c_{\mathbf{k}'-\mathbf{q}+\mathbf{k}''\uparrow}\rangle$$
$$=UN^{-3/2}\sum_{\mathbf{k}'}n_{\mathbf{k}'\uparrow}(1-n_{\mathbf{q}\uparrow}). \tag{22}$$

Finally for $E_{\mathbf{qq}'}$, let us first anticommute the second term in Eq. (20) with $A_{\mathbf{kq}'}$ using Eq. (16):

$$\langle c_{\mathbf{k}'\uparrow}{}^{\dagger}c_{\mathbf{q}\uparrow}d_{\mathbf{k}+\mathbf{k}'-\mathbf{q}\downarrow}A_{\mathbf{kq}'}{}^{\dagger}\rangle$$
$$=\langle c_{\mathbf{k}'\uparrow}{}^{\dagger}c_{\mathbf{q}\uparrow}[d_{\mathbf{k}+\mathbf{k}'-\mathbf{q}\downarrow},c_{\mathbf{k}+\mathbf{k}''-\mathbf{q}\downarrow}{}^{\dagger}]c_{\mathbf{q}'\uparrow}{}^{\dagger}c_{\mathbf{k}''\uparrow}\rangle. \tag{23}$$

We now use Eq. (21), and then factor the operator products as before. For the first term of Eq. (20), we can use the same argument as in Eqs. (18) and (19) giving altogether

$$E_{\mathbf{qq}'}=\delta_{\mathbf{qq}'}N^{-1}\sum_{\mathbf{k}'}(\epsilon_{\mathbf{k}+\mathbf{k}'-\mathbf{q}}+\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'})n_{\mathbf{k}'}(1-n_{\mathbf{q}})$$
$$+UN^{-1}\sum_{\mathbf{k}'}n_{\mathbf{k}'}(1-n_{\mathbf{q}})(1-n_{\mathbf{q}'}). \tag{24}$$

Let us summarize the matrices in block form:

$$N=\begin{pmatrix}1 & 0\\ 0 & \delta_{\mathbf{qq}'}n_{\mathbf{q}\uparrow}(1-n_{\mathbf{q}\uparrow})\end{pmatrix}$$
$$E=\begin{pmatrix}E_k+Un_{\uparrow} & -N^{-1/2}Un_{\uparrow}(1-n_{\mathbf{q}'\uparrow})\\ N^{-1/2}Un_{\uparrow}(1-n_{\mathbf{q}\uparrow}) & \delta_{\mathbf{qq}'}\bar{\epsilon}_{\mathbf{kq}}(1-n_{\mathbf{q}\uparrow})+Un_{\uparrow}(1-n_{\mathbf{q}\uparrow})(1-n_{\mathbf{q}'\uparrow})\end{pmatrix}, \tag{25}$$

where

$$\bar{\epsilon}_{\mathbf{kq}}=(n_{\uparrow}N)^{-1}\sum_{\mathbf{k}'}n_{\mathbf{k}'}(\epsilon_{\mathbf{k}+\mathbf{k}'-\mathbf{q}}+\epsilon_{\mathbf{q}}-\epsilon_{\mathbf{k}'}) \tag{26}$$

is the energy of intermediate particles averaged over hole states, and where $n_{\uparrow}=N^{-1}\sum_{\mathbf{k}}n_{k\uparrow}$ is the number of electrons per site. We notice immediately the factor $1-n_{\mathbf{q}\uparrow}$, which makes N singular unless we restrict $\mathbf{q}$ to unoccupied states, which we shall do. We can then omit the $1-n_{\mathbf{q}}$ factor.

