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[21] The lack of this structure has been pointed out by A. J. Hughes, D. Jones, and A. H. Lettington, J. Phys. C 2, 102 (1969).

[22] M. A. Biondi and A. I. Gurobadia, Phys. Rev. 166, 667 (1968); L. W. Bos and D. W. Lynch, Phys. Rev. Letters 25, 156 (1970).

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[24] The optical mass m_{opt} introduced here will be discussed in Sec. V.

[25] C. J. Powell and J. B. Swan, Phys. Rev. 115, 869 (1959).

[26] This point has already been emphasized by J. C. Phillips, Solid State Phys. 18, 55 (1966), in particular, p. 72.

[27] Although it is not *a priori* obvious that the interband relaxation time τ is the same as the intraband equivalent τ_0, it is nonetheless difficult to see how they can differ substantially.

[28] This rule has been established by P. C. Martin, Phys. Rev. 161, 143 (1967), but only insofar as the system (here nearly free-electron-like metals) can be regarded as translationally invariant.

[29] D. Brust, Solid State Commun. 8, 413 (1970).

[30] It follows that knowing V_{200} alone (as given for example by the position of the principal absorption peak), one can determine a bound on V_{111} by using the measured optical mass. (Strictly speaking this will be a bound on the component of the optical pseudopotential.) If this is done in Al the value of V_{111} so obtained is within a few percent of the Fermi-surface predicted value. In other metals this method may give a useful preliminary estimate of (optical) band gaps as well as imposing an overall limitation on their absolute values.

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Correlation Energy of the Electron Gas at Metallic Densities*

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The electron gas at metallic densities is studied by means of a quadratic boson Hamiltonian which includes the direct and exchange processes among the electrons but neglects the scattering of electron-hole pairs. This Hamiltonian is further separated into two independent parts which describe the singlet and triplet states of the electron-hole pairs. These parts are diagonalized in an approximation in which the exchange interaction is treated on the average. A dielectric function for all momentum transfers is thereby obtained. The correlation energy is the sum of the ground-state energies of the singlet and triplet Hamiltonians. Its value, calculated for the metallic density range ($r_s = 1-6$), is found to be about two-thirds of that in the random-phase approximation. It is consequently numerically smaller than most other estimates. The triplet contribution is very considerable. The triplet ground state is predicted to be unstable for $r_s > 9.4$.

I. INTRODUCTION

The correlation energy of an electron gas was defined by Wigner[1] to be the difference between the true ground-state energy and that calculated in the Hartree-Fock approximation. It is a function of the specific interparticle separation r_s, the Bohr radius a_0 being taken as unity. In the high-density ($r_s \ll 1$) and low-density ($r_s \gg 1$) limits, its value has been calculated very accurately by Gell-Mann and Brueckner[2] and Coldwell-Horsfall and Maradudin,[3] respectively. If we regard the electron gas as a model of real metals, we must consider its behavior in the intermediate-density region $1 < r_s < 6$. A number of estimates of the correlation energy at metallic densities have been made by means of interpolation methods. Wigner[4] and Carr and Maradudin[5] have interpolated between the high- and low-density limits. Another method is to interpolate between the contributions from processes of high- and low-momentum transfers, as was done by Hubbard[6] and Nozières and Pines.[7] There is also a variational calculation by Gaskell.[8] These investigations and many others have indicated that the properties of an electron gas even at metallic densities are very similar to those at high density.

It has been shown by Sawada[9] that the high-density results of Gell-Mann and Brueckner can be obtained from a Hamiltonian quadratic in quasiboson operators. These operators describe the creation and annihilation of electron-hole pairs and approximately obey Bose commutation rules at high density. The Sawada Hamiltonian takes into account the direct interaction between electrons in the singlet state, and is equivalent to the random-phase approximation of Bohm and Pines. As the density is lowered to the metallic region other processes become considerable, and corrections to the Sawada Hamiltonian must be made. The sources of these corrections are four: (i) the exchange interaction, (ii) the contribution from the triplet state, (iii) the deviation from Bose behavior, and (iv) the interaction between electron-hole pairs. These corrections can be systematically calculated by transcribing the electron-gas Hamiltonian in terms of ideal boson operators. This method is due to Usui,[10] who applied it to calculate the exchange corrections to the properties of a spinless electron gas at high density.

In this work we present a calculation of the correlation energy of the electron gas at metallic densities in the approach of the Usui-transformed boson Hamiltonian. In Sec. II the Usui transformation is discussed at some length, leading in Sec. III to a boson Hamiltonian which is a generalization of the one derived by Usui to the case of spin-$\frac{1}{2}$ electrons. In Sec. IV the Hamiltonian is separated into a singlet and a triplet part and diagonalized by a canonical transformation; the resulting eigenvalue equations are solved approximately. In Sec. V further approximations are made so that finally we obtain a dielectric function similar in form to that in the random-phase approximation but modified by a pair of interpolation functions. In Sec. VI the correlation energy is calculated and compared with some previous results. In Sec. VII the stability of the paramagnetic ground state of the electron gas is briefly discussed.

II. TRANSITION TO BOSON OPERATORS

We consider a gas of N electrons at zero temperature in a volume Ω, interacting through the Coulomb potential with one another and with a uniform background of neutralizing positive charge density. Its Hamiltonian is given as follows:

$$\begin{aligned}
H_F &= T + V,\\
T &= \sum_{\vec{p}\sigma} \epsilon_{\vec{p}} a^\dagger_{\vec{p}\sigma} a_{\vec{p}\sigma},\\
V &= \frac{1}{2\Omega} \sum_{\substack{\vec{p}\vec{p}'\vec{q}\\ \sigma\sigma'}} V(\vec{q}) a^\dagger_{\vec{p}+\vec{q}\sigma} a^\dagger_{\vec{p}'-\vec{q}\sigma'} a_{\vec{p}'\sigma'} a_{\vec{p}\sigma},\\
\epsilon_{\vec{p}} &= p^2/2m,\\
V(\vec{q}) &= 4\pi e^2/q^2, \quad q \neq 0\\
&= 0, \qquad\qquad q = 0.
\end{aligned} \tag{2.1}$$

The creation and annihilation operators satisfy the Fermi commutation rules

$$\begin{aligned}
[a_{\vec{p}\sigma}, a^\dagger_{\vec{p}'\sigma'}]_+ &= \delta_{\vec{p}\vec{p}'} \delta_{\sigma\sigma'},\\
[a^\dagger_{\vec{p}\sigma}, a^\dagger_{\vec{p}'\sigma'}]_+ &= 0.
\end{aligned} \tag{2.2}$$

We define the specific interparticle separation r_s by the relation

$$\Omega/N = \tfrac{4}{3}\pi(r_s a_0)^3, \quad a_0 = (me^2)^{-1}. \tag{2.3}$$

In the absence of the interaction the ground state is the paramagnetic Fermi sphere of radius p_F given by

$$(2\pi)^3(N/\Omega) = \tfrac{8}{3}\pi p_F^3, \tag{2.4}$$

each momentum state inside the sphere being occupied by two electrons of opposite spin. The effect of the interaction is to transport electrons from the inside to the outside of the Fermi sphere with conservation of spin. This action can be described by electron-hole-pair creation operators of the form

$$a^\dagger_{\vec{P}\sigma} a_{\vec{p}\sigma}, \quad P > p_F, \quad p < p_F. \tag{2.5}$$

The usefulness of these operators in the study of the electron gas at high density has been demonstrated by Sawada. Thus any paramagnetic state of the electron gas can be obtained by operating on the Fermi sphere with a selected set of the operators (2.5). It is therefore convenient to express the Hamiltonian (2.1) in terms of them. However, these operators obey neither Fermi nor Bose commutation rules, being approximately Bose-like only in the limit of high density. This difficulty can be overcome by a transformation of Usui in which the Hamiltonian is rewritten in terms of ideal boson operators.

