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Electron correlations at metallic densities*

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The effect of correlations on effective interactions in the electron gas is studied. It is argued that because of the strong correlations at short distances, two-body terms make up the dominant contribution to the effective electron-electron interaction for small separations. An interpolated effective electron-electron interaction is proposed which is approximately correct for all separations. This interaction incorporates both the two-body short-distance correlation effects, and the well-known many-body collective behavior at large separations. A number of metallic properties including cohesive energies and plasmon dispersion curves are calculated using this effective interaction, and all are found to be in remarkable agreement with the results of Singwi, Tosi, Land, and Sjölander who calculated the effects of the short-distance correlations using a quite different method.

I. INTRODUCTION

The electron-gas model has proved to be very useful for studying properties of metals which depend strongly on electron-electron interactions and only weakly on the discrete nature of the ion-core lattice. The system that one studies is an interacting electron gas on a uniform positive background. The effect of the background is to neutralize the over-all system. The model is especially well suited for certain phenomena involving the conduction-band electrons of the alkali metals. The Fermi surfaces for these degenerate valence electrons are nearly spherical[1] and fit well within the first Brillouin zone.[2]

For many metallic properties we need to know the electron-gas dielectric function $\epsilon(\vec{q}, \omega)$,[3] which is very closely related to the Fourier transform of the time-dependent pair-correlation function $g(\vec{r}, t)$, Such experimentally accessible quantities as the cohesive energy of a metal or its plasmon dispersion curve, can be directly related to these functions. The electron pair-correlation function is also needed in calculating the buildup of electron density around a positron in a metal.[4]

It is fairly straightforward to evaluate the dielectric function within the random phase approximation (RPA).[5–7] In the RPA, the coupling between different Fourier components of the Coulomb interaction is completely neglected. Because of this it is impossible to build wave packets corresponding to a field of localized charges, and consequently the RPA neglects all localized correlations. The RPA was originally applied to long-wavelength phenomena[5] where such correlations can safely be neglected, since only over-all polarization effects should be important. It has also been shown to be valid for all wavelengths in the high-density limit.[6] At metallic densities, however, phenomena which depend on short-wavelength excitations, such as the electron buildup near a positron or the correlations between two close electrons, are found to be very sensitive to the local-field corrections. Our purpose is to develop an over-all calculational scheme which adequately treats these localized effects, and at the same time retains the RPA results at long wavelengths. We can then investigate how the localized effects affect various metallic properties.

The RPA retains only those terms in the perturbation series for which different momentum components of the interaction are not mixed. The contribution from each particle-hole polarization bubble is given by the Lindhard function[8] $\Pi_0(\vec{q}, \omega)$,

$$\Pi_0(\vec{q}, \omega) = \sum_{\text{spin}} \int \frac{d^4k}{(2\pi)^4} G_0(\vec{q}+\vec{k}, \omega + k^0)\, G_0(\vec{k}, k^0) , \tag{1}$$

where G_0 is the free-electron Green's function

$$G_0(\vec{k}, k^0) = \frac{i}{k^0 - \frac{1}{2}k^2 + i\eta\,\mathrm{sgn}(|\vec{k}| - k_F)} ,$$
$$\eta = 0^+ . \tag{2}$$

The units we use are such that $\hbar^2/m = 1$. Because there is no mixing of momentum components and because the Coulomb interaction $v\vec{q}$ is local, each polarization bubble $\Pi_0(\vec{q}, \omega)$ decouples from its interaction. This makes summing the infinite set of RPA terms straightforward since each term belongs to a geometric series in powers of $\Pi_0(\vec{q}, \omega)\, v\vec{q}$.

Hubbard[7] pointed out that for large momentum transfers the exchange contribution to a given diagram would tend to cancel one-half the direct contribution. Since it is impractical to evaluate all the exchange terms for RPA, Hubbard suggested instead using only the direct terms and approximating exchange effects by replacing $\Pi_0(\vec{q}, \omega)$ with

$$\frac{\Pi_0(\vec{q}, \omega)}{1 + \frac{1}{2}[q^2/(q^2 + k_F^2)]\,\Pi_0(\vec{q}, \omega)} . \tag{3}$$

For small $\vec{q}$ this function remains $\Pi_0(\vec{q}, \omega)$, but for large $\vec{q}$ it becomes $\frac{1}{2}\Pi_0(\vec{q}, \omega)$. Nozières and Pines[9] developed an interpolation procedure based on this same physical idea. For small momentum transfers they used RPA, while for large momentum transfers they used lowest-order perturbation theory and included only antiparallel spins. Since for large $|\vec{q}|$ the RPA series converges rapidly, this is similar to Hubbard's approximation. For intermediate momentum transfer they interpolated between their large and small momentum results.

While both these approaches go beyond the RPA in considering the local correlations caused by exchange, they still completely neglect the important correlative effects arising from the repulsive interaction. Singwi, Tosi, Land, and Sjölander[10] (STLS) successfully included local correlations caused by the interactions. By considering only two-body contributions to the Liouville equation of motion they were able to relate the pair-correlation function to a certain effective interaction, and vice versa. They iterated their calculation until the correlations and the interaction agreed self-consistently. The final effective interaction incorporated local two-body correlations, and since it was represented on the unperturbed-plane-wave basis it could be neatly dovetailed into the RPA scheme by simply replacing each Coulomb interaction in the RPA sum by the effective interaction. Since the effective interaction was also local and static, the RPA-type terms still factorized into powers of the interaction and powers of the polarization bubbles, so the geometric sum could still be performed. A drawback of their method is that because it uses a self-consistent approach, it is difficult to say precisely which terms of the perturbation expansion in the Coulomb interaction are being retained. Since only two-body contributions to the equation of motion were included, it is plausible that only two-body terms from the perturbation expansion are being considered, but it is difficult to be more precise.

A quite different approach to this problem of calculating the short-range correlations caused by the electron repulsion was adopted by Yasuhara[11] and by Hede and Carbotte.[12] Yasuhara calculated the zero-distance pair-correlation function for antiparallel spins using an effective interaction which consisted of the infinite ladder sum of unscreened Coulomb interactions between the two electrons. Hede and Carbotte calculated the same function for small distances, but they used the ladder sum of static RPA interactions for their effective interaction. These ladder-sum approaches are similar to our calculation, and we discuss them further in Sec. III.

II. ELECTRON-ELECTRON EFFECTIVE INTERACTION

We want to construct a two-body effective interaction for the electrons which takes into account the strong correlative effects at small separations caused by both repulsion and exchange, and which at the same time extrapolates smoothly to the retarded RPA interaction for large separations.

A. At short range

Let us first concentrate on constructing the effective interaction for small separations. Two-body contributions to this interaction will tend to dominate for small separations, both because the interaction is everywhere repulsive and also because of the Fermi statistics. If we already have two particles close together, it costs considerable energy for a third particle to approach sufficiently close to them to interact strongly with them. The energy cost is much greater than that incurred in bringing the first two particles together, since the third particle has to approach a double charge. By the uncertainty principle, we would then expect the lifetime of any such third virtual excitation to be short compared to the lifetime of the first two.[13] Hence retardation effects involving a third particle, such as retarded screened-interaction terms or terms of the Bethe-Faddeev type,[14] should not be very important at short distances. The two particles will tend to polarize the medium around them, but since they are both negatively charged, any polarization they cause at distances much greater than their separation will affect both particles equally. We can approximate this effect by adding a weak static external potential. We shall find that in fact our results are not sensitive to such a potential.

Since the electron gas is a spin-$\frac{1}{2}$ fermion system, exchange contributions further diminish the importance of three-body terms. In any three-body term at least two of the electrons must have parallel spin, so that when all three electrons are close together direct and exchange terms will tend to cancel. As an example of how the exchange terms reduce the effects of screening, consider the first- and second-order terms for antiparallel spin electrons shown in Fig. 1. We denote the term corresponding to Fig. 1(a) as D_a, etc. Our calculations indicate that the most important contributions to the zero-separation pair-correlation function come from the momentum-transfer region $q \sim (2-3)k_F$. For $q > k_F$, the ladder terms are all of the same order in k_F/q,

$$D_b/D_a = 0.165 r_s \left[1 + O(k_F^2/q^2)\right], \tag{4}$$

where r_s is a dimensionless parameter defined in Sec. III. Although the screening terms are all smaller than any of the ladder terms,

$$D_c/D_a = 0.110 r_s (k_F^4/q^4) \left[1 + O(k_F^2/q^2)\right], \tag{5}$$

if we include only the direct screening term Fig.