Let us now calculate $\bar{G}=(N\omega-E)^{-1}$:

$$\bar{G}^{-1}=\begin{pmatrix}\omega-\epsilon_k-Un_{\uparrow} & -N^{-1/2}Un_{\uparrow}\\ -N^{-1/2}Un_{\uparrow} & \delta_{\mathbf{qq}'}n_{\uparrow}(\omega-\bar{\epsilon}_{\mathbf{kq}})-Un_{\uparrow}\end{pmatrix}. \tag{27}$$

To find the inverse, we write out the equations for $\bar{G}_{11}$, which from Eqs. (9) and (25) equals G_{11}, and $\bar{G}_{q1}$.

$$(\omega-\epsilon_{\mathbf{k}}-Un_{\uparrow})G_{11}-\sum_{\mathbf{q}}{}'Un_{\uparrow}N^{-1/2}\bar{G}_{q1}=1, \tag{28}$$

$$-Un_{\uparrow}N^{-1/2}G_{11}+n_{\uparrow}(\omega-\bar{\epsilon}_{kq})\bar{G}_{q1}-\sum_{\mathbf{q}'}{}'UnN^{-1}\bar{G}_{\mathbf{q}'1}=0. \tag{29}$$

Solving the second line for $\bar{G}_{q1}$,

$$\bar{G}_{q1}=\frac{U}{\omega-\bar{\epsilon}_{kq}}\left(\frac{G_{11}}{N^{1/2}}+\frac{1}{N}\sum_{q'}{}'\bar{G}_{q'1}\right). \tag{30}$$

Summing this over $\mathbf{q}$, solving for $\sum_{q'}{}'\bar{G}_{q1}$,

Summing this over $\mathbf{q}$, solving for $\sum'\bar{G}_{q1}$, and substituting into Eq. (28), we find

$$[\omega-\epsilon_k-\Sigma(k\omega)]G_{11}=1, \tag{31}$$

where

$$\Sigma(k\omega)=Un_\uparrow\left(1+\frac{U}{N}\sum_q\frac{1-n_q}{\epsilon_{kq}-\omega}\right)^{-1}. \tag{32}$$

This is the result for the reversed-spin one-particle Green's function which we have sought in this section.

COMPARISON WITH OTHER RESULTS

Let us now compare our result with other work. Consider first the two pole approximation for which we take the result of I and specialize to the fully aligned case. In Eqs. (73) and (74) of I, the down-spin one-particle Green's function is expressed in the same form as Eq. (31), with

$$\Sigma(k\omega)=n_\uparrow U\left(1+\frac{U(1-n_\uparrow)}{W_{k\uparrow}-\omega}\right)^{-1}, \tag{33}$$

where from Eq. (21) of I, now specialized to the case where we take all averages in the completely aligned state, we have

$$\begin{aligned}n_\uparrow(1-n_\uparrow)W_{k\uparrow}&=-\sum_{j\neq0}t_{0j}\langle c_{0\uparrow}c_{j\uparrow}\rangle+\sum_{j\neq0}t_{0j}e^{i\mathbf{k}\cdot\mathbf{R}_i}(\langle n_{j\uparrow}n_{0\uparrow}\rangle-n_\uparrow{}^2)\\&=N^{-1}\sum_{k'}\epsilon_{k'}n_{k'\uparrow}-N^{-2}\sum_{k'k''}n_{k'\uparrow}n_{k''\uparrow}\epsilon_{k'+k''-k}.\end{aligned} \tag{34}$$

This is also the result of Ref. 5. Suppose we now consider the result of averaging Eq. (26) for $\tilde{\epsilon}_{kq}$ over the unoccupied $\mathbf{q}$ states. We have

$$\begin{aligned}(1-n_\uparrow)^{-1}\sum_q(1-n_{q\uparrow})\tilde{\epsilon}_{kq}&=[n_\uparrow(1-n_\uparrow)N^2]^{-1}\\&\times\sum_{k'q}n_{k'\uparrow}(1-n_{q\uparrow})(\epsilon_{k'-q+k}+\epsilon_q-\epsilon_{k'}).\end{aligned} \tag{35}$$

A comparison of Eqs. (34) and (35), using the fact that $\sum_k\epsilon_k=0$ shows that the average in Eq. (35) is exactly equal to $W_{k\uparrow}$. Thus, the two-pole approximation in the fully aligned case is obtained from the present result by replacing the denominator in Eq. (32) by its average value.