We shall describe in some detail the Usui transformation. Consider a set of boson operators

$$C^{\vec{P}}_{\vec{p}\sigma}, \quad P > p_F, \quad p < p_F \tag{2.6}$$

satisfying the Bose commutation rules

$$\begin{aligned}
[C^{\vec{P}}_{\vec{p}\sigma}, C^{\vec{P}'\dagger}_{\vec{p}'\sigma'}] &= \delta_{\vec{p}\vec{p}'} \delta_{\vec{P}\vec{P}'} \delta_{\sigma\sigma'},\\
[C^{\vec{P}}_{\vec{p}\sigma}, C^{\vec{P}'}_{\vec{p}'\sigma'}] &= [C^{\vec{P}\dagger}_{\vec{p}\sigma}, C^{\vec{P}'\dagger}_{\vec{p}'\sigma'}] = 0.
\end{aligned} \tag{2.7}$$

We can generate a boson-state space by applying the boson creation operators to the boson vacuum state $|0)$. We then try to set up a one-to-one correspondence between this boson-state space and the paramagnetic-electron-state space generated by the application of the pair creation operators (2.5) to the Fermi sphere $|0\rangle$. First we can easily map the Fermi sphere into the boson vacuum and the one-pair states into the one-boson states; that is,

$$\begin{aligned}
|0\rangle &\to |0),\\
a^\dagger_{\vec{P}\sigma} a_{\vec{p}\sigma} |0\rangle &\to C^{\vec{P}\dagger}_{\vec{p}\sigma} |0).
\end{aligned} \tag{2.8}$$

However, for states containing more than one pair, ambiguities arise. For example, to the two-pair state

$$a^\dagger_{\vec{P}\sigma} a_{\vec{p}\sigma} a^\dagger_{\vec{P}'\sigma} a_{\vec{p}'\sigma} |0\rangle, \tag{2.9}$$

there correspond two two-boson states

$$C^{\vec{P}\dagger}_{\vec{p}\sigma}\, C^{\vec{P}'\dagger}_{\vec{p}'\sigma}|0) , \qquad C^{\vec{P}\dagger}_{\vec{p}'\sigma} C^{\vec{P}'\dagger}_{\vec{p}\sigma} |0). \tag{2.10}$$

Whereas the interchange of the pair of annihilation operators in the fermion state (2.9) produces only a change of sign, the corresponding permutation of the lower indices of the boson state produces a different state which is orthogonal to the former. Moreover, for $\vec{p}=\vec{p}'$, the fermion state vanishes but the boson state does not. A similar situation occurs for fermion states with more than two pairs. What is needed to resolve these ambiguities is a criterion for choosing one particular boson state to correspond to the fermion state. We shall therefore assume that the momentum vectors have been assigned a certain order the nature of which will be specified later. Now the pair creation operators of an arbitrary fermion state can be grouped into two independent classes according to the two values of the spin index. We can treat each class separately. Within each class we have a set of indices $\vec{P}$ and a set of indices $\vec{p}$. Consider all the boson states that can be formed with the same sets of indices. We call that boson state physical if, when the upper indices are permuted into the prescribed order, the lower indices are simultaneously arranged in conformity with that order. The other states, together with those having two or more identical indices, are called unphysical. And we map the fermion state into the physical boson state. Thus we have established a one-to-one correspondence between the fermion-state space and a certain subspace of the boson-state space.

The operator effecting this transformation has been worked out by Usui. Consider the product space of the fermion- and boson-state spaces. Then the operator that transforms a fermion state

$$\Pi\, a^{\dagger}_{\vec{P}\sigma} a_{\vec{p}\sigma} |0\rangle\, |0) \tag{2.11}$$

into the corresponding physical boson state

$$\Pi\, C^{\vec{P}\dagger}_{\vec{p}\sigma} |0\rangle\, |0) \tag{2.12}$$

is given by

$$U= O\Gamma_F \exp\Bigl(\sum_{\vec{P}\vec{p}\sigma} C^{\vec{P}\dagger}_{\vec{p}\sigma}\, a^{\dagger}_{\vec{p}\sigma} a_{\vec{P}\sigma}\Bigr)\Gamma_B \,. \tag{2.13}$$

Here Γ_F, Γ_B, and O are projection operators onto $|0\rangle$, $|0)$, and the physical boson subspace, respectively. In the above, whenever a product of fermion operators occurs, it must be assumed that the momenta are already ordered to remove an ambiguity in sign. The inverse transformation is given by the Hermitian conjugate $U^\dagger$.

III. BOSON HAMILTONIAN

Using the transformation U we can translate the dynamics of the electron gas into that of a system of interacting bosons. The fermion Hamiltonian H_F of (2.1) is transformed into a boson Hamiltonian H_B:

$$H_B = U H_F\, U^\dagger . \tag{3.1}$$

An easy method to calculate H_B is to expand it into a power series of physically ordered normal products of C and $C^\dagger$. The expansion coefficients can be expressed as the vacuum expectation values of certain multiple commutators involving H_B. These can be calculated since they are equal to the expectation values of the corresponding commutators of H_F in the Fermi sphere.

It can be shown that H_B can be decomposed as follows:

$$H_B = H_0 + H_2 + H_3 + H_4, \tag{3.2}$$

where H_0 is a constant and H_2, H_3, and H_4 are quadratic, cubic, and quartic in boson operators, respectively. The linear term vanishes because of translational invariance. There are no terms beyond the quartic because of the restrictions on the momentum indices in (2.6). We have

$$\begin{aligned} H_0 &= (0|H_B|0) = \langle 0|H_F|0\rangle \\ &= 2 \sum_{p<p_F} \epsilon_{\vec{p}} - \frac{1}{\Omega} \sum_{p,p'<p_F} V(\vec{p}-\vec{p}') \,. \end{aligned} \tag{3.3}$$

