calculate

$$s_2(t)=\frac{H_{c2}}{R_n}\left(\frac{\partial R(H)}{\partial H}\right)\bigg|_{H=H_{c2}-0}-\frac{H_{c2}}{R_n}\left(\frac{\partial R(H)}{\partial H}\right)\bigg|_{H=H_{c2}+0}$$

$$=\frac{g(r)}{2\beta_A}\left(\frac{\delta_0}{\xi(t)}\right)^2[2\kappa_2{}^2(t)-1]^{-1},\qquad\text{(A23)}$$

with

$$g(r)=r[1-r+r(2/r-1)^{1/2}].$$

Finally, by combining (A18), (A20), and (A21), we can derive

$$\alpha(t)=\frac{(2/r-1)^{1/2}-1}{s_3(t)}\left(\frac{H_{c3}}{H_{c3}-H_{c2}}\right).\qquad\text{(A24)}$$

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Electron Correlations at Metallic Densities*

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The dielectric function of a degenerate electron gas in the random-phase approximation, and the one proposed by Hubbard, which takes exchange effects into account, have been extensively used in the study of metallic properties. However, both dielectric functions lead to an overestimate of the short-range correlations between particles. This is manifest from the fact that the pair-correlation function is negative for small interparticle separations over the whole range of metallic densities, and implies an overestimate of the correlation energy. An improved expression of the dielectric function is given, which includes explicitly, in an approximate way, the short-range correlations arising from both Coulomb and exchange effects by being a functional of the structure factor. The structure factor and the dielectric function can then be determined in a self-consistent manner. The numerical solution of the self-consistent scheme yields a pair-correlation function which is positive for all values of the density up to $r_s=4$. For $r_s>4$, it is very slightly negative at small separations, but it is so small that it can be considered to be zero for all practical purposes. New estimates of the correlation energy are given for the entire metallic density range, and are smaller than the earlier estimates. These results are used to recalculate the cohesive energy of the alkali metals. A discussion of the plasmon dispersion relation, the compressibility, and the liquid-solid transition, both for the electron system and for an astrophysically interesting system of protons over a background of electrons, is also given.

I. INTRODUCTION

The dielectric formulation of the many-body problem has been found to be very fruitful in studying the degenerate electron gas and the metallic properties which depend strongly on electron-electron interactions. The system that one studies is a degenerate electron gas on a uniform, neutralizing background. The density-fluctuation excitation spectrum, the correlations between the density fluctuations, and the ground-state energy of the system are rigorously expressible in terms of its frequency- and wavelength-dependent dielectric function. This model system serves as a useful guide to the study of many metallic properties, such as the interionic potential and the screening of defects, under the assumption that the dielectric function is not essentially altered by the discrete nature of the ion lattice. It is, therefore, of great importance to have a precise knowledge of this function in the range of electron densities encountered in metals.

The dielectric function first given by Lindhard,[1] which corresponds to the random-phase approximation[2–4] (RPA), is the one which is most commonly used. It provides a good description of the plasmon excitation modes and of long-wavelength screening phenomena, but its validity is otherwise limited to high electron densities ($r_s\ll 1$). The inadequacy of RPA becomes manifest, for instance, from the fact that the pair-distribution function, which is positive-definite, becomes negative[5,6] for small separation between particles, over the entire range of metallic densities ($2\leq r_s\leq 6$). This arises from the failure of the RPA to take account of short-range effects; indeed, no local field correction[7] is made in this theory. The neglect of short-range

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* Based on work performed under the auspices of the U.S. Atomic Energy Commission.

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effects in the evaluation of the dielectric function leads to a large Coulomb hole, resulting in an overestimation of the correlation energy.

Approximate procedures to improve upon the RPA value of the correlation energy have been proposed by Hubbard[4] and by Nozières and Pines.[8] Hubbard's calculation of the correlation energy involved an approximate infinite summation of bubble-ladder diagrams. In this way he was able to take into account the contribution of the exchange terms, which at large momentum transfers tends to cancel one-half the contribution of the direct terms. On the other hand, the method of Nozières and Pines is based on an interpolation procedure between the low and high momentum transfer contributions to the correlation energy. The two methods are in essence based on the same physical idea, that is, that the RPA is approximately valid for small momentum transfers while for large momentum transfers the main contribution to the energy arises from the interactions of electrons with antiparallel spins only. Hubbard's approximation yields a modified expression for the dielectric function. This expression has been extensively used in the study of metallic properties and has been found to yield improved results. However, the pair-distribution function obtained from Hubbard's dielectric function remains negative for small separation between particles, over the entire range of metallic densities.[9] This defect arises, as we now know, from the fact that Hubbard's dielectric function includes the local-field correction only to the extent that it takes into account the exchange hole in the Hartree-Fock approximation. In the region of metallic densities, where the electron-electron interaction plays an increasingly important role, the local-field correction associated with the Coulomb hole must also be taken into account.

Gaskell,[10] on the other hand, has used the Rayleigh-Schrödinger variational method, with a wave function which is the product of a Slater determinant and a correlation function, to calculate the ground-state energy and the pair-correlation function of the electron gas. He finds that the pair-correlation function becomes negative for $r_s > 2.66$.

It has recently been proposed[11] that the short-range correlations responsible for the local-field corrections can be taken into account in the dielectric function in a more satisfactory and self-consistent manner by making the dielectric function a functional of the Fourier transform of the pair-distribution function $g(\mathbf{r})$. This was achieved in the classical case by an *ansatz*, which replaced the two-particle distribution function $f(1, 1')$ in the Liouville equation for the one-particle distribution function $f(1)$ by

$$f(1, 1') = f(1) f(1') g(\mathbf{x}-\mathbf{x}'), \tag{1}$$

thus making it possible to close the hierarchy of equations. On the other hand, the Fourier transform of $g(\mathbf{r})-1$, which is $(1/n)[S(\mathbf{q})-1]$, where n is the number density and $S(\mathbf{q})$ is the usual structure factor, is related to the dielectric function $\epsilon(\mathbf{q}, \omega)$ through the exact relation[12]

$$S(\mathbf{q}) = -\frac{\hbar q^2}{4\pi^2 e^2 n} \int_0^\infty \mathrm{Im}[\epsilon(\mathbf{q}, \omega)]^{-1} d\omega. \tag{2}$$

Since the dielectric function is now a functional of $S(\mathbf{q})$, Eq. (2) imposes a self-consistency requirement on $S(\mathbf{q})$ and $\epsilon(\mathbf{q}, \omega)$. This self-consistent scheme, as was anticipated, yields[13] values of $g(o)$ which remain positive for all values of r_s up to $r_s = 4$, a region which covers the majority of metals with the exception of the heavy alkali metals. For values of $r_s > 4$, the calculated values of $g(o)$ are negative but are so small that for all practical purposes one can consider $g(o)$ to be zero. The *ansatz* (1) is therefore reasonable even for the heavy alkali metals. Similar calculations, based on the above self-consistent scheme,[11] have also been carried out by Hubbard[14] for $r_s \leq 4$. Thus the grave difficulty of a large and negative $g(r)$ for small separations, that the earlier theories had encountered, has been overcome. It therefore encourages one to reinvestigate those metallic properties which are affected by short-range electron correlations. Experimental studies of many phenomena in solids have recently been refined to the point where it has become both interesting and necessary for the theory to incorporate in a satisfactory manner electron-electron interactions.