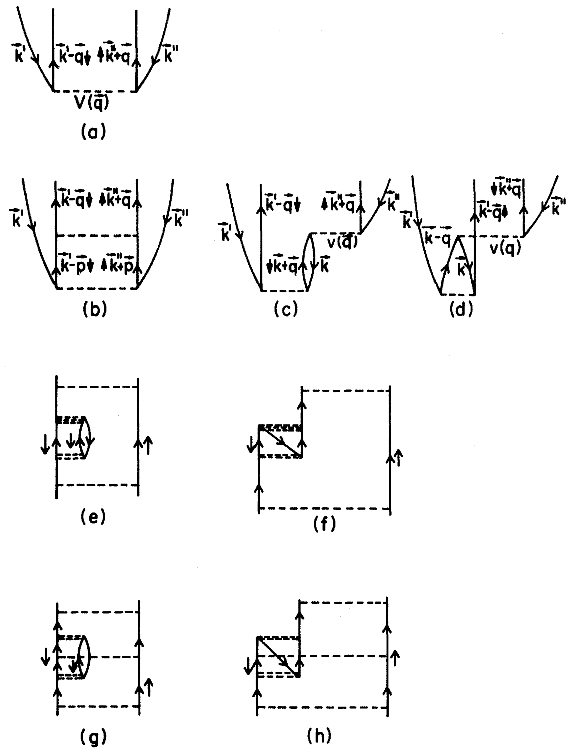

FIG. 1. For $|\vec{q}| > k_F$, first- and second-order ladder contributions (a) and (b) are the same order in k_F/q. Second-order direct screening term (c) is order k_F^4/q^4 smaller than (a) or (b), but (c) plus the exchange screening term (d) is order k_F^6/q^6 smaller than (a) or (b). (e) plus (f), and (g) plus (h) exhibit similar leading-order cancellations between direct and exchange self-energy diagrams, and direct and exchange vertex-correction diagrams, respectively.

1(c), we will still overestimate the effect of screening. Adding the exchange term, we find in this case

$$(D_c + D_d)/D_a = 0.880 r_s (k_F^6/q^6)\,[1 + O(k_F^2/q^2)]\,, \qquad (6)$$

so that there is a cancellation of direct and exchange screening terms to order k_F^2/q^2. This is quite different from Hubbard's exchange cancellation. Here there is complete cancellation in leading order, since the screening electron must have its spin parallel to one of the scattered electrons.

To summarize, since two close electrons will strongly repel other electrons, and since the two electrons will tend to polarize the surrounding medium symmetrically, screening of their interaction at short distance should not be very important; however, retaining only the direct screening terms will still overestimate the effect of screening. Since we intend to account for long-wavelength screening by inserting our effective interaction for short distances into an RPA-type series, we cannot include screening terms in the short-range part of the interaction without double counting. For these reasons, we restrict the short-range part of our effective interaction to be the ladder sum of unscreened Coulomb interactions.

We can also use these arguments to show that the direct self-energy diagrams such as Fig. 1(e) overestimate self-energy effects if we do not also include the self-energy exchange diagram Fig. 1(f). Similarly, the direct vertex correction diagram Fig. 1(g) is partly cancelled by its exchange diagram Fig. 1(h).

We now construct the short-range part of our two-body effective interaction from the ladder sum of Coulomb interactions. For a particular pair of electrons, the sum of all the ladder terms is the solution of the Lippmann-Schwinger integral equation for the effective electron-electron interaction t_{ee},

$$\langle \vec{q}\vec{K}|\,t_{ee}(E)\,|\vec{k}_0\vec{K}\rangle = \langle\vec{q}|\,v\,|\vec{k}_0\rangle + \int \frac{d^3p}{(2\pi)^3}\,\langle\vec{q}|\,v\,|\vec{p}\rangle\,\frac{1}{E - \epsilon_{|\vec{K}/2+\vec{p}|} - \epsilon_{|\vec{K}/2-\vec{p}|}}\,\langle\vec{p}\vec{K}|\,t_{ee}(E)\,|\vec{k}_0\vec{K}\rangle\,, \qquad (7)$$

where $|\vec{q}\,|\vec{K}\rangle$ represents a two-particle plane wave with relative momentum $\vec{q}$ and center-of-mass momentum $\vec{K}$,

$$\langle\vec{q}|\,v\,|\vec{k}_0\rangle = \lim_{\eta\to 0} \frac{4\pi e^2}{|\vec{q}-\vec{k}_0|^2 + \eta^2} \qquad (8)$$

is the unscreened Coulomb interaction, $\epsilon_{|\vec{p}|}$ is the single-particle energy for a propagator of momentum $\vec{p}$, $|\vec{k}_0\vec{K}\rangle$ is an unexcited two-particle state with the restrictions $0 \leq |\frac{1}{2}\vec{K} \pm \vec{k}_0| \leq k_F$, and

$$E = \epsilon_{|\vec{K}/2+\vec{k}_0|} + \epsilon_{|\vec{K}/2-\vec{k}_0|} \qquad (9)$$

is the energy of this initial state.

Since we are neglecting all greater than two-body correlations, the wave functions of all the electrons other than the correlated pair are unperturbed. Because of this, antisymmetrizing the correlated-electron wave functions with the wave functions of the other electrons is equivalent to projecting out from the integral those intermediate states for which $|\frac{1}{2}\vec{K} \pm \vec{p}| \leq k_F$. This point is discussed more fully in a subsequent paper.[4] This gives us the Bethe-Goldstone integral equation[15] for the effective interaction t_{ee} between any two electrons from the antisymmetrized many-electron ground state:

$$\langle\vec{q}\vec{K}|\,t_{ee}(E)\,|\vec{k}_0\vec{K}\rangle = \langle\vec{q}|\,v\,|\vec{k}_0\rangle + \int \frac{d^3p}{(2\pi)^3}\,\langle\vec{q}|\,v\,|\vec{p}\rangle\,\frac{Q(\vec{p},\vec{K},k_F)}{E - \epsilon_{|\vec{K}/2+\vec{p}|} - \epsilon_{|\vec{K}/2-\vec{p}|}}\,\langle\vec{p}\vec{K}|\,t_{ee}(E)\,|\vec{k}_0\vec{K}\rangle\,, \qquad (10)$$

where

$$Q(\vec{p}, \vec{K}, k_F) = \Theta(|\tfrac{1}{2}\vec{K}+\vec{p}| - k_F)\,\Theta(|\tfrac{1}{2}\vec{K}-\vec{p}| - k_F),$$

$$\Theta(k) = \begin{cases} 1 & \text{if } k > 0 \\ 0 & \text{otherwise .} \end{cases} \tag{11}$$

Because the electron pair polarizes the medium, the positive background and the electron medium will not exactly cancel in the vicinity of the pair. To check how this might affect our results, we approximated this polarization field by a constant attractive potential v_{pol}. Since the polarization is approximately symmetric, the field should act equally on both electrons, and we can include it in the single-particle energies $\epsilon_{|\vec{p}|} \to \epsilon_{|\vec{p}|} + v_{\text{pol}}$. Our results turned out to be insensitive to v_{pol} for $-k_F^2 \leqslant v_{\text{pol}} \leqslant 0$, and so we neglected this effect. We have argued that because of exchange cancellations, including only direct self-energy insertions overestimates their importance. However, in those self-energy terms $\Sigma(\vec{p}, \epsilon_{\vec{p}})$ for which $|\vec{p}| < k_F$ exchange is negligible. We may approximate the full self-energy contribution in this region by the RPA term $\Sigma^{(e)}_{\text{RPA}}(\vec{p}, \epsilon_{\vec{p}})$, which has been evaluated by Hedin.[16] Adding this to $\epsilon_{\vec{p}}$ did not appreciably alter our results, so we concluded that it is a good approximation to take the single-particle energy $\epsilon_{|\vec{p}|}$ to be just the kinetic energy

$$\epsilon_{|\vec{p}|} = \tfrac{1}{2}|\vec{p}|^2 \,. \tag{12}$$

The energy denominator in the integral equation then reduces to $(k_0^2 - p^2)$, and the only remaining $\vec{K}$ dependence in the equation is in the Pauli operator Q.