This is recognized as the Hartree-Fock approximation of the ground-state energy. Therefore the ground-state expectation value of the remaining terms in (3.2) is by definition the correlation energy. We represent H_2 as follows:

$$\begin{aligned} H_2 = \sum_{\substack{\vec{P}\vec{p}\sigma \\ \vec{P}'\vec{p}'\sigma'}} \Bigl[& D^{\vec{P}\vec{p}\sigma}_{\vec{P}'\vec{p}'\sigma'} C^{\vec{P}\dagger}_{\vec{p}\sigma} C^{\vec{P}'}_{\vec{p}'\sigma'} \\ & + \tfrac{1}{2} E^{\vec{P}\vec{p}\sigma}_{\vec{P}'\vec{p}'\sigma'} \bigl(C^{\vec{P}\dagger}_{\vec{p}\sigma} C^{\vec{P}'\dagger}_{\vec{p}'\sigma'} + \text{H. c.}\bigr)\Bigr] , \end{aligned} \tag{3.4}$$

where

$$\begin{aligned} D^{\vec{P}\vec{p}\sigma}_{\vec{P}'\vec{p}'\sigma'} &= (0|[[C^{\vec{P}}_{\vec{p}\sigma}, H_B], C^{\vec{P}'\dagger}_{\vec{p}'\sigma'}]|0) \\ &= \langle 0|[[a^{\dagger}_{\vec{p}\sigma} a_{\vec{P}\sigma}, H_F], a^{\dagger}_{\vec{P}'\sigma'} a_{\vec{p}'\sigma'}]|0\rangle \\ &= (\tilde{\epsilon}_{\vec{P}} - \tilde{\epsilon}_{\vec{p}})\delta_{\vec{p}\vec{p}'}\delta_{\vec{P}\vec{P}'}\delta_{\sigma\sigma'} \\ &\quad + \Omega^{-1}[V(\vec{P}-\vec{p}) - \delta_{\sigma\sigma'} V(\vec{p}-\vec{p}')]\delta_{\vec{P}-\vec{p},\vec{P}'-\vec{p}'} \,, \\ E^{\vec{P}\vec{p}\sigma}_{\vec{P}'\vec{p}'\sigma'} &= (0|[C^{\vec{P}'}_{\vec{p}'\sigma'}, [C^{\vec{P}}_{\vec{p}\sigma}, H_B]]|0) \\ &= \langle 0|[a^{\dagger}_{\vec{p}'\sigma'} a_{\vec{P}'\sigma'}, [a^{\dagger}_{\vec{p}\sigma} a_{\vec{P}\sigma}, H_F]]|0\rangle \\ &= \Omega^{-1}[V(\vec{P}-\vec{p}) - \delta_{\sigma\sigma'} V(\vec{P}-\vec{p}\,')]\delta_{\vec{P}+\vec{P}',\vec{p}+\vec{p}'} \,. \end{aligned} \tag{3.5}$$

Here $\tilde{\epsilon}_{\vec{p}}$ is the Hartree-Fock approximation of the electron energy:

$$\tilde{\epsilon}_{\vec{p}} = \epsilon_{\vec{p}} - \frac{1}{\Omega} \sum_{k<p_F} V(\vec{p}-\vec{k}) \,. \tag{3.6}$$

Substituting (3.5) into (3.4) and making a change of notation

$$C^{\vec{P}}_{\vec{p}\sigma} \to C_{\vec{p}\sigma}(\vec{q}) , \tag{3.7}$$

where $\vec{q} = \vec{P} - \vec{p}$ is the momentum transfer, we obtain

$$\begin{aligned} H_2 = &\sum_{\vec{q}\vec{p}\sigma} (\tilde{\epsilon}_{\vec{p}+\vec{q}} - \tilde{\epsilon}_{\vec{p}}) C^\dagger_{\vec{p}\sigma}(\vec{q})\, C_{\vec{p}\sigma}(\vec{q}) \\ &+ \frac{1}{2\Omega} \sum_{\substack{\vec{q}\vec{p}\vec{p}' \\ \sigma\sigma'}} \{2[V(\vec{q}) - \delta_{\sigma\sigma'} V(\vec{p} - \vec{p}')] C^\dagger_{\vec{p}\sigma}(\vec{q}) C_{\vec{p}'\sigma'}(\vec{q}) \\ &+ [V(\vec{q}) - \delta_{\sigma\sigma'} V(\vec{p} + \vec{p}' + \vec{q})] \\ &\times [C^\dagger_{\vec{p}\sigma}(\vec{q}) C^\dagger_{-\vec{p}'\sigma'}(-\vec{q}) + \text{H. c.}]\} . \end{aligned} \tag{3.8}$$

The summation of $\vec{q}$ ranges over the whole momentum space. For each $\vec{q}$ the summations of $\vec{p}$ and $-\vec{p}'$ are restricted to those regions inside the Fermi sphere such that $\vec{p} + \vec{q}$ and $-\vec{p}' - \vec{q}$ lie outside the sphere. These are depicted as regions 1 and 1′, respectively, in Fig. 1 for the special case $q < p_F$. They are formed by the intersections of the Fermi sphere and two other identical spheres centered at $\pm\vec{q}$. They overlap in region 2. For $q > p_F$ region 2 becomes simply connected; and for $q > 2p_F$ all three regions 1, 1′, and 2 coincide with the Fermi sphere.

When $\vec{p}$ and $-\vec{p}'$ both lie in region 2, the summations must be further restricted so that no unphysical ordering of the indices of operator products of the form $C^\dagger C^\dagger$ or CC should occur. The reason for this restriction of ordering is that in region 2 an electron can go out of the Fermi sphere by absorbing either a momentum $\vec{q}$ or $-\vec{q}$. It is convenient to order the momentum vectors according to the magnitude of their projections along $\vec{q}$. Then in the last term of (3.8), when both $\vec{p}$ and $-\vec{p}'$ are in region 2, we should retain only those terms for which $\vec{p} \cdot \vec{q} > -\vec{p}' \cdot \vec{q}$. This means that whenever two electrons in region 2 are to be excited simultaneously out of the Fermi sphere by the absorption of momentum transfers $\vec{q}$ and $-\vec{q}$, we shall adopt the convention that the one whose momentum has a greater projection along $\vec{q}$ acquires the momentum transfer $\vec{q}$. This restriction on the summation is equivalent to the replacement

$$\begin{aligned} &C^\dagger_{\vec{p}\sigma}(\vec{q}) C^\dagger_{-\vec{p}'\sigma'}(-\vec{q}) \\ &\quad \to [1 - \delta_{\sigma\sigma'} \theta_2(-(\vec{p} + \vec{p}') \cdot \vec{q})] C^\dagger_{\vec{p}\sigma}(\vec{q}) C^\dagger_{-\vec{p}'\sigma'}(-\vec{q}), \end{aligned} \tag{3.9}$$

and similarly for the Hermitian conjugate. Here θ_2 is zero outside region 2 and when its argument is negative; otherwise its value is 1. Substituting (3.9) into (3.8), we finally obtain

$$\begin{aligned} H_2 = &\sum_{\vec{q}\vec{p}\sigma} (\tilde{\epsilon}_{\vec{p}+\vec{q}} - \tilde{\epsilon}_{\vec{p}}) C^\dagger_{\vec{p}\sigma}(\vec{q}) C_{\vec{p}\sigma}(\vec{q}) \\ &+ \frac{1}{2\Omega} \sum_{\substack{\vec{q}\vec{p}\vec{p}' \\ \sigma\sigma'}} \{2[V(\vec{q}) - \delta_{\sigma\sigma'} V(\vec{p} - \vec{p}')] C^\dagger_{\vec{p}\sigma}(\vec{q}) C_{\vec{p}'\sigma'}(\vec{q}) \\ &+ [V(\vec{q}) - \delta_{\sigma\sigma'} W(\vec{p} + \vec{p}', \vec{q})] \\ &\times [C^\dagger_{\vec{p}\sigma}(\vec{q}) C^\dagger_{-\vec{p}'\sigma'}(-\vec{q}) + \text{H. c.}]\} , \end{aligned} \tag{3.10}$$

where

$$\begin{aligned} W(\vec{p} + \vec{p}', \vec{q}) = &V(\vec{p} + \vec{p}' + \vec{q}) + \theta_2(-(\vec{p} + \vec{p}') \cdot \vec{q}) \\ &\times [V(\vec{q}) - V(\vec{p} + \vec{p}' + \vec{q})] , \end{aligned} \tag{3.11}$$

which is even under inversion in momentum space.