In this paper, we give a detailed discussion of the theory, present numerical results for the pair-correlation function and the correlation energy over the whole range of metallic densities, and compare them with the results of the earlier theories. A short discussion of the plasma dispersion relation, the compressibility, and the liquid-solid transition, both for the electron system and for an astrophysically interesting system of protons over a background of electrons, is also given. The present estimates of the correlation energy are smaller than those given by the previous theories, since the short-range correlations are no longer overestimated.

II. THEORY

A. Classical Case

The equation of motion for the classical one-particle distribution function $f(\mathbf{x}, \mathbf{p}; t)$ in the presence of an

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[12] See, for instance, D. Pines, *Elementary Excitations in Solids* (W. A. Benjamin, Inc., New York, 1964), p. 129–131.

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[14] J. Hubbard, Phys. Letters **25A**, 709 (1967).

external potential $V_e(\mathbf{x}, t)$ is[15]

$$[\partial f(\mathbf{x}, \mathbf{p}; t)/\partial t]+\boldsymbol{v}\cdot\nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{p}; t) -\nabla_{\mathbf{x}} V_e(\mathbf{x}, t)\cdot\nabla_{\mathbf{p}} f(\mathbf{x}, \mathbf{p}; t) - \int \nabla_{\mathbf{x}}\Phi(\mathbf{x}-\mathbf{x}')\cdot\nabla_{\mathbf{p}} f(\mathbf{x}, \mathbf{p}; \mathbf{x}', \mathbf{p}' \mid t)\, d\mathbf{x}' d\mathbf{p}'=0, \tag{3}$$

where $\Phi(\mathbf{x})$ is the Coulomb interaction potential and $f(\mathbf{x}, \mathbf{p}; \mathbf{x}', \mathbf{p}' \mid t)$ is the two-particle distribution function, and the other symbols have their usual meaning. The equation for the two-particle distribution function contains, in turn, the three-particle distribution function, and so on. We terminate this infinite hierarchy of equations by making the *ansatz*

$$f(\mathbf{x}, \mathbf{p}; \mathbf{x}', \mathbf{p}' \mid t) = f(\mathbf{x}, \mathbf{p}; t) f(\mathbf{x}', \mathbf{p}'; t) g(\mathbf{x}-\mathbf{x}'), \tag{4}$$

where $g(\mathbf{x})$ is taken to be the *equilibrium, static pair-correlation function*. The *ansatz* (4) takes care, in an approximate way, of short-range correlations between the particles, through a function which has a simple physical meaning. The function $g(\mathbf{x})$ tends to unity for large values of its argument, while for small values it is expected to be small, but not necessarily tending to zero in the special case of the Coulomb potential that we are considering. The assumption $g(\mathbf{x})=1$ for all separations in Eq. (4) corresponds to the approximation leading to the Landau-Vlasov equation.[16] The usefulness of the *ansatz* (4) can only be judged *a posteriori*.

If one writes

$$f(\mathbf{x}, \mathbf{p}; t) = f_0(\mathbf{p}) + f_1(\mathbf{x}, \mathbf{p}; t), \tag{5}$$

where $f_1(\mathbf{x}, \mathbf{p}; t)$ denotes the deviation from the equilibrium distribution function $f_0(\mathbf{p})$ induced by the (weak) external potential, and one linearizes Eq. (3), one has the following equation for $f_1(\mathbf{x}, \mathbf{p}; t)$:

$$[(\partial/\partial t)+\boldsymbol{v}\cdot\nabla_{\mathbf{x}}] f_1(\mathbf{x}, \mathbf{p}; t) -\left(\nabla_{\mathbf{x}} V_e(\mathbf{x}, t)+\int \nabla_{\mathbf{x}}\psi(\mathbf{x}-\mathbf{x}') f_1(\mathbf{x}', \mathbf{p}'; t)\, d\mathbf{x}' d\mathbf{p}'\right)\cdot\nabla_{\mathbf{p}} f_0(\mathbf{p})=0, \tag{6}$$

where

$$\nabla_{\mathbf{x}}\psi(\mathbf{x}) = g(\mathbf{x})\nabla_{\mathbf{x}}\Phi(\mathbf{x}). \tag{7}$$

It is apparent from an inspection of Eqs. (6) and (7) that the effective electric field felt by a particle is

$$\mathbf{E}_{\text{eff}}(\mathbf{x}, t) = -\nabla_{\mathbf{x}} V_e(\mathbf{x},t) - \int \nabla_{\mathbf{x}}\Phi(\mathbf{x}-\mathbf{x}') f_1(\mathbf{x}', \mathbf{p}'; t)\, d\mathbf{x}' d\mathbf{p}' - \int [g(\mathbf{x}-\mathbf{x}')-1]\nabla_{\mathbf{x}}\Phi(\mathbf{x}-\mathbf{x}') f_1(\mathbf{x}', \mathbf{p}'; t)\, d\mathbf{x}' d\mathbf{p}', \tag{8}$$

where the first two terms on the right-hand side correspond to the usual macroscopic electric field, and the third term corresponds to the local-field correction in the present approximation. Only the first two terms are taken into account in the RPA.

In the Appendix, we have discussed in a formal way the approximations that are necessary to arrive at Eq. (8) starting from the equation of motion for the density matrix $\langle\psi_\sigma^\dagger(\mathbf{x}, t)\psi_\sigma(\mathbf{x}', t)\rangle$. In this equation the RPA term is isolated, and the remaining term is recast so as to give a nonlocal effective potential which involves the density-density correlation function. If this potential is made local, the density-density correlation function reduces to the pair-correlation function in the presence of the external field. When the latter function is replaced by its equilibrium value, one recovers Eq. (8).