We approximated Q by its angle average $\overline{Q}$,[17] which is defined by the expression

$$\int d\Omega_{\vec{p}\vec{K}}\, Q(\vec{p}, \vec{K}, k_F) = \overline{Q}(p, K, k_F) \int d\Omega_{\vec{p}\vec{K}} \,, \tag{13}$$

so that

$$\overline{Q}(p, K, k_F) = \begin{cases} 0 & \text{if } q^2 + \tfrac{1}{4}K^2 < k_F^2 \\ 1 & \text{if } q - \tfrac{1}{2}K > k_F \\ \dfrac{q^2 + \tfrac{1}{4}K^2 - k_F^2}{qK} & \text{otherwise .} \end{cases} \tag{14}$$

We note that Q and $\overline{Q}$ exclude the same volume in phase space, and they are identical except in the region

$$(k_F + \tfrac{1}{2}K)^2 > q^2 > k_F^2 - \tfrac{1}{4}K^2 \,.$$

For $K = 0$, Q and $\overline{Q}$ are identical. Since our calculated t_{ee}^K was found to be only a slowly varying function of K for $0 \leqslant |\tfrac{1}{2}\vec{K}| \leqslant k_F$, our approximation is reasonable.

Using $\overline{Q}$, t_{ee} becomes a function of only the magnitude of $\vec{K}$, and we can expand t_{ee} in partial waves,

$$\langle\vec{q}|\, t_{ee}^K(E)\, |\vec{k}_0\rangle = 4\pi \sum_{l=0}^{\infty} (2l+1) \times \langle q|\, t_l^K(E)\, |k_0\rangle\, P_l(\hat{\vec{q}} \cdot \hat{\vec{k}}_0) \,. \tag{15}$$

We can also expand v,

$$\langle\vec{q}|\, v\, |\vec{k}_0\rangle = 4\pi \sum_{l=0}^{\infty} (2l+1) \times \langle q|\, v_l\, |k_0\rangle\, P_l(\hat{\vec{q}} \cdot \hat{\vec{k}}_0) \,, \tag{16}$$

where

$$\langle q|\, v_l\, |k_0\rangle = \lim_{\eta\to 0} \frac{e^2}{2qk_0}\, Q_l\!\left(\frac{q^2 + k_0^2 + \eta^2}{2qk_0}\right) . \tag{17}$$

In the above equations P_l and Q_l are the Legendre functions of the first and second kind.

The integral equation decouples into equations for each partial wave,

$$\langle q|\, t_l^K(E = k_0^2)\, |k_0\rangle = \langle q|\, v_l\, |k_0\rangle + \frac{2}{\pi}\int_0^\infty dp\, p^2 \langle q|\, v_1\, |p\rangle \times \frac{\overline{Q}(p, K, k_F)}{k_0^2 - p^2}\, \langle p|\, t_l^K(E)\, |k_0\rangle \,. \tag{18}$$

Each of these equations is well behaved, and we can solve them numerically on a suitable mesh of points.

B. Interpolation procedure

For $|\vec{q}| \ll k_F$, we found that because of the Pauli operator $\langle\vec{q}|\, t_{ee}^K(k_0^2)\, |\vec{k}_0\rangle$ tends to $\langle\vec{q}|\, v\, |\vec{k}_0\rangle$. When $|\vec{q}| \gg k_F$, the partial-wave series converged rapidly. In this limit, we found that $\langle\vec{q}|\, t_{ee}^K(k_0^2)\, |\vec{k}_0\rangle$ was only a slowly varying function of K and $\vec{k}_0$ for $0 \leqslant |\tfrac{1}{2}\vec{K}|,\ |\vec{k}_0| \leqslant k_F$, so that it is approximately a local function. We averaged over $\vec{K}$ and $\vec{k}_0$ to obtain the local function $t_{ee}^{\text{loc}}(\vec{q})$,

$$t_{ee}^{\text{loc}}(\vec{q}) = \frac{1}{N_{\text{av}}} \int \frac{d^3k_0}{(2\pi)^3} \int \frac{d^3K}{(2\pi)^3}\, [1 - Q(\vec{k}_0, \vec{K}, k_F)] \times \langle\vec{q} + \vec{k}_0|\, t_{ee}^K(E = k_0^2)\, |\vec{k}_0\rangle \,, \tag{19}$$

where

$$N_{\text{av}} = \int \frac{d^3k_0}{(2\pi)^3} \int \frac{d^3K}{(2\pi)^3}\, [1 - Q(\vec{k}_0, \vec{K}, k_F)] \,. \tag{20}$$

For small $|\vec{q}|$, $t_{ee}^{\text{loc}}(\vec{q})$ becomes just $v(\vec{q})$, and for large $|\vec{q}|$ it provides a good local approximation for $\langle\vec{q} + \vec{k}_0|\, t_{ee}^K(k_0^2)\, |\vec{k}_0\rangle$.

The following effective interaction interpolates smoothly between $\langle\vec{q} + \vec{k}_0|\, t_{ee}^K(k_0^2)\, |\vec{k}_0\rangle$ for large $|\vec{q}|$ and the RPA effective interaction for small $|\vec{q}|$ (Fig. 2),

$$\langle\vec{q} + \vec{k}_0;\, \omega + E|\, t_{\text{eff}}^K\, |\vec{k}_0; E\rangle = \frac{\langle\vec{q} + \vec{k}_0|\, t_{ee}^K(E)\, |\vec{k}_0\rangle}{\tilde{\epsilon}(\vec{q}, \omega)} \,, \tag{21}$$

where

$$\tilde{\epsilon}(\vec{q}, \omega) = 1 - t_{ee}^{\text{loc}}(\vec{q})\,\Pi_0(\vec{q}, \omega) \,. \tag{22}$$

For large $|\vec{q}|$, $\Pi_0(\vec{q}, \omega)$ vanishes[18] as $|\vec{q}|^{-2}$, so that

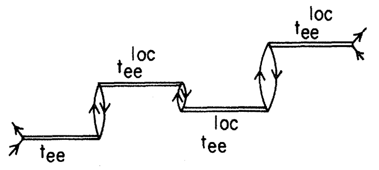

FIG. 2. Typical contribution to the effective electron-electron interaction t_{eff}. t_{ee} is the effective interaction for short distances, t_{ee}^{loc} is a local approximation to t_{ee}. Each polarization bubble represents a Lindhard function $\Pi_0(\vec{q}, \omega)$.

$$\langle \vec{q}+\vec{k}_0;\, \omega+E \,|\, t^K_{\text{eff}} \,|\, \vec{k}_0;\, E\rangle \to \langle \vec{q}+\vec{k}_0 \,|\, t^K_{ee}(E) \,|\, \vec{k}_0\rangle \,. \tag{23}$$

For small $|\vec{q}|$,

$$\langle \vec{q}+\vec{k}_0 \,|\, t^K_{ee}(k_0^2) \,|\, \vec{k}_0\rangle \to v(\vec{q})$$

and

$$t^{\text{loc}}_{ee}(\vec{q}) \to v(\vec{q}) \,,$$

so

$$\langle \vec{q}+\vec{k}_0;\, \omega+k_0^2 \,|\, t^K_{\text{eff}} \,|\, \vec{k}_0;\, k_0^2\rangle \to v(\vec{q})/[1-v(\vec{q})\Pi_0(\vec{q}, \omega)] \,, \tag{24}$$

which is just the RPA interaction.

In the small-$|\vec{q}|$ region, the function $\epsilon(\vec{q}, \omega)$ defined in Eq. (22) does not include the leading-order corrections to the Lindhard function $\Pi_0(\vec{q}, \omega)$ corresponding to self-energy insertions and dynamic-vertex correction terms inside the particle-hole polarization bubble. The self-energy insertions would take into account the polarization of the medium caused by the electron and the hole, while the vertex corrections would treat the mutual scatterint of the electron-hole pair. Our formalism would permit the inclusion of these additional terms. However, calculations by Du Bois and Kivelson[19] and Beeferman and Ehrenreich[20] indicate that these corrections are too small by an order of magnitude to account for the discrepancy between the RPA and experimental results for plasmon damping and optical properties of metals. This suggests that for real metals the dominant correction terms to the RPA in the small-$|\vec{q}|$ limit arise from effects of the metallic lattice rather than from perturbation corrections within the framework of the electron-gas model.