The cubic and quartic parts of (3.2) can be calculated and treated in a similar manner. They describe the scattering processes of the electron-hole pairs. In this work, however, they will be taken to be negligible and discarded. This is equivalent to assuming that even at metallic densities the fraction of electrons excited out of the Fermi sphere is still small.

IV. DIAGONALIZATION

We introduce singlet and triplet operators A and B, respectively, as follows:

$$\begin{aligned} A_{\vec{p}}(\vec{q}) &= \tfrac{1}{2}\sqrt{2}\, [C_{\vec{p}\uparrow}(\vec{q}) + C_{\vec{p}\downarrow}(\vec{q})] , \\ B_{\vec{p}}(\vec{q}) &= \tfrac{1}{2}\sqrt{2}\, [C_{\vec{p}\uparrow}(\vec{q}) - C_{\vec{p}\downarrow}(\vec{q})] . \end{aligned} \tag{4.1}$$

By (2.7) these satisfy the Bose commutation rules

$$[A_{\vec{p}}(\vec{q}), A^\dagger_{\vec{p}'}(\vec{q}')] = [B_{\vec{p}}(\vec{q}), B^\dagger_{\vec{p}'}(\vec{q}')] = \delta_{\vec{p}\vec{p}'} \delta_{\vec{q}\vec{q}'} , \tag{4.2}$$

all other commutators vanishing. In terms of A and B, H_2 is separated into two independent parts:

$$H_2 = H^{(1)} + H^{(3)} , \tag{4.3}$$

where

$$\begin{aligned} H^{(1)} = &\sum_{\vec{q}\vec{p}} (\tilde{\epsilon}_{\vec{p}+\vec{q}} - \tilde{\epsilon}_{\vec{p}}) A^\dagger_{\vec{p}}(\vec{q}) A_{\vec{p}}(\vec{q}) \\ &+ \frac{1}{2\Omega} \sum_{\vec{q}\vec{p}\vec{p}'} \{2[2V(\vec{q}) - V(\vec{p} - \vec{p}')] A^\dagger_{\vec{p}}(\vec{q}) A_{\vec{p}'}(\vec{q}) \\ &+ [2V(\vec{q}) - W(\vec{p} + \vec{p}', \vec{q})][A^\dagger_{\vec{p}}(\vec{q}) A^\dagger_{-\vec{p}'}(-\vec{q}) + \text{H. c.}]\} , \end{aligned} \tag{4.4}$$

$$\begin{aligned} H^{(3)} = &\sum_{\vec{q}\vec{p}} (\tilde{\epsilon}_{\vec{p}+\vec{q}} - \tilde{\epsilon}_{\vec{p}}) B^\dagger_{\vec{p}}(\vec{q}) B_{\vec{p}}(\vec{q}) \\ &- \frac{1}{2\Omega} \sum_{\vec{q}\vec{p}\vec{p}'} \{2V(\vec{p} - \vec{p}') B^\dagger_{\vec{p}}(\vec{q}) B_{\vec{p}'}(\vec{q}) \end{aligned}$$

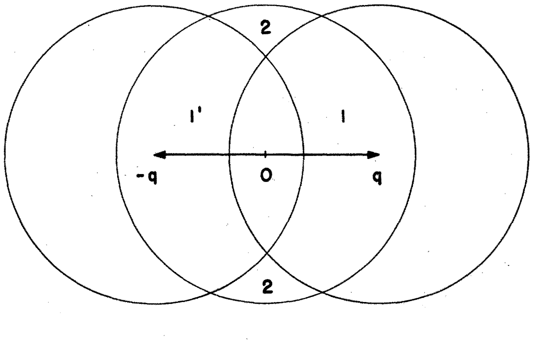

FIG. 1. Regions of summation in momentum space ($q < p_F$).

$$+\,W(\vec{p}+\vec{p}\,',\vec{q})[B^{\dagger}_{\vec{p}}(\vec{q})B^{\dagger}_{-\vec{p}\,'}(-\vec{q})+\mathrm{H.\,c.}]\}\;. \tag{4.5}$$

Both $\vec{p}$ and $\vec{p}\,'$ are summed over region 1. The singlet Hamiltonian $H^{(1)}$ is a generalization of the Sawada Hamiltonian. The electron kinetic energy is now replaced by the quasiparticle energy in the Hartree-Fock approximation. The terms in $V(\vec{q})$ represent the direct interaction. Those in W containing θ_2 represent the deviation of the electron-hole pairs from true Bose behavior. They may be regarded as a kinematical interaction whose origin can be traced back to the Pauli exclusion principle. The remaining terms can be identified with the matrix elements for various exchange processes. In the following calculations we need only consider $H^{(1)}$; the corresponding results for the triplet Hamiltonian $H^{(3)}$ can be obtained by setting the direct interaction equal to zero.

The correlation energy of the electron gas is now the sum of the ground-state energies of $H^{(1)}$ and $H^{(3)}$. Both the ground-state energies and the excitation spectra can be obtained by diagonalizing the Hamiltonians by a canonical transformation. Consider the transformation to a set of new boson operators $\tilde{A}$:

$$\tilde{A}_{\vec{k}}(\vec{q})=\sum_{\vec{p}}^{1}[\alpha_{\vec{k}\vec{p}}(\vec{q})A_{\vec{p}}(\vec{q})+\beta_{\vec{k}\vec{p}}(\vec{q})A^{\dagger}_{-\vec{p}}(-\vec{q})]\;. \tag{4.6}$$

The superscript 1 indicates the region of summation. α and β are real, having the symmetry properties

$$\begin{aligned}\alpha_{-\vec{k},-\vec{p}}(-\vec{q})&=\alpha_{\vec{k}\vec{p}}(\vec{q})\;,\\ \beta_{-\vec{k},-\vec{p}}(-\vec{q})&=\beta_{\vec{k}\vec{p}}(\vec{q})\;,\end{aligned} \tag{4.7}$$

and satisfying the identities

$$\begin{aligned}&\sum_{\vec{p}}^{1}[\alpha_{\vec{k}\vec{p}}(\vec{q})\alpha_{\vec{k}'\vec{p}}(\vec{q})-\beta_{\vec{k}\vec{p}}(\vec{q})\beta_{\vec{k}'\vec{p}}(\vec{q})]=\delta_{\vec{k}\vec{k}'}\;,\\ &\sum_{\vec{k}}^{\vec{q}}[\alpha_{\vec{k}\vec{p}}(\vec{q})\alpha_{\vec{k}\vec{p}'}(\vec{q})-\beta_{\vec{k}\vec{p}}(\vec{q})\beta_{\vec{k}\vec{p}'}(\vec{q})]=\delta_{\vec{p}\vec{p}'}\;,\\ &\sum_{\vec{p}}^{1}[\alpha_{\vec{k}\vec{p}}(\vec{q})\beta_{\vec{k}'\vec{p}}(\vec{q})-\alpha_{\vec{k}'\vec{p}}(\vec{q})\beta_{\vec{k}\vec{p}}(\vec{q})]=0\;,\\ &\sum_{\vec{k}}^{\vec{q}}[\alpha_{\vec{k}\vec{p}}(\vec{q})\beta_{\vec{k}\vec{p}'}(\vec{q})-\alpha_{\vec{k}\vec{p}'}(\vec{q})\beta_{\vec{k}\vec{p}}(\vec{q})]=0\;.\end{aligned} \tag{4.8}$$