Because of the linearity of Eq. (6) we can find its solution by considering a single Fourier component of the external potential:

$$V_e(\mathbf{x}, t) = V_e(\mathbf{q}, \omega)\exp[i(\mathbf{q}\cdot\mathbf{x}-\omega t)+\eta t]+\text{c.c.}, \tag{9}$$

where η is a positive infinitesimal. Proceeding in a standard manner, one finds the induced charge density

$$\rho_{\text{ind}}(\mathbf{q}, \omega) = \int f_1(\mathbf{q}, \omega; \mathbf{p})\, d\mathbf{p} = -\frac{Q_0(\mathbf{q}, \omega)}{\Phi(\mathbf{q})+\psi(\mathbf{q})Q_0(\mathbf{q}, \omega)} V_e(\mathbf{q}, \omega), \tag{10}$$

where

$$\Phi(\mathbf{q}) = 4\pi e^2/q^2, \tag{11}$$

$$\psi(\mathbf{q}) = \Phi(\mathbf{q}) + n^{-1}\int \frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\Phi(\mathbf{q}')[S(\mathbf{q}-\mathbf{q}')-1]\frac{d\mathbf{q}'}{(2\pi)^3}, \tag{12}$$

and

$$Q_0(\mathbf{q}, \omega) = -\Phi(\mathbf{q})\chi^0(\mathbf{q}, \omega), \tag{13}$$

$\chi^0(\mathbf{q}, \omega)$ being the usual free-electron polarizability. The dielectric function is, therefore, given by

$$\epsilon(\mathbf{q}, \omega) = 1 + \frac{Q_0(\mathbf{q}, \omega)}{1-G(\mathbf{q})Q_0(\mathbf{q}, \omega)}, \tag{14}$$

with

$$G(\mathbf{q}) = -n^{-1}\int \frac{\mathbf{q}\cdot\mathbf{q}'}{q'^2}[S(\mathbf{q}-\mathbf{q}')-1]\frac{d\mathbf{q}'}{(2\pi)^3}. \tag{15}$$

Equations (14) and (15), together with Eq. (2), provide a set of equations which have to be solved *self-consistently*.

It is easy to show that in the limit of large frequencies Eq. (14) reduces to

$$\epsilon(\mathbf{q}, \omega) = 1 - (\omega_p^2/\omega^2),$$

where ω_p is the plasma frequency. From the analytical properties of $\epsilon(\mathbf{q}, \omega)$ and the above asymptotic be-

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[15] See, for instance, E. G. D. Cohen, *Fundamental Problems in Statistical Mechanics* (North-Holland Publishing Co., Amsterdam, 1962).

[16] See, for instance, R. Brout and P. Carruthers, *Lectures on the Many-Electron Problem* (John Wiley & Sons, Inc., New York, 1963), p. 34.

havior, it follows that

$$\int_0^\infty \omega \operatorname{Im}[\epsilon(\mathbf{q}, \omega)]^{-1} d\omega = -\tfrac{1}{2}\pi\omega_p^2$$

and

$$\int_0^\infty \omega \operatorname{Im}[\epsilon(\mathbf{q}, \omega)] d\omega = \tfrac{1}{2}\pi\omega_p^2.$$

Equation (14) also satisfies the "perfect" screening requirement,

$$\lim_{\mathbf{q}\to 0}[\epsilon(\mathbf{q}, 0)]^{-1} = 0.$$

The compressibility sum rule is discussed in detail in Sec. IV B.

B. Quantum Mechanical Case

Our basic assumption consists in taking over the results of the preceding classical analysis of the dielectric function to the quantum mechanical case, merely replacing the classical free-electron polarizability and the classical structure factor by their quantum mechanical analogs. Clearly this assumption is made in the same spirit as the self-consistent–field method, in that the system responds to a screened electric potential through the free-particle polarizability. The only difference from the RPA is that one has allowed for a local depletion of the electron density around any given particle, which is associated with its Coulomb and exchange holes. Indeed, Eq. (14) reduces to the RPA expression of the dielectric function if one neglects all local-field corrections. On the other hand, as we shall see, it reduces to the Hubbard expression if one calculates $G(\mathbf{q})$ by Eq. (15) using the Hartree–Fock expression for the structure factor.

The non-RPA term in the equation of motion for the density fluctuation $\rho_\mathbf{q}$ in the absence of an external field can, indeed, be approximated to give an effective interaction between the electrons which is given by Eq. (12) with $S(\mathbf{q})$ replaced by its quantum mechanical analog. The equation of motion[17] of $\rho_\mathbf{q}$ is

$$\ddot{\rho}_\mathbf{q} = -\sum_i \left(\frac{\mathbf{q}\cdot\mathbf{p}_i}{m} + \frac{\hbar q^2}{2m}\right)^2 \exp(-i\mathbf{q}\cdot\mathbf{r}_i) - \Phi(\mathbf{q})\,\frac{q^2}{m}\,n\rho_\mathbf{q} - \sum_{\mathbf{q}'(\neq\mathbf{q})} \Phi(\mathbf{q}')(\mathbf{q}\cdot\mathbf{q}'/m)\rho_{\mathbf{q}-\mathbf{q}'}\rho_{\mathbf{q}'}. \tag{16}$$

The last term in Eq. (16) can be written as

$$m^{-1} \sum_{\mathbf{q}'(\neq\mathbf{q})} (\mathbf{q}\cdot\mathbf{q}')\Phi(\mathbf{q}') \sum_i \exp(i\mathbf{q}\cdot\mathbf{r}_i) \times \sum_j \exp[i(\mathbf{q}'-\mathbf{q})\cdot(\mathbf{r}_i-\mathbf{r}_j)],$$

where $\mathbf{r}_i$ is the position of the ith electron at time t. If we now replace the sum over j by its *static* average value, i.e.,

$$\begin{aligned}\langle\sum_j \exp[i(\mathbf{q}'-\mathbf{q})\cdot(\mathbf{r}_i-\mathbf{r}_j)]\rangle &= n^{-1}\langle\sum_{ij} \exp[i(\mathbf{q}'-\mathbf{q})\cdot(\mathbf{r}_i-\mathbf{r}_j)]\rangle \\ &= S(\mathbf{q}'-\mathbf{q}),\end{aligned} \tag{17}$$

Eq. (16) can be rewritten as

$$\ddot{\rho}_\mathbf{q} = -\sum_i \left(\frac{\mathbf{q}\cdot\mathbf{p}_i}{m} + \frac{\hbar q^2}{2m}\right)^2 \exp(-i\mathbf{q}\cdot\mathbf{r}_i) - \psi(\mathbf{q})\,\frac{q^2}{m}\,n\rho_\mathbf{q}. \tag{18}$$

The last term in the above equation has the same structure as the RPA term except that $\Phi(\mathbf{q})$ has been replaced by $\psi(\mathbf{q})$. If we remember this fact we can derive Eq. (14) proceeding in the same manner as in the RPA. One starts with the equation of motion for the particle-hole pair in the presence of an external field and calculates the induced charge density $\langle\rho_\mathbf{q}\rangle$. In the expression for the latter one then replaces the polarization field $\Phi(\mathbf{q})\langle\rho_\mathbf{q}\rangle$ by $\psi(\mathbf{q})\langle\rho_\mathbf{q}\rangle$.