C. Response function

The density-density response function $\chi(\vec{q}, q^0)$ obtained using the effective interaction defined in Eq. (21) is

$$\begin{aligned}\chi(\vec{q}, q^0) = \Pi_0(\vec{q}, q^0) + \int d^4k_1/(2\pi)^4 \int [d^4k_2/(2\pi)^4] \\ \times G_0(k_1)G_0(k_1+q)G_0(k_2)G_0(k_2-q) \\ \times \langle \vec{q}+\vec{k};\, q^0+E \,|\, t^K_{\text{eff}}(E) \,|\, \vec{k};\, E\rangle \,,\end{aligned} \tag{25}$$

where

$$k_1 = \tfrac{1}{2}K + k \,;\quad k_2 = \tfrac{1}{2}K - k \,;\quad E = k_1^0 + k_2^0 \,. \tag{26}$$

In the small-$|\vec{q}|$ limit $\chi(\vec{q}, q^0)$ reduces to the RPA expression

$$\lim_{|\vec{q}|\to 0} \chi(\vec{q}, q^0) = \Pi_0(\vec{q}, q^0) + \frac{\Pi_0^2(\vec{q}, q^0)v(\vec{q})}{1-v(\vec{q})\Pi_0(\vec{q}, q^0)} \,. \tag{27}$$

D. Correlation function

We define the instantaneous two-body correlated wave function to be (Fig. 3)

$$\langle \vec{K}, \,|\vec{k}+\vec{q}|\, |\psi^{(\vec{K},\vec{k})}\rangle = \langle \vec{K}, \,|\vec{k}+\vec{q}|\, |\vec{K}, \vec{k}\rangle + \int \frac{dk_1^0}{2\pi} \int \frac{dk_2^0}{2\pi} \int \frac{dq^0}{2\pi}\, G_0(k_1)G_0(k_1+q)G_0(k_2)G_0(k_2-q)\, \frac{\langle \vec{k}+\vec{q} \,|\, t^K_{ee}(E) \,|\, \vec{k}\rangle}{\tilde{\epsilon}(\vec{q}, q^0)} \,, \tag{28}$$

with k_1, k_2, and E defined in Eq. (26). This wave function reduces to familiar forms in the large- and small-$|\vec{q}|$ limits. For large $|\vec{q}|$, $|\psi\rangle$ is the correlated wave function for a ladder sum of Coulomb interactions.

$$\lim_{|\vec{q}|\to\infty} \langle \vec{K}, \vec{k}+\vec{q} \,|\, \psi^{(\vec{K},\vec{k})}\rangle = \langle \vec{k}+\vec{q} \,|\, v^{-1}\, t^K_{ee}(E=\tfrac{1}{2}k^2) \,|\, \vec{k}\rangle \,, \tag{29}$$

while for small $|\vec{q}|$, upon averaging $|\psi\rangle$ over $\vec{k}$ and $\vec{K}$, we get back the correlated wave function for RPA,

$$\frac{1}{\rho^2} \int \frac{d^3K}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \lim_{|\vec{q}|\to 0} \langle \vec{K}, \vec{k}+\vec{q} \,|\, \psi^{(\vec{K},\vec{k})}\rangle = \delta^3(\vec{q}) + \frac{1}{\rho^2} \int \frac{dq^0}{2\pi}\, \Pi_0^2(\vec{q}, q^0)\, \frac{\langle \vec{k}+\vec{q} \,|\, v \,|\, \vec{k}\rangle}{\epsilon_{\text{RPA}}(\vec{q}, q^0)} \,. \tag{30}$$

Here ρ is the average density and ϵ_{RPA} the RPA dielectric function.

Let us calculate the spatial wave function $\psi(r)$ for small $k_F r \ll 1$. From this we can determine the short-range pair-correlation function $g(r)$:

$$\begin{aligned}\psi^{(K,\vec{k})}(\vec{r}, t=0) = e^{i\vec{k}\cdot\vec{r}} - \int \frac{dk_1^0}{2\pi} \int \frac{dk_2^0}{2\pi} \int \frac{d^4q}{(2\pi)^4}\, e^{i(\vec{k}+\vec{q})\cdot\vec{r}}\, \frac{\langle \vec{k}+\vec{q} \,|\, t^K_{ee}(E) \,|\, \vec{k}\rangle}{\tilde{\epsilon}(\vec{q}, q^0)} \\ \times \frac{1}{\frac{1}{2}\vec{k}_1^2 - k_1^0 - i\eta}\, \frac{1}{\frac{1}{2}|\vec{k}_1+\vec{q}|^2 - k_1^0 - q^0 + i\eta}\, \frac{1}{\frac{1}{2}\vec{k}_2^2 - k_2^0 - i\eta}\, \frac{1}{\frac{1}{2}|\vec{k}_2-\vec{q}|^2 - k_2^0 - q^0 + i\eta} \,.\end{aligned} \tag{31}$$

Defining $\vec{q}\,'=\vec{k}+\vec{q}$, and carrying out the integrations over the energy variables,

$$\psi^{(K,\vec{k})}(\vec{r},t=0)=e^{i\vec{k}\cdot\vec{r}}-\int\frac{d^3q'}{(2\pi)^3}\,e^{i\vec{q}\,'\cdot\vec{r}}$$

$$\times\frac{\langle\vec{q}\,'|t_{ee}^{K}(E=\tfrac{1}{4}K^2+k^2)|\vec{k}\rangle}{\epsilon(|\vec{q}\,'-\vec{k}|,q^0=\tfrac{1}{2}[q'^2+k^2+\vec{K}\cdot(\vec{q}\,'-\vec{k})])}\,\frac{\Theta(|\tfrac{1}{2}\vec{K}+\vec{q}\,'|-k_F)\,\Theta(|\tfrac{1}{2}\vec{K}-\vec{q}\,'|-k_F)}{q'^2-k^2}+\chi_{\mathrm{pl}}^{(K,\vec{k})}(\vec{r})\,,\qquad(32)$$

where $\chi_{\mathrm{pl}}^{(K,\vec{k})}(\vec{r})$ is the contribution to ψ from the plasmon pole, $\epsilon(\vec{q},q^0)=0$ at $q^0=\omega_{\mathrm{q}}^{\mathrm{pl}}$ for $|\vec{q}|<q_c$. In the Appendix we estimate that $\chi_{\mathrm{pl}}^{(K,\vec{k})}(\vec{r})$ is negligible compared with the first two terms, and we do not consider it further. The remaining expression does not change for small $k_F r$ if we replace ϵ by 1, and the expression for $\psi(r)$ reduces to the contribution from a single ladder sum,

$$\psi^{(K,\vec{k})}(\vec{r},t=0)=e^{i\vec{k}\cdot\vec{r}}-\int\frac{d^3q'}{(2\pi)^3}\,e^{i\vec{q}\,'\circ\vec{r}}\;\frac{\langle\vec{q}\,'|\,t_{ee}^{K}(E=\tfrac{1}{4}K^2+k^2)|\vec{k}\rangle}{q'^2-k^2}\;Q(\vec{q}\,',\vec{K},k_F)\,.\qquad(33)$$

Once again approximating the Pauli operator Q by its angle average $\overline{Q}$, and expanding both t_{ee} and the exponentials in partial waves, we get, after performing the angular integration $\hat{\vec{q}}\,'$,

$$\psi^{(K,\vec{k})}(\vec{r},t=0)=\sum_{l}(2l+1)\,i^{l}\,P_l(\hat{\vec{k}}\circ\hat{\vec{r}})\,\psi_l^{(K,k)}(r)\,,\qquad(34)$$

where

$$\psi_l^{(K,k)}(r)=j_l(kr)-(2/\pi)\int_0^{\infty}dq'\,q'^2\,j_l(q'r)[\langle q'|t_l^{K}(E)|k\rangle/(q'^2-k^2)]\,\overline{Q}(q',K,k_F)\,.\qquad(35)$$

For small $k_F r$, the partial-wave series converges rapidly. The instantaneous pair-correlation function within our approximations is

$$g(r)=\sum_{\sigma}{}'\sum_{\vec{K}}{}'\sum_{\vec{k}}{}'\;|\,\psi_{\sigma}^{(K,\vec{k})}(\vec{r},t=0)|^2,\qquad(36)$$

σ indicating the relative spin of the pair, and $\sum'$ the average over the appropriate quantity,

$$0\leqq|\tfrac{1}{2}\vec{K}|,\;|\vec{k}|\leqq k_F;\quad\sigma=\uparrow\uparrow,\uparrow\downarrow\;.$$