The superscript $\vec{q}$ indicates that the set of indices $\vec{k}$ summed over is dependent on $\vec{q}$. Then $H^{(1)}$ can be brought into the diagonal form

$$H^{(1)}=\sum_{\vec{q}\vec{k}}\Omega_{\vec{k}}(\vec{q})\tilde{A}^{\dagger}_{\vec{k}}(\vec{q})\tilde{A}_{\vec{k}}(\vec{q})+E_0 \tag{4.9}$$

such that $\Omega_{\vec{k}}(\vec{q})$ is positive and

$$\Omega_{-\vec{k}}(-\vec{q})=\Omega_{\vec{k}}(\vec{q})\;, \tag{4.10}$$

provided that α and β satisfy the eigenvalue equations

$$[\Omega_{\vec{k}}(\vec{q})-\omega_{\vec{p}}(\vec{q})]\alpha_{\vec{k}\vec{p}}(\vec{q})-\frac{2V(\vec{q})}{\Omega}\sum_{\vec{p}'}^{1}[\alpha_{\vec{k}\vec{p}'}(\vec{q})-\beta_{\vec{k}\vec{p}'}(\vec{q})]$$

$$\begin{aligned}&=\frac{1}{\Omega}\sum_{p'<p_F}[V(\vec{p}-\vec{p}\,')-V(\vec{p}-\vec{p}\,'+\vec{q})]\,\alpha_{\vec{k}\vec{p}}(\vec{q})\\ &\quad-\frac{1}{\Omega}\sum_{\vec{p}'}^{1}V(\vec{p}-\vec{p}\,')\,\alpha_{\vec{k}\vec{p}'}(\vec{q})+\frac{1}{\Omega}\sum_{\vec{p}'}^{1}W(\vec{p}+\vec{p}\,',\vec{q})\beta_{\vec{k}\vec{p}'}(\vec{q})\;,\end{aligned} \tag{4.11}$$

$$[\Omega_{\vec{k}}(\vec{q})+\omega_{\vec{p}}(\vec{q})]\beta_{\vec{k}\vec{p}}(\vec{q})-\frac{2V(\vec{q})}{\Omega}\sum_{\vec{p}'}^{1}[\alpha_{\vec{k}\vec{p}'}(\vec{q})-\beta_{\vec{k}\vec{p}'}(\vec{q})]$$

$$\begin{aligned}&=-\frac{1}{\Omega}\sum_{p'<p_F}[V(\vec{p}-\vec{p}\,')-V(\vec{p}-\vec{p}\,'+\vec{q})]\beta_{\vec{k}\vec{p}}(\vec{q})\\ &\quad+\frac{1}{\Omega}\sum_{\vec{p}'}^{1}V(\vec{p}-\vec{p}\,')\,\beta_{\vec{k}\vec{p}'}(\vec{q})-\frac{1}{\Omega}\sum_{\vec{p}'}^{1}W(\vec{p}+\vec{p}\,',\vec{q})\,\alpha_{\vec{k}\vec{p}'}(\vec{q})\;,\end{aligned}$$

where

$$\omega_{\vec{p}}(\vec{q})=\epsilon_{\vec{p}+\vec{q}}-\epsilon_{\vec{p}}\;. \tag{4.12}$$

The ground-state energy is given by

$$E_0=-\sum_{\vec{q}\vec{k}\vec{p}}\Omega_{\vec{k}}(\vec{q})\beta^{2}_{\vec{k}\vec{p}}(\vec{q})\;. \tag{4.13}$$

Equations (4.11) are a set of homogeneous linear equations which cannot be solved exactly. In the random-phase approximation the right-hand sides are put equal to zero. In this work we adopt the approximation in which α and β on the right-hand sides are replaced by their average values in region 1:

$$\begin{aligned}\alpha_{\vec{k}\vec{p}}(\vec{q})\rightarrow\alpha_{\vec{k}}(\vec{q})&=\frac{1}{\mu(q)\Omega}\sum_{\vec{p}}^{1}\alpha_{\vec{k}\vec{p}}(\vec{q})\;,\\ \beta_{\vec{k}\vec{p}}(\vec{q})\rightarrow\beta_{\vec{k}}(\vec{q})&=\frac{1}{\mu(q)\Omega}\sum_{\vec{p}}^{1}\beta_{\vec{k}\vec{p}}(\vec{q})\;,\end{aligned} \tag{4.14}$$

where

$$\mu(q)=\frac{1}{\Omega}\sum_{\vec{p}}^{1}1\;. \tag{4.15}$$

This amounts to treating the direct interaction exactly and the exchange interaction more or less on the average. Substituting (4.14) into (4.11), we obtain the approximate eigenvalue equations

$$\begin{aligned}[\Omega_{\vec{k}}(\vec{q})-\omega_{\vec{p}}(\vec{q})]\,\alpha_{\vec{k}\vec{p}}(\vec{q})&=2\mu(q)\\ &\quad\times[F_{\vec{p}}(\vec{q})\,\alpha_{\vec{k}}(\vec{q})-G_{\vec{p}}(\vec{q})\,\beta_{\vec{k}}(\vec{q})]\;,\\ [\Omega_{\vec{k}}(\vec{q})+\omega_{\vec{p}}(\vec{q})]\,\beta_{\vec{k}\vec{p}}(\vec{q})&=2\mu(q)\\ &\quad\times[G_{\vec{p}}(\vec{q})\,\alpha_{\vec{k}}(\vec{q})-F_{\vec{p}}(\vec{q})\,\beta_{\vec{k}}(\vec{q})]\;,\end{aligned} \tag{4.16}$$

where

$$\begin{aligned}F_{\vec{p}}(\vec{q})&=V(\vec{q})+f_{\vec{p}}(\vec{q})\;,\\ G_{\vec{p}}(\vec{q})&=V(\vec{q})+g_{\vec{p}}(\vec{q})\;,\end{aligned} \tag{4.17}$$

and

$$f_{\vec{p}}(\vec{q})=-\frac{1}{2\mu(q)\Omega}\left(\sum_{p'<p_F}V(\vec{p}-\vec{p}\,'+\vec{q})-\sum_{p'<p_F}V(\vec{p}-\vec{p}\,')+\sum_{\vec{p}'}^{1}V(\vec{p}-\vec{p}\,')\right)\;,$$

$$g_{\vec{p}}(\vec{q}) = -\frac{1}{2\mu(q)\Omega}\sum_{\vec{p}'}^{1} W(\vec{p}+\vec{p}', \vec{q}) \ . \tag{4.18}$$