III. REDUCTION TO THE HUBBARD DIELECTRIC FUNCTION

The simplest assumption that one can make in Eq. (15) is to take the Hartree-Fock value for the structure factor, which corresponds to neglecting the Coulomb interactions in the calculation of $G(\mathbf{q})$. In this case one has

$$S(\mathbf{q}) = -\frac{2}{(2\pi)^3 n}\int_{(k\leq q_F)} d\mathbf{k} \int_{(k'\leq q_F)} d\mathbf{k}'\,\delta(\mathbf{k}-\mathbf{k}'+\mathbf{q}), \tag{19}$$

where q_F is the Fermi momentum. Substituting Eq. (19) into Eq. (15) we have

$$G(\mathbf{q}) = \frac{2}{(2\pi)^6 n^2}\int_{(k\leq q_F)} d\mathbf{k} \int_{(k'\leq q_F)} d\mathbf{k}'\,\frac{\mathbf{q}\cdot(\mathbf{q}+\mathbf{k}-\mathbf{k}')}{|\mathbf{q}+\mathbf{k}-\mathbf{k}'|^2}. \tag{20}$$

If in the above integral we replace the factor $|\mathbf{q}+\mathbf{k}-\mathbf{k}'|^{-2}$ in the integrand by $(q^2+q_F^2)^{-1}$, as also done by Hubbard,[4] we find

$$G(\mathbf{q}) = \tfrac{1}{2}[q^2/(q^2+q_F^2)]. \tag{21}$$

With this value of $G(\mathbf{q})$, Eq. (14) is precisely the expression of the dielectric function given by Hubbard. Thus the Hubbard approximation for the exchange correction corresponds simply to using the Hartree–Fock value of the pair correlation function (representing the Pauli hole) in the present formulation.

In our case it is, however, not necessary to make the Hubbard approximation in evaluating the integral (20). The evaluation of the integral is rather lengthy but can

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[17] Reference 12, p. 99.

TABLE I. Values of γ.

r_s	1	2	3	4	5	6	10	20
γ	0.4561	0.4894	0.5107	0.5261	0.5378	0.5471	0.5715	0.5986

be done exactly. The result is

$$G(\mathbf{q})=\frac{9}{32}\left(\frac{q}{q_F}\right)^2\left\{\frac{2}{105}\left[24\left(\frac{q_F}{q}\right)^2+44+\left(\frac{q}{q_F}\right)^2\right]\right.$$
$$-2\frac{q_F}{q}\left[\frac{8}{35}\left(\frac{q_F}{q}\right)^2-\frac{4}{15}+\frac{1}{6}\left(\frac{q}{q_F}\right)^2\right]\ln\left|\frac{q+2q_F}{q-2q_F}\right|$$
$$\left.+\left(\frac{q}{q_F}\right)^2\left[\frac{1}{210}\left(\frac{q}{q_F}\right)^2-\frac{2}{15}\right]\ln\left|\frac{q^2-4q_F^2}{q^2}\right|\right\}. \quad (22)$$

From this the two limiting cases follow:

$$\lim_{\mathbf{q}\to\infty} G(\mathbf{q})=\tfrac{1}{2} \quad (23)$$

and

$$\lim_{\mathbf{q}\to 0} G(\mathbf{q})=\tfrac{3}{8}(q/q_F)^2. \quad (24)$$

The Hubbard approximation given by Eq. (21) is correct in the former limit, but gives

$$\lim_{\mathbf{q}\to 0} G(\mathbf{q})=\tfrac{1}{2}(q/q_F)^2$$

instead of Eq. (24). In Fig. 1, the Hubbard factor (21) is compared with the result (22). Since the two curves are very nearly the same, one does not expect to find large discrepancies between integrated properties calculated by either formula.

The effective potential $\psi(\mathbf{q})$,

$$\psi(\mathbf{q})=(4\pi e^2/q^2)[1-G(\mathbf{q})], \quad (25)$$

enters the effective ion-ion interaction in the calculation of phonon frequencies. Different forms of $G(\mathbf{q})$ have been used by various authors. Sham[18] and Vosko *et al.*[19] have used slightly modified forms of the Hubbard $G(\mathbf{q})$ reported in Eq. (21). Toya,[20] on the other hand, has used the expression (24) for all wave vectors up to $q^2=(8/3)q_F^2$, and unity otherwise.

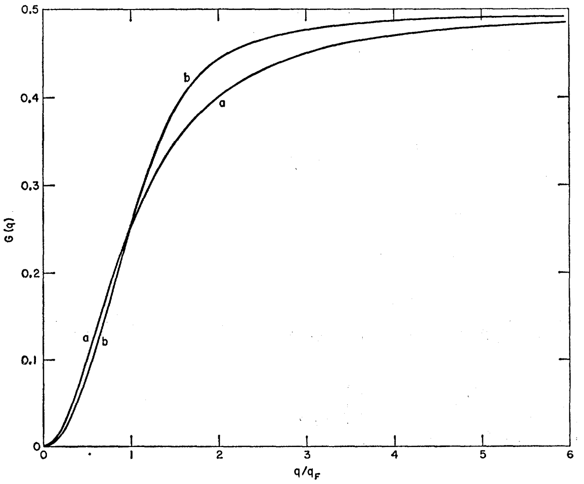

FIG. 1. $G(q)$ versus q/q_F in the Hartree-Fock approximation. Curve a is based on Hubbard's approximation [Eq. (21)] and curve b on Eq. (22).

IV. LONG-WAVELENGTH LIMIT

A. Plasma Dispersion

The dielectric function (14) in the limit $\mathbf{q}\to 0$ and ω finite has the form

$$\epsilon(\mathbf{q},\omega)=1-(\omega_P^2/\omega^2)[1+(9/5)(q/q_{FT})^2$$
$$-\gamma(q/q_F)^2]+\cdots, \quad (26)$$

where $\omega_P=(4\pi ne^2/m)^{1/2}$, $q_{FT}^2=(4me^2/\pi\hbar^2)q_F$, and

$$\gamma=-(2q_F)^{-1}\int_0^\infty[S(q)-1]dq. \quad (27)$$

In the present formulation the quantity γ has to be determined from $S(\mathbf{q})$ evaluated self-consistently. Since γ is an important quantity and occurs often in the present calculations, its values for different values of r_s are given in Table I. On the other hand, in the Hubbard case γ has the value $\frac{1}{2}$ if determined from Eq. (21) or the value $\frac{3}{8}$ if determined from Eq. (24). In the RPA, $\gamma=0$. From Eq. (26) follows the plasma dispersion relation:

$$\omega_p(q)=\omega_p\{1+[(9/10)-\tfrac{1}{2}\gamma(q_{FT}/q_F)^2](q/q_{FT})^2+\cdots\}. \quad (28)$$

It is interesting to note that for $r_s>5$, $\omega_p(q)$ is initially decreasing as q increases in both the Hubbard and the present theory.