This expression for $g(r)$ is within the spirit of our use of the Brueckner formalism with retarded interactions. Certain processes which cannot be included in the square of a correlated wave function are neglected. In either short- or long-range limit, the neglected terms are unimportant. Performing the angular integration over $\vec{k}$ and $\vec{K}$, and carrying out the spin sum, we get finally

$$g_{\mathrm{av}}(r)=\sum_{|\vec{K}|}{}'\sum_{|\vec{k}|}{}'\left(\frac{1}{2}\sum_{l\text{ even}}+\frac{3}{2}\sum_{l\text{ odd}}\right)$$

$$\times(2l+1)\,|\psi_l^{(K,k)}(r)|^2.\qquad(37)$$

The different weighting for even and odd partial waves is due to exchange. If we omit the sum over spins and specify $\sigma=\uparrow\downarrow$, we get the correlations from the repulsion alone without exchange,

$$g_{\uparrow\downarrow}(r)=\sum_{|\vec{K}|}{}'\sum_{|\vec{k}|}{}'\sum_{l}(2l+1)\,|\psi_l^{(K,k)}(r)|^2.\qquad(38)$$

Let us now look at the region $k_F r\gg 1$, to check that with our effective interaction t_{eff}, $g(r)$ does indeed give the RPA result in this limit. For $k_F r\gg 1$, the exponential in the integrand will oscillate destructively for large $|\vec{q}|$, so we need only consider the integrand in the region of small $|\vec{q}|$ where

$$\langle\vec{q}+\vec{k}\,|\,t_{ee}^{K}(E)\,|\vec{k}\rangle=v(\vec{q})+O(1)\,,$$

$$t_{ee}^{\mathrm{loc}}(\vec{q})=v(\vec{q})+O(1)\,,\qquad(39)$$

$$\tilde{\epsilon}(\vec{q},q^0)=\epsilon_{\mathrm{RPA}}(\vec{q},q^0)=1-v(\vec{q})\,\Pi_0(\vec{q},q^0).$$

Thus for large r, our expression for $g(r)$ reduces to

$$g(r)=\sum_{\sigma}{}'\frac{1}{\rho}\int_{|\vec{k}_1|<k_F}\frac{d^3k_1}{(2\pi)^3}\,\frac{1}{\rho}\int_{|\vec{k}_2|<k_F}\frac{d^3k_2}{(2\pi)^3}\left|e^{i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}/2}+\int\frac{dk_1^0}{2\pi}\int\frac{dk_2^0}{2\pi}\int\frac{d^4q}{(2\pi)^4}\right.$$

$$\left.\times\left(e^{i(\vec{q}+\vec{k}_1/2-\vec{k}_2/2)\cdot\vec{r}}\,\frac{v(\vec{q})}{\epsilon_{\mathrm{RPA}}(\vec{q},q^0)}\,G_0(k_1)G_0(k_1+q)G_0(k_2)G_0(k_2-q)\right)\right|^2\,,\qquad(40)$$

where ρ is the average density. Expanding the squared term, this becomes

$$g(r)=1+\sum_{\sigma}{}'\frac{2}{\rho^2}\int_{|\vec{k}_1|<k_F}\frac{d^4k_1}{(2\pi)^4}\int_{|\vec{k}_2|<k_F}\frac{d^4k_2}{(2\pi)^4}\int\frac{d^4q}{(2\pi)^4}\cos(\vec{q}\cdot\vec{r})\,\frac{v(\vec{q})}{\epsilon_{\mathrm{RPA}}(\vec{q},q^0)}$$

$$\times[G_0(k_1)G_0(k_1+q)G_0(k_2)G_0(k_2-q)]+\sum_\sigma{}' \frac{1}{\rho^2}\int_{|\vec{k}_1|<k_F}\frac{d^3k_1}{(2\pi)^3}\int_{|\vec{k}_2|<k_F}\frac{d^3k_2}{(2\pi)^3}$$

$$\times\left|\int\frac{dk_1^0}{2\pi}\int\frac{dk_2^0}{2\pi}\int\frac{d^4q}{(2\pi)^4}e^{i(\vec{q}+\vec{k}_1/2-\vec{k}_2/2)\cdot\vec{r}}\frac{v(\vec{q})}{\epsilon_{\mathrm{RPA}}(\vec{q},q^0)}G_0(k_1)G_0(k_1+q)G_0(k_2)G_0(k_2-q)\right|^2 . \tag{41}$$

Thus our expression for the pair-correlation function at large separations reduces to the square of the RPA wave function. The advantage of this expression over the more commonly used RPA pair-correlation function,[21]

$$g_{\mathrm{RPA}}^{\uparrow\downarrow}=1-\frac{1}{\rho^2}\frac{1}{4\pi^2}\int dq^0\int dq\,q^2 \times\frac{v(\vec{q})}{\epsilon_{\mathrm{RPA}}(|\vec{q}|,q^0)}\Pi_0^2(|\vec{q}|,q^0)\frac{\sin qr}{qr} , \tag{42}$$

is that the former is explicitly non-negative. At metallic densities, the RPA terms are only dominant for large separations where the pair-correlation function is nearly unity.[16] In this case we may neglect the squared term in Eq. (41), and expressions (41) and (42) become identical.

We conclude that the effective electron-electron interaction t_{eff} which we have constructed does indeed interpolate between the RPA interaction at large distances and the ladder sum of Coulomb interactions at small distances.

III. RESULTS OF CALCULATION

A. Correlation function

Our calculated pair-correlation functions $g_{\mathrm{av}}(r)$ and $g_{\uparrow\downarrow}(r)$ are shown in Figs. 4 and 5 for different electron densities, covering the range of densities for valence electrons in the alkali metals. We measure density in terms of the dimensionless parameter r_s which is the average electron spacing in units of Bohr radii. We may express r_s in terms of the Fermi momentum k_F, and the Bohr radius $a_0 \simeq 0.52$ Å,

$$r_s^3 = 9/4\pi a_0^3 k_F^3 . \tag{43}$$

Comparing $g_{\mathrm{av}}(r)$ with the corresponding quantity computed by STLS, also shown in Fig. 4, we see the agreement between the two for all metallic densities and all separations is remarkable, recalling that the two calculations are quite different. The good agreement suggests that the STLS interaction at short distances is closely related to the ladder sum of unscreened Coulomb interactions. This is reasonable, since STLS did in fact consider only two-body correlations. In Figs. 5 we show $g_{\uparrow\downarrow}(r)$ and the long-range part of $g_{\uparrow\downarrow}^{\mathrm{RPA}}(r)$, and confirm that the two functions agree at large distances.

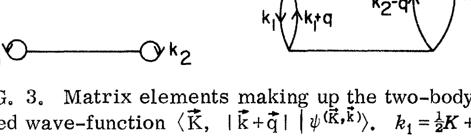

FIG. 3. Matrix elements making up the two-body correlated wave-function $\langle\vec{K}, \ |\vec{k}+\vec{q}|\ |\psi^{(\vec{K},\vec{k})}\rangle$. $k_1=\frac{1}{2}K+k$ and $k_2=\frac{1}{2}K-k$.

Yasuhara[11] also calculated $g_{\uparrow\downarrow}(r)$ for small r from a ladder sum of bare Coulomb interactions. However, he approximated the Coulomb interaction by

$$v(\vec{q}-\vec{k})\simeq\begin{cases}4\pi e^2/|\vec{q}|^2 & |\vec{q}|>|\vec{k}|\\ 4\pi e^2/|\vec{k}|^2 & |\vec{k}|>|\vec{q}| .\end{cases} \tag{44}$$

Such an approximation is of doubtful validity and leads to the retention of only the s-wave contribution to $g(r)$. We find that our higher partial waves give significant contributions to $g(r)$ for small but nonzero r. Our results do support Yasuhara's further assumption that his neglect of the electron starting momenta is a good approximation provided r is much less than the average electronic separation.