Solving (4.16) for $\alpha_{\vec{k}\vec{p}}(\vec{q})$ and $\beta_{\vec{k}\vec{p}}(\vec{q})$ and taking the averages over region 1, we obtain a pair of homogeneous linear equations for $\alpha_{\vec{k}}(\vec{q})$ and $\beta_{\vec{k}}(\vec{q})$. The vanishing of the determinant yields the dispersion relation for the eigenfrequencies $\Omega_{\vec{k}}(\vec{q})$:

$$\epsilon(\vec{q}, \Omega_{\vec{k}}(\vec{q})) = 0 , \tag{4.19}$$

where

$$\epsilon(\vec{q}, \omega) = \left[1 - \frac{2}{\Omega}\sum_{\vec{p}}^{1} \frac{F_{\vec{p}}(\vec{q})}{\omega - \omega_{\vec{p}}(\vec{q})}\right]\left[1 + \frac{2}{\Omega}\sum_{\vec{p}}^{1} \frac{F_{\vec{p}}(\vec{q})}{\omega + \omega_{\vec{p}}(\vec{q})}\right] + \left[\frac{2}{\Omega}\sum_{\vec{p}}^{1} \frac{G_{\vec{p}}(\vec{q})}{\omega - \omega_{\vec{p}}(\vec{q})}\right]\left[\frac{2}{\Omega}\sum_{\vec{p}}^{1} \frac{G_{\vec{p}}(\vec{q})}{\omega + \omega_{\vec{p}}(\vec{q})}\right] \ . \tag{4.20}$$

This is a generalization of the Bohm-Pines dispersion relation, and reduces to it at low-momentum transfer. For large q,

$$f_{\vec{p}}(\vec{q}),\ g_{\vec{p}}(\vec{q}) \to -\tfrac{1}{2}V(\vec{q}) \ , \tag{4.21}$$

and we recover the well-known result that the exchange processes reduce the direct interaction by one-half at high-momentum transfer. Our expressions $f_{\vec{p}}(\vec{q})$ and $g_{\vec{p}}(\vec{q})$ in (4.18) provide us with a means for interpolating between these two limits.

From (4.8), (4.13), and (4.16) it can be shown that

$$E_0 = \tfrac{1}{2}\sum_{\vec{q}}\left\{\sum_{\vec{k}}^{\vec{q}} \Omega_{\vec{k}}(\vec{q}) - \sum_{\vec{p}}^{1}\left[\omega_{\vec{p}}(\vec{q}) + \frac{2}{\Omega} F_{\vec{p}}(\vec{q})\right]\right\} \ . \tag{4.22}$$

V. DIELECTRIC FUNCTION

$\epsilon(\vec{q}, \omega)$ defined in (4.20) can be regarded as a dielectric function for the electron gas. It is doubtful whether the expression could be evaluated exactly. Even if it were possible, such an exact treatment is perhaps unnecessary in view of the approximation we have made in Sec. IV. It is simpler, and probably no worse, to continue making the averaging approximation. First we replace all the summands in (4.18) by their averages over the Fermi sphere, thereby obtaining

$$f_{\vec{p}}(\vec{q}) \simeq -\frac{1}{2\mu(q)}\left[\frac{1}{\Omega}\sum_{p'<p_F} V(\vec{p}-\vec{p}'+\vec{q}) - \left(1 - \frac{\mu(q)}{\mu(2p_F)}\right)\frac{1}{\Omega}\sum_{p'<p_F} V(\vec{p}-\vec{p}')\right], \tag{5.1}$$

$$g_{\vec{p}}(\vec{q}) \simeq -\frac{\mu(q)-\nu(q)}{2\mu(q)\,\mu(2p_F)}\,\frac{1}{\Omega} \times \sum_{p'<p_F} V(\vec{p}-\vec{p}'+\vec{q}) - \frac{\nu(q)}{2\mu(q)}\ V(\vec{q}) \ ,$$

where

$$\mu(2p_F) = \frac{1}{\Omega}\sum_{p'<p_F} 1 \ ,$$

$$\nu(q) = \frac{1}{\Omega}\sum_{\vec{p}'}^{1} \theta_2(-(\vec{p}+\vec{p}')\cdot\vec{q}) \simeq \frac{1}{2\Omega}\sum_{\vec{p}'}^{2} 1 \ , \tag{5.2}$$

$$\frac{1}{\Omega}\sum_{p'<p_F} V(\vec{p}-\vec{p}') = \frac{e^2 p_F}{2\pi}\left[2 + \frac{p_F^2 - p^2}{p_F p}\ \ln\left|\frac{p_F + p}{p_F - p}\right|\right] .$$

Equation (5.1) is still too complicated for the evaluation of (4.20). Therefore we again replace f and g by their averages over region 1:

$$f_{\vec{p}}(\vec{q}) \to f(\vec{q}) = \frac{1}{\mu(q)\Omega}\sum_{\vec{p}}^{1} f_{\vec{p}}(\vec{q}) \ ,$$
$$g_{\vec{p}}(\vec{q}) \to g(\vec{q}) = \frac{1}{\mu(q)\Omega}\sum_{\vec{p}}^{1} g_{\vec{p}}(\vec{q}) \ . \tag{5.3}$$

This time it would not be a good approximation to average over the whole Fermi sphere. With these simplifications the dielectric function becomes

$$\epsilon(\vec{q}, \omega) = 1 - \frac{2F(\vec{q})}{\Omega}\sum_{\vec{p}}^{1} \frac{2\omega_{\vec{p}}(\vec{q})}{\omega^2 - \omega_{\vec{p}}^2(\vec{q})} - 4\left[F^2(\vec{q}) - G^2(\vec{q})\right] \times \left[\frac{1}{\Omega}\sum_{\vec{p}}^{1} \frac{1}{\omega - \omega_{\vec{p}}(\vec{q})}\right]\left[\frac{1}{\Omega}\sum_{\vec{p}}^{1} \frac{1}{\omega + \omega_{\vec{p}}(\vec{q})}\right] , \tag{5.4}$$

where

$$F(\vec{q}) = V(\vec{q}) + f(\vec{q}) \ ,$$
$$G(\vec{q}) = V(\vec{q}) + g(\vec{q}) \ . \tag{5.5}$$

We therefore assimilate the effects of the exchange interaction by a pair of effective direct potentials $f(\vec{q})$ and $g(\vec{q})$.

The evaluation of $f(\vec{q})$ and $g(\vec{q})$ in (5.3) is straightforward but lengthy. We list the relevant results in terms of a dimensionless variable x:

$$\begin{aligned}
x &= q/p_F \ , \\
\mu(2p_F) &= (2\pi)^{-3}\tfrac{4}{3}\pi p_F^3 \ , \\
\mu(q) &= \mu(2p_F)\,\mu(x) \ , \\
\mu(x) &= \tfrac{3}{4}(x - \tfrac{1}{12}x^3) \ , && 0 < x < 2 \\
&= 1 \ , && x > 2 \\
\nu(q) &= \mu(2p_F)\,\nu(x) \ , \\
\nu(x) &= \tfrac{3}{16}x^3 \ , && 0 < x < 1 \\
&= \tfrac{1}{16}(12x - x^3 - 8) \ , && 1 < x < 2 \\
&= \tfrac{1}{2} \ , && x > 2 \ .
\end{aligned} \tag{5.6}$$