In comparing our results with T-matrix approximations, we find that there are several formalisms, all of which give the same result at low densities. Let us consider that of Kanamori[6] who obtains an energy shift $\Delta E(\mathbf{kk}')$ for two electrons $\mathbf{k}$ and $\mathbf{k}'$, which we suppose have down and up spins, respectively, and let us generalize the result to cover unequal occupancy of up and down spins.

$$\Delta E_\downarrow(\mathbf{kk}')=UN^{-1}(1+Ug_\downarrow(\mathbf{kk}'))^{-1}, \tag{36}$$

where

$$g_\downarrow(\mathbf{kk}')=\frac{1}{N}\sum_q\frac{(1-n_{q\uparrow})(1-n_{k+k'-q\uparrow})}{\epsilon_{k+k'-q}+\epsilon_q-\epsilon_{k'}-\epsilon_k}. \tag{37}$$

The self-energy is now

$$\Sigma(\mathbf{k},\epsilon_k)=\sum_{k'}n_{k'\uparrow}\Delta E_\downarrow(\mathbf{kk}'). \tag{38}$$

We note that in Eq. (38), we have a sum over occupied states. If we replace ϵ_k by ω in Eq. (37) (i.e., go off the energy shell), and if we average the denominator over the occupied k' states noting that $n_{k\downarrow}=0$, we obtain the result of the present work.

A rather commonly used approximation to the T-matrix result is to place ϵ_k and $\epsilon_{k'}$ by the band edge energies, and so to obtain Eq. (36) with

$$g(\mathbf{kk}')=g(00)=\frac{1}{N}\sum_q\frac{(1-n_{q\uparrow})(1-n_{q\downarrow})}{2(\epsilon_q-\epsilon_b)}. \tag{39}$$

We shall refer to this as the Kanamori result and we shall compare it with the present calculation in the numerical example.

NUMERICAL RESULTS

We now wish to apply our result to the case of a simple cubic lattice with nearest-neighbor (nn) interaction, as in I. In order to carry out the integrals readily, we shall make one further approximation. That is, in Eq. (26), we would like to average the right-hand side over surfaces of constant energy in $\mathbf{q}$ as well as in $\mathbf{k}'$. This is the same as performing a cubic average. We can make the replacement

$$\epsilon_{k+k'-q}=t\sum_{R(\mathrm{nn})}e^{i\mathbf{k}\cdot\mathbf{R}}e^{i\mathbf{k}'\cdot\mathbf{R}}e^{-i\mathbf{q}\cdot\mathbf{R}}\rightarrow\frac{\epsilon_k\epsilon_{k'}\epsilon_q}{(tz)^2} \tag{40}$$

because all nn contribute alike to an average over constant energy surfaces which have cubic symmetry. Thus we can put

$$\tilde{\epsilon}_{kq}=y-y\epsilon_k\epsilon_q/(tz)^2+\epsilon_q, \tag{41}$$

where

$$y=(n_\uparrow N)^{-1}\sum_{k'}n_{k'\uparrow}\epsilon_{k'} \tag{42}$$

is the negative of the average electron energy in the occupied band. Using this approximation, we have for the self-energy

$$\Sigma(\mathbf{k}\omega)=Un_\uparrow\left(1+\frac{U}{N}\sum_q\frac{1-n_{q\uparrow}}{\epsilon_q[1-\epsilon_k y/(tz)^2]+y-\omega}\right)^{-1}. \tag{43}$$

We should point out that this approximation would also result from choosing for our basis set not c_k and A_{kq},

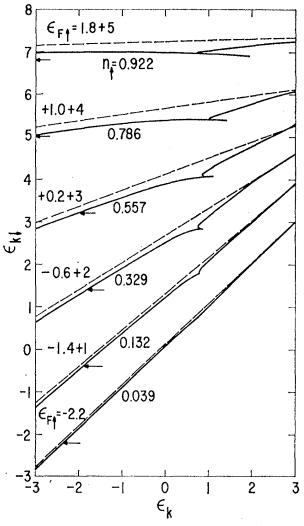

FIG. 1. Solid curves are the reversed-spin bands given by the solution of the equation $\omega_k=\epsilon_k+\mathrm{Re}\,\Sigma(\mathbf{k},\omega_k)$ as a function of $\mathbf{k}$ via the up-spin energy $\epsilon_k=\cos k_x a+\cos k_y a+\cos k_z a$, for varous values of the number $n_\uparrow$ of up spin electrons per site, and for $U\to\infty$. All curves but the lowest have been displaced upwards. Up-spin Fermi energy is given for each curve in terms of the original value plus the displacement, and is also indicated by the arrow. Dashed lines give the two pole approximation results. Units are such that the bandwidth is six.