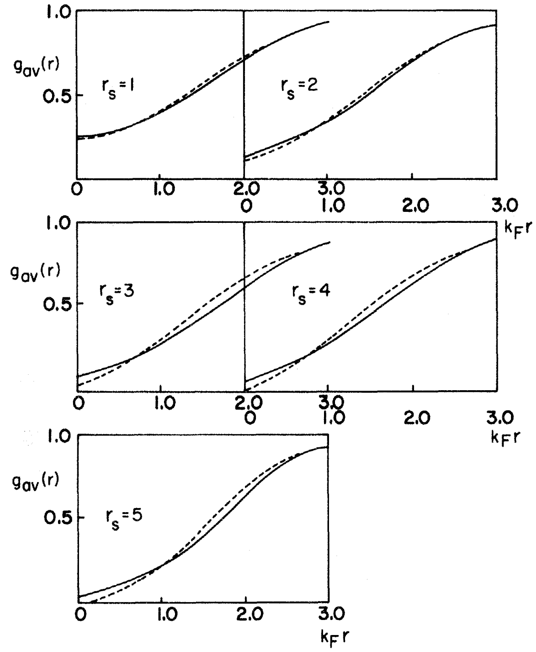

FIG. 4. Pair-correlation function $g(r)$ averaged over spin for different densities. The solid line is $g_{\mathrm{av}}(r)$ using our effective interaction t_{eff}. It is always non-negative. The broken line is $g_{\mathrm{av}}(r)$ calculated by STLS.

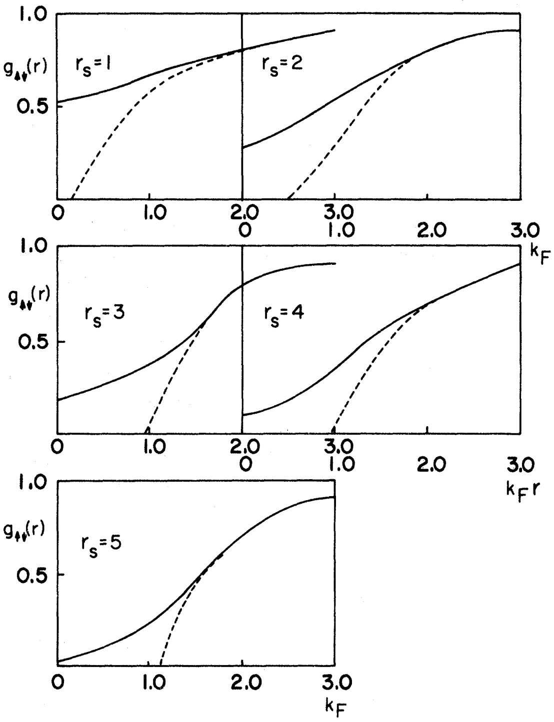

FIG. 5. Pair-correlation function $g(r)$ for antiparallel spin. This represents the correlations in the absence of exchange. The solid line is $g_{\uparrow\downarrow}(r)$ using our effective interaction t_{eff}. The broken line is $g_{\uparrow\downarrow}(r)$ in the RPA.

Yasuhara[22] has proposed the dielectric function

$$\epsilon^{-1}(\vec{q},\omega)=1+v(q)\Pi_0(\vec{q},\omega)/[1-\Phi(\vec{q})\Pi_0(\vec{q},\omega)] \quad (45)$$

for use at all values of $|\vec{q}|$. The effective potential $\Phi(\vec{q})$ is adjusted away from the Coulomb potential $v(\vec{q})$ until the resultant change in the ground-state energy equals the binding energy calculated from his ladder sum.

Hede and Carbotte[12] used the ladder sum of static RPA interactions to compute $g_{\uparrow\downarrow}(r)$ for small r. Our arguments in Sec. II suggest that retardation effects from additional electrons should not be important, so it is reasonable to approximate screening by its static limit. The value $g_{\uparrow\downarrow}(r)$ computed by Hede and Carbotte differs from both ours and Yasuhara's and this could suggest that screening terms are important. We showed in Sec. II that exchange cancellations were important for screening terms, but in the case of the static approximation the importance of exchange terms is not clear. We find it extremely puzzling, however, that their $g_{\uparrow\downarrow}(r)$ becomes negative for small r at low densities $r_s \gtrsim 5$, since it follows from the symmetry of the diagrams summed, that the complete ladder sum of any static interaction leads to a non-negative pair-correlation function (Fig. 6).

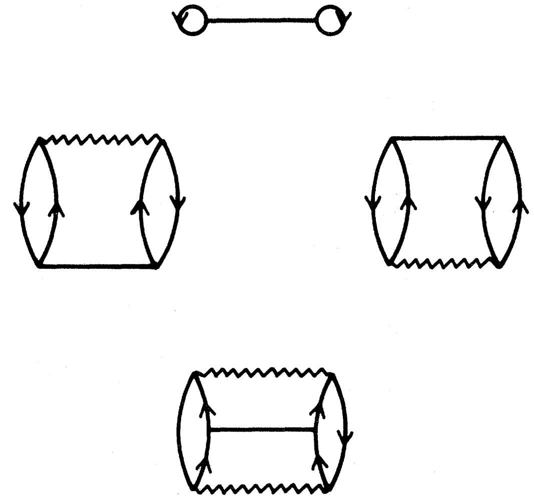

FIG. 6. Contributions to the pair-correlation function for the ladder sum of *any* static interaction. The wavy line represents the complete ladder sum. The horizontal straight line represents the square of the density operator. The sum of these four terms make up an absolute square, $\psi^*\psi$.

B. Correlation energy

We can compute the correlation energy per particle from $g_{\text{av}}(r)$ using

$$E_{\text{corr}}(r_s)=0.92/r_s+(4\pi/r_s^2)(9\pi/4)^{1/3}\times\int_0^{r_s}d\lambda\int_0^{\infty}d(k_Fr)\,(k_Fr)\times[g_{\text{av}}^{(\lambda)}(k_Fr)-g_{\text{HF}}(k_Fr)]\,\text{Ry}\,, \quad (46)$$

where $g_{\text{av}}^{(\lambda)}(k_Fr)$ is the value of $g_{\text{av}}(k_Fr)$ for density $r_s=\lambda$, and $g_{\text{HF}}(k_Fr)$ is the Hartree–Fock pair-correlation function which is independent of λ:

$$g_{\text{HF}}(k_Fr)=1-\tfrac{1}{2}\{[3/(k_Fr)^3]\times[\sin k_Fr-k_Fr\cos k_Fr]\}^2\,. \quad (47)$$

Knowing $g_{\text{av}}^{(\lambda)}(k_Fr)$ for all densities $\lambda\le r_s$, we can then evaluate $E_{\text{corr}}(r_s)$ directly.

Our computed values for $E_{\text{corr}}(r_s)$ are shown in Table I, together with the values from STLS. The two are in close agreement.

C. Cohesive energy

These values of the correlation energy can be used to predict the cohesive energies of the alkali metals, following the procedure discussed by Nozières and Pines,[23] and using their values for m_{kin}

TABLE I. Correlation energy per particle (eV).

r_s	Present calc	STLS
1	−1.70	−1.69
2	−1.25	−1.25
3	−1.01	−1.02
4	−0.85	−0.87
5	−0.74	−0.76

and E_{ion}. We must assume that the correlation energy per particle, E_{corr}, is not sensitive to the form of the positive background. (Recall that the electron-gas model uses a uniform positive background instead of a discrete array of positive ions.) This is a reasonable assumption, since we find that most of the contributions to E_{corr} occur when the electrons are close to each other compared with their average spacing. In alkali metals the average electron spacing equals the ion-core spacing, so while the electrons are strongly interacting with each other they should remain in a nearly constant potential from the lattice. In Sec. II, our results were found to be insensitive to just such a constant potential v_{pol}. However, this approximation will always underestimate E_{corr} to some extent, since the additional polarization of the electrons by the ions will increase the binding energy. Hence we will also underestimate the cohesive energy.

The cohesive energies we calculated are shown in Table II, together with the experimentally measured cohesive energies of three alkali metals,[24] and also the cohesive energies calculated by STLS. We use the customary units kcal mole^{-1}(= 0.0433 eV particle^{-1}). Our calculated values are about 10% less than the measured values. Part of this difference is caused by our neglect of electron polarization by the ions.