Then

$$F(\vec{q}) = \frac{4\pi e^2}{p_F^2}\,F(x) = \frac{4\pi e^2}{p_F^2}\left(\frac{1}{x^2} + f(x)\right),$$

$$G(\vec{q})=\frac{4\pi e^2}{p_F^2}\,G(x)=\frac{4\pi e^2}{p_F^2}\left(\frac{1}{x^2}+g(x)\right),$$

$$f(x)=-\frac{1}{\mu^2(x)}\,\{X(x)-[1-\mu(x)]\,Y(x)\}\,, \qquad (5.7)$$

$$g(x)=-\frac{1}{\mu^2(x)}\,[\mu(x)-\nu(x)]\,X(x)-\frac{\nu(x)}{2\mu(x)x^2}\,,$$

where

$$\frac{1}{\Omega}\sum_{\vec{p}}^{1}\frac{1}{\Omega}\sum_{p'<p_F}V(\vec{p}-\vec{p}\,'+\vec{q})=\frac{8\pi e^2}{p_F^2}\,\mu^2(2p_F)\,X(x)\,,$$

$$\frac{1}{\Omega}\sum_{\vec{p}}^{1}\frac{1}{\Omega}\sum_{p'<p_F}V(\vec{p}-\vec{p}\,')=\frac{8\pi e^2}{p_F^2}\,\mu^2(2p_F)\,Y(x)\,,$$

$$\begin{aligned}X(x)&=\tfrac{1}{2}\,\mu(x)-\tfrac{3}{4}(1-\tfrac{1}{2}x)\ln 2+\phi_1(x)\,, && 0<x<2\\ &=\tfrac{1}{2}+\phi_2(x)\,, && x>2 \qquad (5.8)\\ Y(x)&=\tfrac{1}{2}\,\mu(x)+\tfrac{3}{4}(1+\tfrac{1}{2}x)\ln 2-\phi_1(-x)\,, && 0<x<2\end{aligned}$$

$$\phi_1(x)=\frac{3}{16x}\int_1^{1+x}dt\,(t-x)K(t)\,,$$

$$\phi_2(x)=\frac{3}{16x}\int_{x-1}^{x+1}dt\,(t-x)K(t)\,;$$

$$K(t)=(2-t)(1+t)^2\ln|1+t|+(2+t)(1-t)^2\ln|1-t|\,. \qquad (5.9)$$

The evaluation of the ϕ's is elementary and the results can be expressed in terms of the function

$$\begin{aligned}\psi(\xi,\eta)=\eta^3\{&[\tfrac{1}{5}\eta^2-\tfrac{1}{4}\eta(4+\xi)+(1+\xi)]\ln|\eta|\\ &-[\tfrac{1}{25}\eta^2-\tfrac{1}{16}\eta(4+\xi)+\tfrac{1}{3}(1+\xi)]\}\,, \qquad (5.10)\end{aligned}$$

whereby

$$\phi_1(x)=\frac{3}{16x}\,[\psi(x,2)-\psi(x,2+x)-\psi(-x,-x)]\,,$$

$$\begin{aligned}\phi_2(x)=\frac{3}{16x}\,[&\psi(x,x)+\psi(-x,2-x) \qquad (5.11)\\ &-\psi(x,2+x)-\psi(-x,-x)]\,.\end{aligned}$$

In Fig. 2 we plot the interpolation functions $f(x)$ and $g(x)$ and compare them with Hubbard's interpolation function $h(x)$:

$$h(x)=-[2(x^2+1)]^{-1}\,. \qquad (5.12)$$

If we set $f(x)=g(x)=h(x)$ in (5.4), we would obtain the dielectric function in the Hubbard approximation. We note that $f(x)$ is positive for $x<1$ and is finite at $x=0$. For large x all three functions approach the form $-\frac{1}{2}x^{-2}$.

VI. CORRELATION ENERGY

The dielectric function (5.4) has the product representation

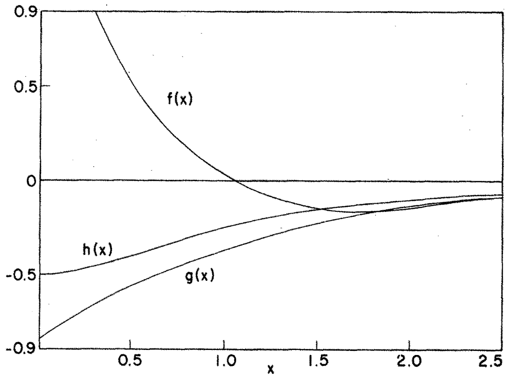

FIG. 2. Interpolation functions.

$$\epsilon(\vec{q},\omega)=\prod_{\vec{k}}^{\vec{q}}[\omega^2-\Omega_{\vec{k}}^2(\vec{q})]\Big/\prod_{\vec{p}}^{1}[\omega^2-\omega_{\vec{p}}^2(\vec{q})]\,. \qquad (6.1)$$

By a transformation of Wentzel[11] it can be shown that

$$\frac{1}{2}\left[\sum_{\vec{k}}^{\vec{q}}\Omega_{\vec{k}}(\vec{q})-\sum_{\vec{p}}^{1}\omega_{\vec{p}}(\vec{q})\right]=\frac{1}{4\pi}\int_{-\infty}^{\infty}du\,\ln\epsilon(\vec{q},iu)\,. \qquad (6.2)$$

Replacing $F_{\vec{p}}(\vec{q})$ in (4.22) by $F(\vec{q})$ and using the identity

$$\frac{1}{\pi}\int_{-\infty}^{\infty}du\,\frac{\omega_{\vec{p}}(\vec{q})}{u^2+\omega_{\vec{p}}^2(\vec{q})}=1\,, \qquad (6.3)$$

we obtain

$$E_0=\frac{1}{4\pi}\sum_{\vec{q}}\int_{-\infty}^{\infty}du \times\left(\ln\epsilon(\vec{q},iu)-\frac{2F(\vec{q})}{\Omega}\sum_{\vec{p}}^{1}\frac{2\omega_{\vec{p}}(\vec{q})}{u^2+\omega_{\vec{p}}^2(\vec{q})}\right). \qquad (6.4)$$

This expression enables us to calculate the ground-state energy without an explicit expression for the eigenfrequencies. We introduce a dimensionless variable y:

$$\begin{aligned}y&=u/E_F\,,\\ E_F&=p_F^2/2m\,. \qquad (6.5)\end{aligned}$$

In terms of x and y we have

$$\frac{1}{\Omega}\sum_{\vec{p}}^{1}\frac{1}{iu-\omega_{\vec{p}}(\vec{q})}=-\frac{mp_F}{8\pi^2}\,[R(x,y)+iI(x,y)]\,, \qquad (6.6)$$

where

$$\begin{aligned}R(x,y)=1&+\frac{y^2+4x^2-x^4}{8x^3}\ln\frac{(2x+x^2)^2+y^2}{(2x-x^2)^2+y^2}\\ &-\frac{y}{2x}\left(\tan^{-1}\frac{2x+x^2}{y}+\tan^{-1}\frac{2x-x^2}{y}\right),\end{aligned}$$

$$I(x,y)=\frac{y^2+4x^2-x^4}{4x^3}\left(\tan^{-1}\frac{2x+x^2}{y}-\tan^{-1}\frac{2x-x^2}{y}\right)$$

$$+\frac{y}{4x}\ln\frac{[(2x+x^2)^2+y^2][(2x-x^2)^2+y^2]}{y^4}-\frac{y}{2x}\ ,$$

$$0<x<2$$

$$=\frac{y^2+4x^2-x^4}{4x^3}\left(\tan^{-1}\frac{2x+x^2}{y}+\tan^{-1}\frac{2x-x^2}{y}\right)$$

$$+\frac{y}{4x}\ln\frac{(2x+x^2)^2+y^2}{(2x-x^2)^2+y^2}-\frac{y}{x^2}\ ,\quad x>2\ . \qquad (6.7)$$