but c_k and A_{kq} averaged over surfaces of constant energy in $\mathbf{q}$. The simplification also depends on the nearest-neighbor feature. We have not looked into how good the approximation is; however, for $\mathbf{k}=0$, Eq. (43) is equal to Eq. (32).

We can now calculate the Green's function given the density of states calculated by Wolfram and Calloway[11] in another context. We shall find that for some values of $\mathbf{k}$ and ϵ_F, the self energy is real, while for other regions it has an imaginary part. Neglecting at first the imaginary part, let us examine the reversed-spin energy given

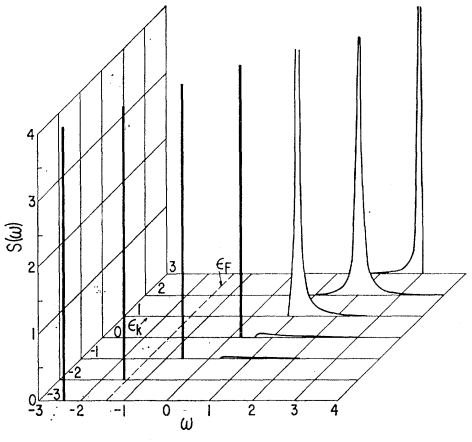

FIG. 2. Spectral function $S(\omega)=(1/\pi)\,\mathrm{Im}G(\omega)$ for reversed spin, for various wave vectors labeled by the associated energies ϵ_k and for $n=0.132$, $\epsilon_F=-1.4$, $U\to\infty$. The area under $S(\omega)$ is $1-n_\uparrow$ and the height of the δ function is scaled so that the area would be correct if it were a rectangle of width 0.2.

[11] T. Wolfram and J. Calloway, Phys. Rev. **130**, 2207 (1963).

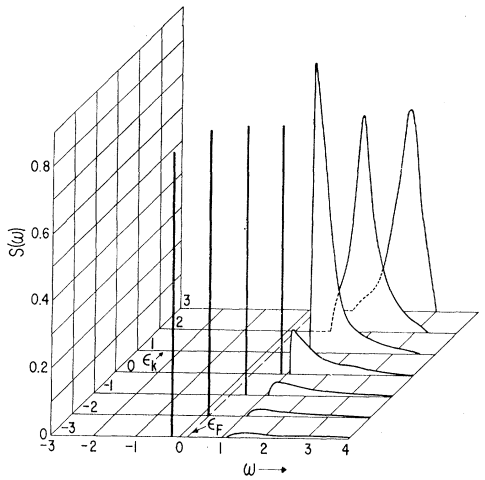

FIG. 3. Spectral function $S(\omega)=(1/\pi)\,\mathrm{Im}G_k(\omega)$ for reversed spin, for various wave vectors labeled by the associated energies ϵ_k, and for $n=0.557$, $\epsilon_F=0.2$, $U\to\infty$. The area under $S(\omega)$ is $1-n_\uparrow$, and the height of the δ function is scaled so that the area would be correct if it were a rectangle of width 1.

as the solution of the equation

$$\omega_k=\epsilon_k+\mathrm{Re}\Sigma(\mathbf{k},\omega_k). \tag{44}$$

This can be solved by Newton's method. Actually for $U\to\infty$, we use the following scheme. We let

$$\omega_k=\omega_1[1-\epsilon_k y/(tz)^2]+y, \tag{45}$$

where ω_1 is an auxiliary variable. Then for $U\to\infty$, Eq. (44) becomes

$$\omega_1(1-\epsilon_k y/(tz)^2)+y = \epsilon_k+\mathrm{Re}\left[n_\uparrow\left(\frac{1-\epsilon_k y}{(tz)^2}\right)\Big/\int_{\epsilon_F}^{\epsilon_t}\frac{\rho(\epsilon')}{(\epsilon'-\omega_1)\,d\epsilon'}\right]. \tag{46}$$