In Fig. 2 are given the plasma frequencies as a function of q for a few values of r_s, as evaluated from the zeros of the dielectric function (14), with $S(\mathbf{q})$ determined self-consistently as discussed in the following section. The difference between these curves and those obtained from the Hubbard dielectric function is quite small, amounting to about 3% for $r_s=6$; whereas the difference from the RPA values reaches as much as 10% at this value of r_s. The decrease of $\omega_p(q)$ with increasing q becomes significant at $r_s=10$. In this case

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[20] T. Toya, J. Res. Inst. Catalysis, Hokkaido Univ. **6,** 161 (1958); **6,** 183 (1958); **7,** 60 (1959).

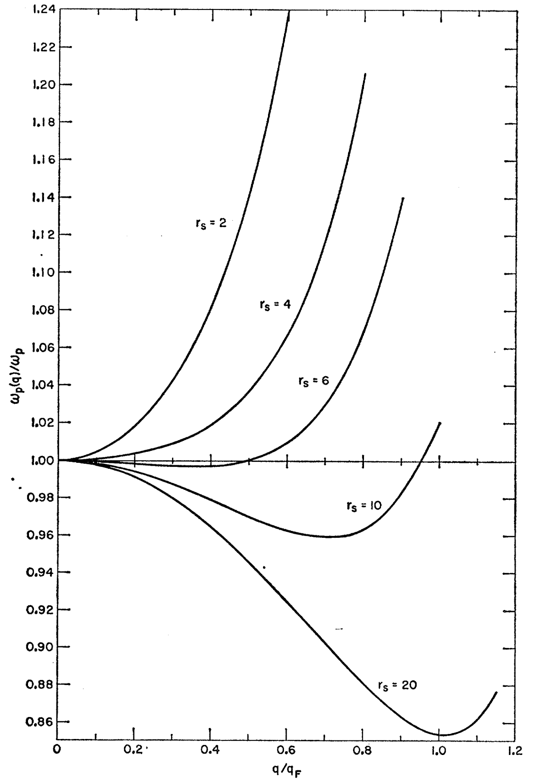

FIG. 2. Plasma dispersion curve for various values of r_s. Each curve ends near the onset of the pertinent particle-hole continuum.

the plasma frequency reaches its minimum value for $q=0.7k_F$, and then increases again. This decrease becomes even more pronounced at $r_s=20$. Thus, as the density is decreased, sufficient short-range correlations are present in the system that it requires less energy to excite a collective mode in which the electrons are to some extent localized than to excite a collective mode of infinite wavelength. The decrease in $\omega_p(q)$ is in fact qualitatively similar to the decrease of the longitudinal optical mode in the electron solid. In any comparison of the theory with experiment, it must be borne in mind, however, that the computed values of γ are probably much too large, as is indicated by the violation of the compressibility sum rule discussed in the following section.

B. Compressibility

The dielectric function (14) in the limit $\mathbf{q}\to 0$ at zero ω has the form

$$\lim_{\mathbf{q}\to 0}\epsilon(\mathbf{q},0)=1+\frac{(q_{FT}/q)^2}{1-\gamma(q_{FT}/q_F)^2}. \tag{29}$$

From the compressibility sum rule one finds

$$K_{\text{free}}/K=1-\gamma(q_{FT}/q_F)^2, \tag{30}$$

where K_{free} is the compressibility of the noninteracting gas. It turns out that the compressibility, when calculated from Eq. (30), is negative for $r_s\geq 3$ in both the Hubbard and the present theory. It is worth pointing out that the values of the compressibility calculated from the sum rule are different from those calculated from the second derivative of the ground-state energy (see Sec. V). This inconsistency, which occurs also in the RPA, arises from the fact that Eq. (30) represents a lower order of approximation to the compressibility. More generally, different values for the Landau short-range interaction parameters are obtained from an approximate transport equation such as Eq. (6) (in the macroscopic limit) than from the functional differentiation of the approximate energy expression. This inconsistency is characteristic of all perturbation theoretic calculations.

V. CALCULATIONS

A. General Formulas and Self-Consistency Requirement

The real and the imaginary parts of the Lindhard[1] free-electron polarizability $Q_0(\mathbf{q},\omega)$ are

$$\mathrm{Re}Q_0(\mathbf{q},\omega)=\frac{\kappa^2}{q^2}\left\{\tfrac{1}{2}+(4q)^{-1}\left[1-\left(\frac{\omega+q^2}{2q}\right)^2\right]\ln\left|\frac{\omega+2q+q^2}{\omega-2q+q^2}\right|+(4q)^{-1}\left[1-\left(\frac{\omega-q^2}{2q}\right)^2\right]\ln\left|\frac{\omega-2q-q^2}{\omega+2q-q^2}\right|\right\}, \tag{31}$$

$$\begin{aligned}\mathrm{Im}Q_0(\mathbf{q},\omega)&=\tfrac{1}{4}\pi(\kappa^2\omega/q^3), & \omega&\leq 2q-q^2\\ &=\tfrac{1}{4}\pi(\kappa^2/q^3)\{1-[(\omega-q^2)/2q]^2\}, & |2q-q^2|&\leq\omega\leq 2q+q^2\\ &=0, & \omega&\geq 2q+q^2\end{aligned} \tag{32}$$

where ω is expressed in units of $\hbar q_F^2/2m$, q is expressed in units of q_F, and $\kappa^2=q_{FT}^2/q_F^2$. In the same units, Eq. (15) becomes

$$G(q)=-\frac{3}{4}\int_0^\infty q'^2[S(q')-1]\left\{1+\frac{q^2-q'^2}{2q'q}\ln\left|\frac{q+q'}{q-q'}\right|\right\}dq'. \tag{33}$$

The self-consistency condition (2) can be written as

$$S(q)=-\frac{3}{2\pi}\int_0^{2q+q^2}\mathrm{Im}[\epsilon(q,\omega)]^{-1}d\omega+\frac{3}{2}\frac{q^2}{\kappa^2}\left(\frac{\partial\,\mathrm{Re}\epsilon(q,\omega)}{\partial\omega}\right)^{-1}_{\omega=\omega_p(q)}, \tag{34}$$

where we have written explicitly the contributions of the single-particle excitations and of the plasmon excitations to the structure factor.