Then the correlation energy per electron arising from the singlet Hamiltonian is given by

$$E^{(1)}_{\text{corr}}=\frac{3}{4\pi}E_F\int_0^\infty dx\int_0^\infty dy\, x^2 A(x,y)\ , \qquad (6.8)$$

$$A(x,y)=\ln[1+\gamma\Pi_1(x,y)+\gamma^2\Pi_2(x,y)]-\gamma\Pi_1(x,y)\ ,$$

where

$$\gamma=\frac{2}{\pi}\left(\frac{4}{9\pi}\right)^{1/3}r_s\simeq 0.332 r_s\ ,$$

$$\Pi_1(x,y)=F(x)R(x,y)\ , \qquad (6.9)$$

$$\Pi_2(x,y)=\tfrac{1}{4}[F^2(x)-G^2(x)][R^2(x,y)+I^2(x,y)]\ .$$

In units of rydbergs ($=e^2/2a_0$), E_F is given by

$$E_F=\left(\frac{9\pi}{4}\right)^{2/3}\frac{1}{r_s^2}\simeq\frac{3.683}{r_s^2}\ . \qquad (6.10)$$

The correlation energy per electron arising from the triplet Hamiltonian is obtained from (6.8) and (6.9) with the replacements of $F(x)$ and $G(x)$ by $f(x)$ and $g(x)$.

The two-dimensional integral in (6.8) is evaluated numerically for $r_s = 1$–6. In Fig. 3 we display the result of the y integration,

$$B(x)=x^2\int_0^\infty dy\, A(x,y) \qquad (6.11)$$

for $r_s = 4$. $B(x)$ measures the contribution to the correlation energy from processes of various momentum transfers. For comparison we also plot the corresponding result in the random-phase approximation obtained by setting $f(x)=g(x)=0$. We note that the triplet Hamiltonian gives substantial contributions for $x > 0.5$, whereas in the random-phase approximation these are zero. The total contribution from the singlet and triplet Hamiltonians is about two-thirds of that in the random-phase approximation. The final results of the integration are shown in Table I and compared with those obtained in other works. Our results are in general numerically smaller than those of other authors. The triplet contribution is practically constant.

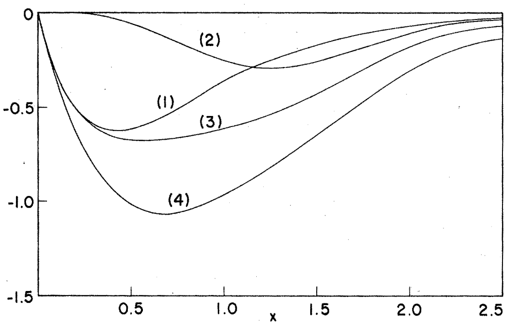

FIG. 3. Contributions to correlation energy from processes of various momentum transfers for $r_s = 4$: (1) singlet, (2) triplet, (3) singlet and triplet, (4) random-phase approximation.

VII. STABILITY OF PARAMAGNETIC GROUND STATE

The reality of the correlation energy indicates that the paramagnetic ground state of the electron gas is stable at metallic densities. The singlet contribution is always real since the interaction between electrons in the singlet state is repulsive. The triplet contribution is real predominantly because $f(x)$ is positive at small x. However, as r_s is increased, the triplet contribution may become complex, signifying an instability in the triplet ground state. This occurs when the argument of the logarithm in (6.8) becomes negative. Putting $R(x,y)$ and $I(x,y)$ equal to their optimum values at $y=0$, we obtain an equation for the determination of the critical value:

$$1+\gamma R(x,0)f(x)+\tfrac{1}{4}\gamma^2 R^2(x,0)[f^2(x)-g^2(x)]=0\ . \qquad (7.1)$$

TABLE I. Correlation energy per electron in Ry.

r_s	1	2	3	4	5	6
Singlet	−0.082	−0.058	−0.047	−0.040	−0.035	−0.031
Triplet	−0.020	−0.020	−0.020	−0.021	−0.021	−0.022
Total	−0.102	−0.078	−0.067	−0.060	−0.056	−0.053
Random-phase approximation	−0.157	−0.123	−0.105	−0.093	−0.084	−0.078
Hubbard (Ref. 6)	...	−0.099	−0.086	−0.074	−0.067	...
Nozières and Pines (Ref. 7)	...	−0.094	−0.081	−0.072	−0.065	...
Singwi *et al.* (Ref. 12)	−0.124	−0.092	−0.075	−0.064	−0.056	−0.050

The solution is

$$\gamma = -2\{R(x,0)[f(x)+g(x)]\}^{-1}. \tag{7.2}$$

The right-hand side has a positive minimum of 3.1 at $x \simeq 1.2$, giving a critical value

$$r_s \simeq 9.4. \tag{7.3}$$

At this point the electron gas presumably becomes ferromagnetic. If we had used instead of $f(x)$ and $g(x)$ the Hubbard interpolation function $h(x)$ in (7.1), we would have obtained a critical value $r_s \simeq 3.0$.

VIII. SUMMARY

The results obtained in this work are summarized as follows.

(i) A dielectric function for all momentum transfers is derived.

(ii) The separate contributions to the correlation energy from the singlet and triplet states are calculated.

(iii) The stability of the paramagnetic ground state is put in evidence.

(iv) The limit of stability is estimated.

Although our approximation procedures greatly simplify the problem and lead to reasonable results, their accuracy and range of validity are hard to assess. This lack of knowledge precludes us from studying the effects of the cubic and quartic Hamiltonians. It is perhaps more appropriate to investigate at this stage the other properties of the electron gas in the present approximation.

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Nuclear-Magnetic-Resonance Study of the Hydrogen Nucleus in OH^- in the Potassium Chloride Lattice*

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Experimental data are presented on the nuclear-magnetic-resonance signal from the hydrogen magnetic-dipole moment in the OH^- ion substituted for Cl^- in a KCl lattice. The recovery rate of the signal after saturation is measured for OH^- concentrations down to 1.2×10^{19} OH^-/cm^3. This rate is used to deduce a displacement distance $= 0.4\times10^{-8}$ cm for the hydrogen nucleus from the halogen vacancy site when the OH^- ion has $\langle 100\rangle$-directed localized states in a rigid lattice and a correlation time $= 4\times10^{-8}$ sec. The effects of librating states of the OH^- and lattice relaxation are estimated. A discussion of the dependence of the displacement distance on the correlation time is included.

I. INTRODUCTION

In recent years a great deal of experimental and theoretical work has been done on alkali halides with OH^- ions substituted as an impurity.[1] The OH^- is known to go into the KCl lattice by substituting for Cl^- ion, and the potential minima of the OH^- ion are believed to be such that alignment of the OH^-