This can be solved for ϵ_k in terms of ω_1, and through Eq. (45) we obtain ω_k as a function of ϵ_k. The results are plotted in Fig. 1 for a number of values of the up-spin Fermi level, which is a measure of the number of electrons. The reversed-spin energies are plotted against the corresponding up spin energy which is a measure of the wave vector $\mathbf{k}$.

We can compare this result with the two-pole approximation result which is

$$\omega_k=\epsilon_k(1-n_\uparrow)+n_\uparrow W_{k\uparrow}, \tag{47}$$

where from Eqs. (34) and (42),

$$W_k=y(1-yn_\uparrow\epsilon_k/(tz)^2)/(1-n_\uparrow). \tag{48}$$

We have also included these results in the figure.

We see that the over-all behavior of the reversed-spin band is similar for the two approximations, but there is more structure in the present approximation results. We find that for small $\mathbf{k}$, the self-energy is real so that we are plotting the position of a simple pole in the Green's function. This can be interpreted as the energy of the down-spin quasiparticle. At a finite value of ϵ_k, the pole

becomes swallowed up by the continuum; this occurs at the position of the cusp in Fig. 1. We note that there are several solutions of Eq. (44) near this point, which indicates that the quasiparticle picture is breaking down in this region. Actually part of the detailed structure is an artifact of our approximation of averaging quantities over constant energy surfaces, and we find that the self-energy is going to zero as an inverse logarithm. Above the cusp the quasiparticle picture reemerges provided the broadening is not too great.

The reason for the behavior of the level width can be seen by examining the energy denominator in Eq. (32), which vanishes for

$$\omega=\epsilon_q+(n_\uparrow N)^{-1}\sum_{\mathbf{k}'}(\epsilon_{\mathbf{k}'+\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}'})n_{\mathbf{k}'\uparrow}. \tag{49}$$

The second term here is just the energy of a spin wave in the random-phase approximation.[5,12] Thus, the process which contributes to the broadening is the reversed-spin electron $\mathbf{k}$ going into an up-spin electron $\mathbf{q}$ plus a spin wave of wave vector $\mathbf{k}-\mathbf{q}$. This becomes possible when the reversed-spin band crosses the up-spin band, and the crossing occurs because of the band narrowing effect. At smaller k values, the reversed-spin electron should have a level broadening due to emission of up spin electron-hole pairs, but we have neglected this in our treatment.

To examine further the characteristics of the reversed-spin states, we have plotted the spectral function for three values of the up-spin Fermi energy in Figs. 2–4. We can see that for the lowest value of ϵ_F given, the quasiparticle states are generally well defined but for large ϵ_F (or n close to 1) the broadening becomes extreme and we can hardly talk about bands. Even for small $\mathbf{k}$, the δ function is losing strength to the continuum. We should remark that the two-pole approximation corresponds to replacing the spectral function by a single δ-function peak placed at the center of gravity.

We notice in Fig. 1 that for $\epsilon_F=1$, the lowest down-spin state has gone above the Fermi level. (Actually interpolating, we find that this occurs at $\epsilon_F=0.9$, $n_\uparrow=0.76$.) Above this value of ϵ_F, the ferromagnetic state is stable, while below it is unstable, although as pointed out in the Introduction, we can still study the reversed-spin states to compare approximations.