Starting from the known expression of $S(q)$ in the Hartree–Fock approximation, $G(q)$ was calculated by Eq. (33) and the result was inserted in Eq. (14), which was then used to recalculate $\omega_p(q)$ from the zero of $\epsilon(q,\omega)$ and $S(q)$ by Eq. (34). After the initial two iterations, the average of the structure factors obtained from the two previous iterations was used as input for each subsequent iteration. About 10 iterations were necessary to obtain convergence in $G(q)$ within 0.1%. This implies on closer inspection a much higher accuracy in $S(q)$. It was checked that alternative starting points [in particular, the assumption $S(q)=1$] lead to the same final result.

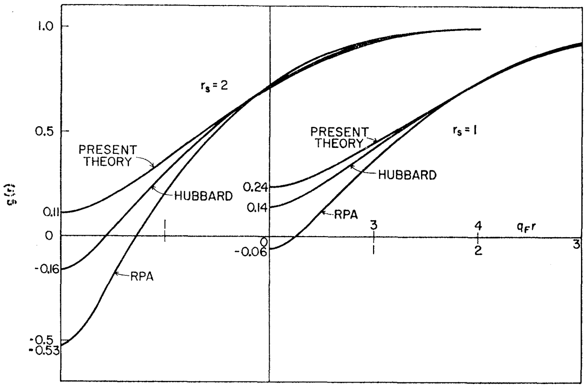

FIG. 3. Pair-correlation function $g(r)$ versus $q_F r$ for $r_s=1$ and $r_s=2$.

B. Pair-Correlation Function

The pair-correlation function $g(r)$ is given by

$$g(r)=1+\frac{3}{2r}\int_0^\infty q(\sin qr)\,[S(q)-1]dq, \qquad (35)$$

where r is expressed in units of q_F^{-1}. The self-consistent values of $S(q)$ obtained as mentioned above were used in Eq. (35) to calculate $g(r)$. The results are shown graphically in Figs. 3–5 for values of r_s of interest. For comparison the corresponding curves obtained in the Hubbard approximation and in the RPA are also given.

The most important point to notice is that in the present theory $g(r)$ remains positive for all values of r_s up to $r_s=4$, whereas for values of $r_s>4$ our calculated values of $g(r)$ become negative for very small values of r but are so small that for all practical purposes they may indeed be considered to be zero. Thus in the entire region of metallic densities, including the heavy alkali metals, the *ansatz* (4) is proved to be reasonable. On the other hand, the previous theories give a pair-correlation function which not only is negative and large for $r=0$ over the metallic density range, but also remains negative over a sizable range of separation (up to $rk_F\simeq 1$). We may also note that our value of $g(o)$ for $r_s=1$ is in close agreement with that of Ueda[21] [$g(o)=0.22$, as recalculated by Hedin[6]], who used a Green's-function approach valid at small r_s.

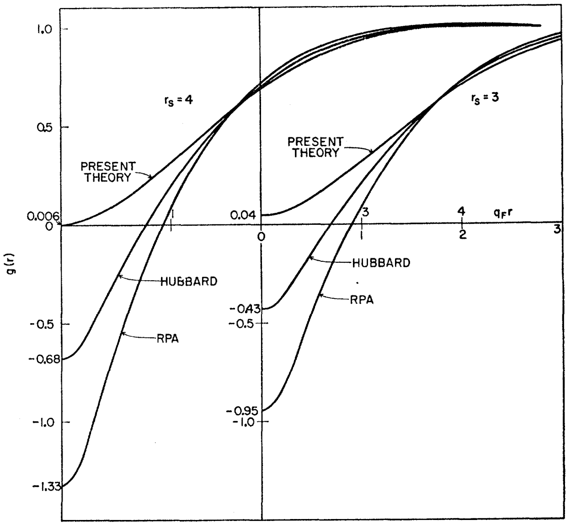

FIG. 4. Pair-correlation function $g(r)$ versus $q_F r$ for $r_s=3$ and $r_s=4$.

For large values of r, $g(r)$ exhibits an oscillatory behavior, which is not displayed in the figures. However, the oscillations have a very small amplitude and are very broad. This amplitude increases with r_s, but even at $r_s=6$ the first peak (at $rq_F=4.2$) has a value

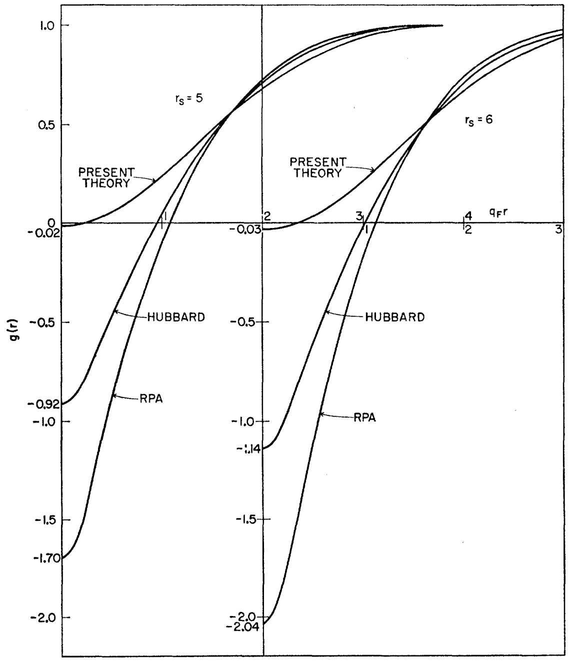

FIG. 5. Pair-correlation function $g(r)$ versus $q_F r$ for $r_s=5$ and $r_s=6$.

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[21] S. Ueda, Progr. Theoret. Phys. (Kyoto) **26**, 45 (1961).

TABLE II. Correlation energy (Ry/electron).

r_s	1	2	3	4	5	6	10	20
Present theory	−0.124	−0.092	−0.075	−0.064	−0.056	−0.050	−0.036	−0.022
Hubbard	−0.131	−0.102	−0.086	−0.076	−0.069	−0.064	...	...
Nozières-Pines	−0.115	−0.094	−0.081	−0.072	−0.065	−0.060	...	...
RPA	−0.157	−0.124	−0.105	−0.094	−0.085	−0.078	...	...

of only 1.013. This result is in agreement with the results reported by Gaskell[10] for his variational calculation.

The behavior of the pair-correlation function in the electron liquid is therefore very different from the behavior to which one is accustomed in classical liquids. In the latter, $g(r)$ exhibits a very pronounced, narrow peak followed by secondary peaks. This is understandable, since, in contrast to classical liquids, in the electron liquid the interparticle potential is very soft and quantum effects disfavor localization of the particles. A similar effect[22] occurs in liquid He^3, where, in spite of the very hard character of the potential, the first peak in $g(r)$ is much smaller and broader than that in classical liquids.