D. Plasma-dispersion curve

Our short-distance correlations also change the plasma-dispersion curve from its RPA form. The plasmon frequency $\omega_p(\vec{q})$ is the solution of the equation[18]

$$\epsilon(\vec{q}, \omega_p(\vec{q})) = 0 = 1 - \frac{4\pi e^2}{|\vec{q}|^2}\Pi_0(\vec{q}, \omega_p(\vec{q})) \times\left[1 - \left(t_{ee}^{\mathrm{loc}}(\vec{q}) - \frac{4\pi e^2}{|\vec{q}|^2}\right)\Pi_0(\vec{q}, \omega_p(\vec{q}))\right]^{-1} \quad (48)$$

The small-$|\vec{q}|$ limit of the Lindhard function $\Pi_0(\vec{q}, \omega)$ is given by[18]

$$\lim_{|\vec{q}|\to 0}\Pi_0(\vec{q}, \omega) = \frac{k_F^3}{3\pi^2}\frac{|\vec{q}|^2}{m\omega^2}\left(1 + \frac{3}{5}\frac{\hbar^2 k_F^2}{m^2}\frac{|\vec{q}|^2}{\omega^2} + 0(|\vec{q}|^4)\right). \quad (49)$$

We also need the small-$|\vec{q}|$ limit of $t_{ee}^{\mathrm{loc}}(\vec{q})$. Since $\langle\vec{q}+\vec{k}_0|t_{ee}^{K}(k_0^2)|\vec{k}_0\rangle$ is a slowly varying function of $\vec{k}_0$ and K for $0 \leq \frac{1}{2}K$, $|\vec{k}| \leq k_F$, we approximate

$$t_{ee}^{\mathrm{loc}}(\vec{q}) \simeq \langle\vec{q}\,|\,t_{ee}^{0}(0)\,|\,\vec{0}\,\rangle$$

Then,

$$t_{ee}^{\mathrm{loc}}(\vec{q}) = \frac{4\pi e^2}{q^2} + \int_{|\vec{p}|>k_F} d^3p\,\frac{4\pi e^2}{|\vec{q}-\vec{p}|^2}\frac{1}{p^2}t_{ee}^{\mathrm{loc}}(\vec{p}) \;. \quad (50)$$

For $|\vec{q}| < k_F$, an iterative expansion of this equation shows that each of the integrals goes as $O((q/k_F)^0)$ to leading order, i.e., independently of $|\vec{q}|$. Accordingly, we may expand the integral equation as

$$\lim_{|\vec{q}|\to 0} t_{ee}^{\mathrm{loc}}(|\vec{q}|) = \frac{4\pi e^2}{|\vec{q}|^2} + \int_{|\vec{p}|>k_F} d^3p\,\frac{4\pi e^2}{|\vec{p}|^2}\frac{1}{|\vec{p}|^2} \times t_{ee}^{\mathrm{loc}}(|\vec{p}|) + O\left(\frac{|\vec{q}|}{k_F^3}\right) \;. \quad (51)$$

We rewrite this

$$\lim_{|\vec{q}|\to 0} t_{ee}^{\mathrm{loc}}(|\vec{q}|) = \frac{4\pi e^2}{|\vec{q}|^2}\left[1 + \frac{|\vec{q}|^2}{k_F^2}\gamma + O\left(\frac{|\vec{q}|^3}{k_F^3}\right)\right], \quad (52)$$

where

$$\gamma = \int_0^\infty d(k_F r)(k_F r)[\tilde{\psi}(k_F r) - 1], \;\; \langle q\,|\,v\,|\,\tilde{\psi}\rangle = t_{ee}^{\mathrm{loc}}(|\vec{q}|) \;. \quad (53)$$

Then,

$$\lim_{|\vec{q}|\to 0}\epsilon(\vec{q}, \omega) = 1 - \frac{4\pi e^2}{|\vec{q}|^2}\frac{k_F^2}{3\pi^2}\frac{|\vec{q}|^2}{m\omega^2} \times\left(1 + \frac{3}{5}\frac{\hbar^2 k_F^2}{m^2}\frac{|\vec{q}|^2}{\omega^2}\right)\left(1 + \frac{4\pi e^2}{\gamma k_F^2}\frac{k_F^2}{3\pi^2}\frac{|\vec{q}|^2}{m\omega^2}\right) \;. \quad (54)$$

For $|\vec{q}| = 0$, $\epsilon(0, \omega_p) = 0$ still gives the RPA solution

$$\omega_p^2 = \frac{k_F^3}{3\pi^2}\frac{4\pi e^2}{m} \;, \quad (55)$$

but for $|\vec{q}| \neq 0$ we get as a solution,

$$\omega_p^2(q) = \omega_p^2\{1 + [\tfrac{9}{5} + \gamma(k_{\mathrm{TF}}/k_F)^2] \times q^2/k_{\mathrm{TF}}^2 + \cdots\} \;, \quad (56)$$

where k_{TF} is the Thomas-Fermi wave number.

The quantity γ contains all our information about short-distance correlations. In the RPA,

$$t_{ee}^{\mathrm{loc}}(|\vec{q}|) = v(\vec{q}) \;, \quad (57)$$

so that $\gamma = 0$, while in the Hubbard approximation $\gamma = -\frac{1}{2}$.[10] Our calculated values of γ vary between -0.51 and -0.58 over the density range $2 \leq r_s \leq 5$, and while our resultant dispersion curves differ considerably from the RPA curves, they agree closely with the curves from both the Hubbard approximation and from STLS. In Fig. 7 we show our dispersion curves for $r_s = 2$, 3, and 4, and the corresponding RPA curves. The difference between the curves represents the effect of short-distance correlations. The experimental points were deduced from data for aluminum, lithium, and sodium.[25] They lie between the two curves but closer to the RPA curve. This could indicate a breakdown in our calculations for the interme-

TABLE II. Cohesive energy of alkali metals (kcal mole^{-1}).

Metal	Expt	Present calc	STLS
Li	−38.4	−35.8	−36.0
Na	−25.9	−23.4	−23.9
K	−21.5	−19.4	−19.9

diate region, but it is also possible that the ion lattice significantly affects the measured values, indicating that the electron gas itself is not an adequate model for this property.

E. Compressibility

We can calculate the compressibility of the electron gas from the correlation energy per particle [Eq. (46)] using the thermodynamic expression

$$\frac{1}{\kappa}=\Omega\frac{d^2E_0}{d\Omega^2}, \tag{58}$$

which relates the compressibility κ to the total ground state energy E_0. Ω is the volume per particle, $\Omega=\frac{4}{3}\pi r_0^3$. It follows that

$$\frac{1}{\kappa}=\frac{1}{12\pi r_s a_0^3}\left(\frac{d^2E_0}{dr_s^2}-\frac{2}{r_s}\frac{dE_0}{dr_s}\right) \tag{59}$$

and

$$\frac{\kappa^{\text{free}}}{\kappa}=1-\frac{\alpha}{\pi}r_s+\frac{\alpha^2}{3e^2}r_s^4a_0\left(\frac{d^2E_{\text{corr}}}{dr_s^2}-\frac{2}{r_s}\frac{dE_{\text{corr}}}{dr_s}\right), \tag{60}$$

where κ^{free} is the compressibility of the noninteracting gas and $\alpha=(4/9\pi)^{1/3}$.

The first two terms correspond to the Hartree-Fock expression, which predicts a negative compressibility when $r_s \gtrsim 6$. In our calculation the third term is small and negative, and the compressibility becomes negative at an even higher density, for $r_s \gtrsim 5$. In Table III we show $\kappa^{\text{free}}/\kappa$ for our theory, for STLS, and for Hartree-Fock. While it is not possible to check calculated compressibilities against experiment, the compressibility sum rule[23] does provide a consistency test for them. Within our theory this sum rule requires that our computed ratio $\kappa^{\text{free}}/\kappa$ be equal to

$$1+\gamma(k_{\text{TF}}/k_F)^2 \tag{61}$$

where $k_{\text{TF}}^2=4me^2k_F/\pi\hbar^2$ is the Thomas-Fermi wave number. We find in our theory that this sum rule is violated over the entire density range. This is not very surprising since compressibility is a quantity which is sensitive to the region between the large and small separation limits, and it is this region in which we use an interpolation procedure. STLS also violates this sum rule. Vashishta and Singwi[26] have extended STLS to include density derivatives of the pair-correlation function. With these additional terms their theory satisfies the compressibility sum rule well. Including such derivatives incorporates higher than two-particle correlations in the short-distance effective interaction. We intend in subsequent paper to include certain three-body terms in our effective interaction. It can be shown that inclusion of such terms must improve the agreement with the sum rule.