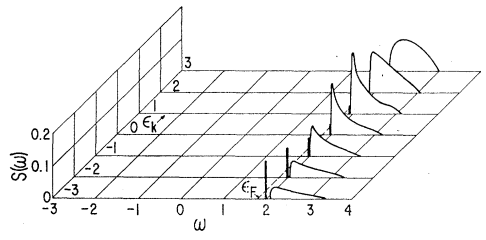

FIG. 4. Spectral function $S(\omega)=(1/\pi)\,\mathrm{Im}G_k(\omega)$ for reversed spin, for various wave vectors labeled by the associated energies ϵ_k, and for $n=0.922$, $\epsilon_F=1.8$, $U\to\infty$. The area under $S(\omega)$ is $1-n_\uparrow$ and the height of the δ function is scaled so that the area would be correct if it were a rectangle of width 0.5.

[12] T. Izuyama, Progr. Theoret. Phys. (Kyoto) **23**, 969 (1960).

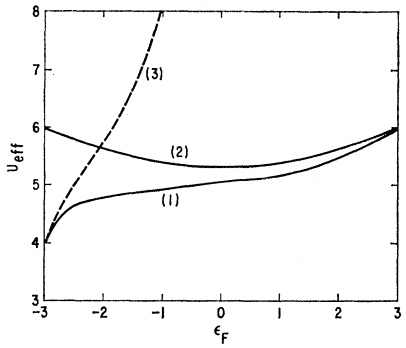

FIG. 5. Effective exchang splitting parameter $U_{\mathrm{eff}}=\sum(0,\omega_0)/n_\uparrow$, for $U\to\infty$, versus up-spin Fermi energy. (1) Present calculation, (2) two-pole approximation, and (3) Kanamori result.

To make a comparison with the Kanamori result, let us consider the $\mathbf{k}=0$ down-spin state, and let us define a quantity U_{eff} in the following way:

$$E_\downarrow(\mathbf{k}=0)-\epsilon_b=n_\uparrow U_{\mathrm{eff}}. \tag{50}$$

We shall call the value of U_{eff} we obtain in the present calculation, $U_{\mathrm{eff}}{}^{(1)}$. The two-pole approximation gives

$$U_{\mathrm{eff}}{}^{(2)}=-\epsilon_b+W_{\mathrm{k}}, \tag{51}$$

and the Kanamori result gives

$$U_{\mathrm{eff}}{}^{(3)}=\left[\frac{1}{2N}\sum_{\mathrm{q}}\frac{1-n_{\mathrm{q}}}{\epsilon_{\mathrm{q}}-\epsilon_b}\right]^{-1}. \tag{52}$$

The three are plotted in Fig. 5. We see that the present approximation agrees with the Kanamori result for very small n, but that as n increases, the Kanamori result increases much more rapidly than either of our results. This appears to be due to the neglect of the frequency dependence of the self-energy.

It is interesting to note that for intermediate values of occupation of the bands, the two-pole result and the present result for U_{eff} are quite close together.

We can also calculate the residue Z at the pole in the Green's function, or the spectral weight of the state. The results are plotted versus ϵ_F in Fig. 6, for both the two-pole approximation, in which case it is given by

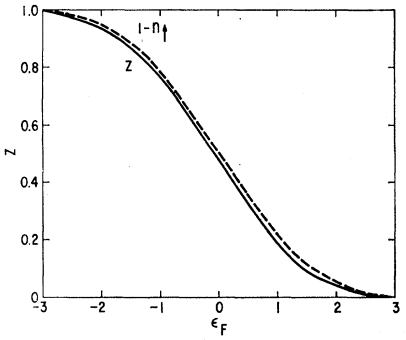

FIG. 6. Residue Z at the pole in the Green's function for $\mathbf{k}=0$, $U\to\infty$, versus up-spin Fermi energy. Solid line is the present work, dashed line is the two-pole approximation.

$1-n_\uparrow$, and for the improved calculation, for which

$$Z=1/(1-d\Sigma/d\omega). \tag{53}$$

We see that the two results are almost identical.