We have also evaluated the pair-correlation function up to $r_s=20$. It is gratifying to note that, even for such larger values of r_s, $g(o)$ is never smaller than -0.05. This gives us some confidence to estimate the correlation energy of the gas at low densities by the present method (see Sec. VI). The height of the first peak in $g(r)$ is only 1.04 at $r_s=20$.

C. Correlation Energy

The interaction energy per particle is given by

$$E_{\rm int}(r_s)=\sum_{\mathbf{q}}(2\pi e^2/q^2)[S(\mathbf{q})-1], \qquad (36)$$

which, in the notation introduced previously, is

$$E_{\rm int}(r_s)=-(4/\pi r_s)(9\pi/4)^{1/3}\gamma(r_s)\ \text{Ry}. \qquad (37)$$

It is easily seen that the Ferrell condition[23] on the ground-state energy, which is equivalent to

$$(d/dr_s)[E_{\rm int}(r_s)/r_s]\leq 0, \qquad (38)$$

is satisfied with the values of γ given in Table I.

The total energy per particle is given by

$$E_0=\frac{2.2099}{r_s^2}\ \text{Ry}+\int_0^{e^2}\frac{d\lambda}{\lambda}E_{\rm int}(\lambda), \qquad (39)$$

where λ is a parameter representing the strength of the interaction. Equation (39) can be rewritten as

$$E_0=\left[\frac{2.2099}{r_s^2}-\frac{4}{\pi r_s^2}\left(\frac{9\pi}{4}\right)^{1/3}\int_0^{r_s}\gamma(r_s)dr_s\right]\text{Ry} \qquad (40)$$

and the correlation energy per particle is given by

$$E_{\rm corr}=\frac{1}{r_s^2}\int_0^{r_s}\left[-\frac{4}{\pi}(\tfrac{9}{4}\pi)^{1/3}\gamma(r_s)+0.9163\right]dr_s\ \text{Ry}. \qquad (41)$$

Using our computed values of $\gamma(r_s)$, the correlation energy has been evaluated from Eq. (41) and the results are given in Table II. For the sake of comparison the corresponding values of the correlation energy in the RPA and in the Hubbard approximation and those of Nozières and Pines[8] are also given. The values of Gaskell[4] are quite close to those given by Hubbard and by Nozières and Pines.

It is important to note that the present estimates of the correlation energy are smaller than earlier estimates, because the correlation at small distances is no longer overestimated. The deviation becomes as large as 20–30% at $r_s=6$.

Following the procedure discussed by Nozières and Pines,[24] we have reevaluated the cohesive energy of the alkali metals under the assumption that the correlation energy is the same as for the electron gas on a uniform positive background. In Table III, the values of the cohesive energy calculated on the present theory are compared with those calculated by Nozières and Pines and with the experimental values. It is seen that on the whole the values of Nozières and Pines are closer to the experimental values. However, it should be noted that the polarization of the electron gas by the discrete ions will tend to increase the magnitude of the cohesive energy.

TABLE III. Cohesive energy of the alkali metals (kcal/mole.[a])

	Li	Na	K	Rb	Cs
Present theory	−36.0	−23.9	−19.9	−17.8	−17.6
Nozières-Pines	−38.1	−26.4	−22.6	−20.6	−20.4
Experimental	−38.4	−25.9	−21.5	−19.5	−18.7

[a] In the calculation of the theoretical cohesive energy, we have taken the values of the kinetic mass and of $E_{\rm ion}$ adopted by D. Pines and P. Nozières, Ref. 24. The theoretical values in the second row differ slightly from those given in Ref. 24. The experimental values are taken from G. N. Lewis and M. Randall, *Thermodynamics* (revised by K. S. Pitzer and L. Brewer) (McGraw-Hill Book Co., New York, 1961), Appendix 7.

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[22] Y. Narahara, J. Phys. Soc. Japan **24**, 169 (1968).

[23] R. A. Ferrell, Phys. Rev. Letters **1**, 443 (1958).

[24] D. Pines and P. Nozières, *The] Theory of Quantum Fluids* (W. A. Benjamin, Inc., New York, 1966), Vol. I, p. 333–336.

D. Compressibility

The thermodynamic definition of the compressibility yields the expression

$$K_{\text{free}}/K=\left(\frac{4}{9\pi}\right)^{2/3}\tfrac{1}{6}r_s^4\left[\frac{d^2E_0}{dr_s^2}-\frac{2}{r_s}\frac{dE_0}{dr_s}\right], \tag{42}$$

which may be rewritten as

$$K_{\text{free}}/K=1-\left(\frac{4}{9\pi}\right)^{2/3}\frac{r_s}{\pi}+\left(\frac{4}{9\pi}\right)\tfrac{1}{6}r_s^4\left(\frac{d^2E_{\text{corr}}}{dr_s^2}-\frac{2}{r_s}\frac{dE_{\text{corr}}}{dr_s}\right). \tag{43}$$

The first two terms in Eq. (43) represent, respectively, the contributions from the free-gas kinetic energy and from the Hartree-Fock exchange energy, while the last term represents the contribution from the correlation energy.

In Table IV are given the values of the compressibility for various values of r_s, as calculated from Eq. (43) by different theories. It is important to note that the compressibility becomes negative in all cases for $r_s \gtrsim 5$. The electron gas on a uniform background becomes, therefore, unstable for values of r_s larger than 5, in the sense that an infinitesimal fluctuation in the density would lead the system to fly apart. In fact, the correlation contribution to the compressibility is small compared with either of the first two terms in Eq. (43). Therefore, the occurrence of the instability, although not its precise location, is determined by the vanishing of the two leading terms at $r_s \simeq 6$, and is essentially independent of the approximation involved in the estimation of the correlation term. It is apparent from Table IV that all the existing theories of electron correlations give essentially the same values for the compressibility as a function of r_s, even though the corresponding pair-correlation functions are widely different.

VI. WIGNER SOLID

We have seen in the foregoing section that the electron liquid becomes unstable for $r_s \gtrsim 5$. One might think that the liquid would undergo a transition to the solid state, first discussed by Wigner,[25] when the instability occurs. In fact, the available theories predict that this is not so. First of all, as Van Horn[26] has shown using the energy of the electron solid evaluated by Carr *et al.*,[27] the solid itself becomes unstable at $r_s=6.4$, because its compressibility becomes negative. On the other hand, the liquid is stable and its chemical potential is lower than that of the solid for all values of the pressure at which the solid is stable. This is illustrated in Fig. 6. The foregoing analysis then suggests that the liquid-solid transition could not occur. One would arrive at the same conclusion if one were to use the expression for the correlation energy given by Nozières and Pines.