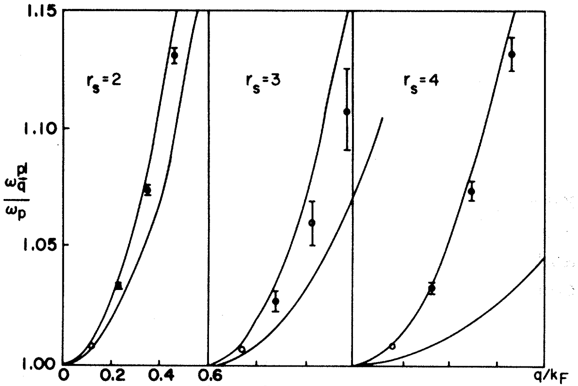

FIG. 7. Plasma-dispersion curves for different values of r_s. Each curve ends when $\omega_p(q)$ crosses the single-particle excitation spectrum. The lower curves are from our calculations, the higher curves from the RPA. The experimental points are from data for Al, Li, and Na (Ref. 25).

TABLE III. Ratio of compressibilities $\kappa^{\text{free}}/\kappa$.

r_s	Present calc.	STLS	Hartree-Fock
1	0.83	0.83	0.83
2	0.64	0.64	0.67
3	0.45	0.45	0.50
4	0.25	0.25	0.34
5	0.05	0.05	0.17

IV. CONCLUDING REMARKS

In this paper we have developed a calculational scheme which interpolates between the dominant terms for the two-body effective interaction at large and small separations. It is of considerable pedagogical interest to correctly treat the short-distance correlations in a pure electron gas satisfactorily, but the results do not lead to many predictions which can be tested experimentally. Further, such quantities as the compressibility or the plasmon dispersion relation are sensitive to the value of the pair-correlation function in the intermediate separation region where we must rely on a nonunique interpolation between our long- and short-distance results. However, it is shown in a subsequent paper that the annihilation rate of positrons in an electron gas is sensitive to the short-distance electron-electron correlations,[4] and this provides us with a test of the validity of our effective electron-electron interaction.

The agreement between our results and those of STLS over a wide range of electron densities indicates a close relation between the STLS self-consistent approach and our diagrammatic method.

ACKNOWLEDGMENT

The authors would like to acknowledge useful discussions with Professor A. Sjölander.

APPENDIX: PLASMON CONTRIBUTION TO SHORT-RANGE ELECTRON CORRELATIONS

We want to estimate the plasmon contribution to the electron-correlated wave function $\psi^{(K,\vec{k})}(\vec{r}, t=0)$ for $k_F r \ll 1$. The complete expression for $\psi^{(K,\vec{k})}(\vec{r}, t=0)$ is

$$\psi^{(K,\vec{k})}(\vec{r}, t=0) = e^{i\vec{k}\cdot\vec{r}} - \int \frac{dk_1^0}{2\pi} \int \frac{dk_2^0}{2\pi} \int \frac{d^4q}{(2\pi)^4}\, e^{i(\vec{k}+\vec{q})\cdot\vec{r}}\, \frac{\langle \vec{k}+\vec{q}\,|\,t_{ee}^{K}(E)\,|\,\vec{k}\rangle}{\epsilon(\vec{q}, q^0)}\, G_0(k_1)G_0(k_1+q)G_0(k_2)G_0(k_2-q). \tag{A1}$$

For $|\vec{q}| < q_c$, $\epsilon^{-1}(\vec{q}, q^0)$ has a pole at $q^0 = \omega_{\vec{q}}^{\mathrm{pl}}$, and the plasmon contribution to ψ comes from the residue of this pole. Defining the residue to be $R(|\vec{q}|)$ and averaging over K, $\vec{k}$, and σ, the plasmon contribution for $r=0$ is

$$\chi_{\mathrm{pl}}(r=0) = \sum_{\sigma}{}' \int_{|\vec{q}|<q_c} \frac{d^3q}{(2\pi)^3} R(|\vec{q}|) \frac{1}{\rho} \int_{|\vec{k}_1|<k_F} \frac{d^4k_1}{(2\pi)^4} G_0(k_1)G_0(k_1+q)$$

$$\times \frac{1}{\rho} \int_{|\vec{k}_2|<k_F} \frac{d^4k_2}{(2\pi)^4} G_0(k_2)G_0(k_2-q)\langle \vec{k}+\vec{q}\,|\,t_{ee}^{K}\,|\,\vec{k}\rangle \Big|_{q^0=\omega_{\vec{q}}^{\mathrm{pl}}}. \tag{A2}$$

At metallic densities the momentum q_c, at which the plasmon pole intersects with the single-particle excitation spectrum, is such that $q_c/k_F \lesssim 1$.[23] We may then approximate $\langle \vec{k}+\vec{q}\,|\,t_{ee}^{K}\,|\,\vec{k}\rangle$ in the integrand by $v(|\vec{q}|)$, so that

$$\chi_{\mathrm{pl}}(r=0) = \frac{1}{2\rho^2} \int_{|\vec{q}|<q_c} \frac{d^3q}{(2\pi)^3} R(|\vec{q}|)$$

$$\times \Pi_0^2(|\vec{q}|, \omega_{|\vec{q}|}^{\mathrm{pl}}) v(|\vec{q}|). \tag{A3}$$

By definition

$$\lim_{q^0 \to \omega_{\vec{q}}^{\mathrm{pl}}} \epsilon^{-1}(\vec{q}, q^0) = \frac{R(\vec{q})}{q^0 - \omega_{\vec{q}}^{\mathrm{pl}}} \tag{A4}$$

and

$$\epsilon^{-1}(\vec{q}, q^0) = \frac{1}{1 - \Pi_0(\vec{q}, q^0)\, t_{ee}^{\mathrm{loc}}(\vec{q})} \tag{A5}$$

$$\simeq \frac{1}{1 - \Pi_0(\vec{q}, q^0)\, v(|\vec{q}|)} \quad \text{for } |\vec{q}|/k_F \lesssim 1. \tag{A6}$$

Also,[18]

$$\lim_{|\vec{q}|\to 0} \Pi_0(\vec{q}, q^0) = \frac{\hbar^2}{m^2} \frac{k_F^3}{3\pi^2} \frac{|\vec{q}|^2}{(q^0)^2}, \tag{A7}$$

so that

$$\lim_{|\vec{q}|\to 0} (\omega_{\vec{q}}^{\mathrm{pl}})^2 \equiv \omega_p^2 = \left(\frac{\hbar^2}{m^2} \frac{k_F^2}{3\pi^2} |\vec{q}|^2\right) \frac{4\pi e^2}{|\vec{q}|^2}, \tag{A8}$$

$$\lim_{q^0 \to \omega_{\vec{q}}^{\mathrm{pl}}} \lim_{|\vec{q}|\to 0} \epsilon^{-1}(\vec{q}, q^0) = \frac{1}{1 - \omega_p^2/(q^0)^2}$$

$$= \frac{\omega_p^2}{2\omega_p(q^0 - \omega_p)}. \tag{A9}$$

It therefore follows

$$\lim_{|\vec{q}|\to 0} R(\vec{q}) = \tfrac{1}{2}\omega_p, \tag{A10}$$

$$\lim_{|\vec{q}|\to 0} \Pi_0(\vec{q}, \omega_{\vec{q}}^{\mathrm{pl}}) = \left(\frac{4\pi e^2}{|\vec{q}|^2}\right)^{-1}. \tag{A11}$$

Since we want only an order-of-magnitude estimate for $\chi_{\mathrm{pl}}(r=0)$, we replace $R(\vec{q})$ and $\Pi_0(\vec{q}, \omega_{\vec{q}}^{\mathrm{pl}})$ by their limits for $|\vec{q}| \to 0$,

$$\chi_{\mathrm{pl}}(r=0) \simeq \frac{1}{2\rho^2} \int_{|\vec{q}|<q_c} \frac{d^3q}{(2\pi)^3} \frac{1}{2}\, \omega_p \left(\frac{4\pi e^2}{|\vec{q}|^2}\right)^{-1}. \tag{A12}$$

Taking $q_c \simeq 0.47\sqrt{r_s}\, k_F$,[23] this reduces to

$$\chi_{\mathrm{pl}}(r=0) \simeq 8.2\times 10^{-3}/r_s^{1/2}. \tag{A13}$$

For metallic densities, $r_s \gtrsim 2$, $\chi_{\mathrm{pl}}(r=0)$ is much smaller than the other correlation corrections to the unperturbed wave function $e^{i\vec{k}\cdot\vec{r}}$. Hence we are justified in neglecting χ_{pl} for small r.

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