DISCUSSION

Perhaps the most interesting result of the present work is that for U_{eff} in Fig. 5. If U_{eff} is to be equated with the exchange splitting in the Stoner model, then we find that the Kanamori result for this quantity departs more rapidly from the low-density result than does the present calculation, as the number of carriers increases. If we believe that an improved calculation gives more correlation reduction of this quantity, then we must say that our result is an improvement and that the Kanamori result overestimates the increase of U_{eff}. The above belief would be a fact if the claim made in I for a minimum principle were verified. At any rate, these considerations may have serious consequences as for example in the work of Calloway's[8] recent article in which he finds that the increase in U_{eff} is very important in stabilizing the ferromagnetic state for small but finite n. This effect seems also to be important in Ni.[7]

There are several mitigating factors here. One is that we are considering the worst possible case, namely, $U\to\infty$. Secondly, we are using the scnn model, and the work of Calloway in particular is based on a second-neighbor face-centered cubic model which has, like nickel, a peak in the density of states near the band edge. The argument here is that the Kanamori result should be good in this case, as the Fermi level is very close to the band edge. We should examine U_{eff} in this case and hope to do so in the future. Calloway has also applied his result to Ni[13] and the same remarks apply, with the additional factor that he considers, and we neglect, degeneracy. Finally, to compare our work with that of Lang and Ehrenreich,[7] for example, we need to find the corresponding quantity for the paramagnetic state. U_{eff} may not be the same for the ferromagnetic and paramagnetic states, as pointed out recently by Penn.[14]

Nevertheless, it does appear that the Kanamori result can be improved upon and extended to higher densities by methods based on the present work, and also that the two pole approximation gives a reasonable value for U_{eff} at finite carrier densities.

[13] J. Calloway and H. M. Zhaver, Phys. Letters **28A**, 292 (1969).
[14] D. R. Penn, Phys. Rev. **177**, 839 (1969).

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Friedel Density Oscillations about a Coulombic Impurity in a High Magnetic Field

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The density perturbation $\delta\rho(\mathbf{r})$ about a Coulombic impurity in strong magnetic fields is analyzed in the degenerate case. The results show that (a) anisotropic Friedel oscillatory behavior is discernible along the direction parallel to the magnetic field, and (b) exponential decay along the direction perpendicular to the magnetic field deprives the result of long-range character. These results are in accord with those of Rensink, save for the fact that the δ-function impurity used by Rensink results in a Gaussian decay in the perpendicular direction, in contrast to the exponential decay in the perpendicular direction seen to result from a Coulombic impurity here. This indicates that the qualitative nature of the spatial decay in the perpendicular direction is dependent upon the character of the impurity potential. The results obtained here are valid at large distances from the impurity for a wide range of field strengths. A qualitative discussion of low-field behavior in the approach to the zero-field limit is presented, and the role of self-consistent aspects of response is briefly indicated.

I. INTRODUCTION AND FORMULATION

THE study[1] of the dynamical properties of a quantum plasma in a high magnetic field has revealed the existence of interesting physical effects due to Landau quantization and nonlocality. Moreover, one may expect static properties to be correspondingly

[1] N. J. Horing, Ann. Phys. (N. Y.) **31**, (1965). The notation of this reference will be maintained here, and a brief review follows: $\omega_p=(4\pi e^2\rho/m)^{1/2}$; ρ is the density; m is the effective mass; ω_c is the cyclotron frequency ($=eH/mc$); $\mathbf{p}$ is the wave vector $[=(p_z,\tilde{p})]$; $\mathbf{r}$ is the position vector from impurity $[=(r_z,\tilde{r})]$; $\mathbf{H}$ is the magnetic field along the z axis; $\beta=(KT)^{-1}$; K is Boltzmann's constant; T is the absolute temperature; ζ is the chemical potential, equal to the Fermi energy E_F in the degenerate limit; $f_0(\omega)$ is the Fermi-Dirac distribution function $[=(1+e^{(\omega-\zeta)\beta})^{-1}]$; p_F is the Fermi wave number $[=(2m\zeta)^{1/2}/\hbar]$; and p_D is the Debye-Thomas-Fermi (DTF) wave number $[=(4\pi e^2\partial\rho/\partial\zeta)^{1/2}]$. (Also, r_0 is the interparticle spacing, a_0 is the Bohr radius, and $r_s=r_0/a_0$.) Note that two-vectors referring to the plane perpendicular to the magnetic field are represented by lightface barred letters.