TABLE IV. Ratio of compressibilities K_{free}/K.

r_s	1	2	3	4	5	6
Present theory	0.83	0.64	0.45	0.25	0.05	−0.17
Hubbard	0.83	0.65	0.46	0.26	0.06	−0.15
Nozières-Pines	0.83	0.65	0.46	0.27	0.07	−0.15
RPA	0.83	0.64	0.45	0.24	0.03	−0.19

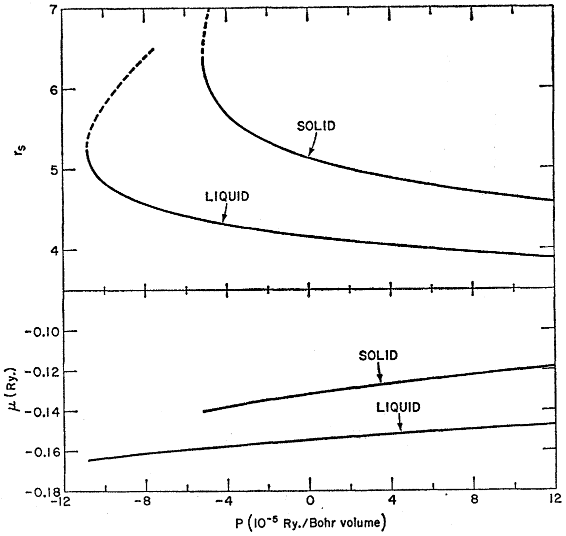

FIG. 6. The quantity r_s and the chemical potential μ versus pressure for the electron liquid and the electron solid.

An interesting aspect of the Wigner solid, which might have some astrophysical significance, has been discussed recently by Van Horn.[26] One deals here with a liquid or a solid of protons on a neutralizing background of electrons at such high densities (occurring in white dwarf stars) that the electrons can be treated as noninteracting. In contrast to the electron liquid discussed above, the system is now stabilized by the electron background. Since the difference in density of the solid and the liquid phases of the proton system at the transition is very small, as pointed out by Van Horn, the equilibrium condition of the two phases after linearization reduces to the condition that their energies be equal at the same density. The contribution of the background to the equilibrium condition cancels, and it is sufficient to consider the energy of the proton solid and that of the proton liquid as functions of r_s, which, except for a trivial change of units, are given by the corresponding energies of the electron system on a uniform background.

In Fig. 7, we have plotted the energy of the electron solid and that of the liquid as functions of r_s. The

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[25] E. P. Wigner, Trans. Faraday Soc. **34**, 678 (1938).
[26] H. M. Van Horn, Phys. Rev. **157**, 342 (1967).
[27] W. J. Carr, Jr., R. A. Coldwell-Horsfall, and A. E. Fein, Phys. Rev. **124**, 747 (1961).

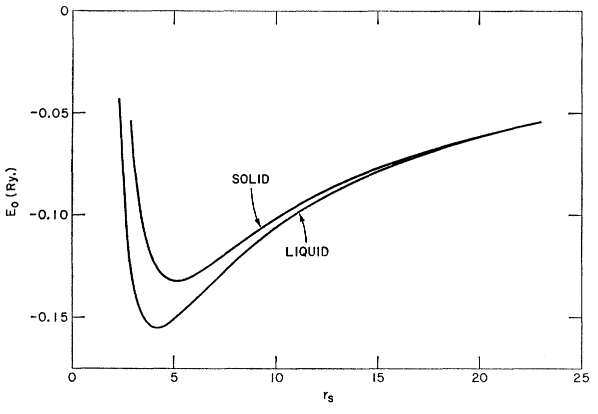

FIG. 7. Ground-state energy E_0 per particle versus r_s for the electron liquid and the electron solid.

former has been evaluated from the formula given by Carr *et al.*,[27] and the latter has been obtained from the present theory of the electron liquid. It is seen that the transition from the liquid to the solid occurs at $r_s \simeq 20$. However, the shapes of the two curves near the crossing are so close that, in view of the uncertainties of the calculation, the critical r_s may be uncertain by as much as 20%. In view of this uncertainty, the good agreement between our value of the critical r_s and that given by Van Horn ($r_s=22$) must be considered as accidental. The density of the proton system at which the transition occurs is given by

$$\rho=(3/4\pi r_s^3)M_0(M_0e^2/\hbar^2)^3, \tag{44}$$

where M_0 is the proton mass. For $r_s=20$ one finds

$$\rho=2\times 10^6\ \mathrm{g/cm^3}. \tag{45}$$

This gives the highest density at which the solid-state model[28] for calculating the proton-proton reaction rates in a model white dwarf star can be used.

VII. CONCLUDING REMARKS

In this paper we have attempted to show that our expression of the dielectric function for an interacting electron gas, which includes the effect of short-range correlations, is a reasonable one to use in the entire range of metallic densities. It marks a definite improvement over the expressions given by the earlier theories. One is, therefore, encouraged to use this dielectric function for the calculation of metallic properties. The present dielectric function leads to more effective screening of the bare potential than that given by the dielectric functions of the earlier theories, and consequently one expects an enhancement in the piling up of induced charge on a foreign charge. It appears that this will lead to an improvement in the theoretical results for the annihilation rate of positrons and for the phonon frequencies at large wave vector in the alkali metals. These questions, besides others, are now being investigated in detail.

APPENDIX

The equation of motion for the field operator $\psi_\sigma(\mathbf{x}, t)$ in the presence of an external potential $V_e(\mathbf{x}, t)$ is

$$[i\hbar(\partial/\partial t)-h(\mathbf{x})-V_e(\mathbf{x},t)]\psi_\sigma(\mathbf{x},t) - \int \Phi(\mathbf{x}-\mathbf{x}'')\rho(\mathbf{x}'',t)\psi_\sigma(\mathbf{x},t)d\mathbf{x}''=0, \tag{A1}$$

where $h(\mathbf{x})$ includes the kinetic-energy operator and the interaction with the background, and $\rho(\mathbf{x}, t)$ is the density operator. The equation of motion of the density matrix $\langle\psi_\sigma^\dagger(\mathbf{x}, t)\psi_\sigma(\mathbf{x}', t)\rangle$ is then

$$[-i\hbar(\partial/\partial t)-h(\mathbf{x})+h(\mathbf{x}')-V_e(\mathbf{x},t)+V_e(\mathbf{x}',t)] \times\langle\psi_\sigma^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x}',t)\rangle = \int d\mathbf{x}''[\Phi(\mathbf{x}-\mathbf{x}'')-\Phi(\mathbf{x}'-\mathbf{x}'')] \times\langle\psi_\sigma^\dagger(\mathbf{x},t)\rho(\mathbf{x}'',t)\psi_\sigma(\mathbf{x}',t)\rangle. \tag{A2}$$

Using the relation[29]

$$i\hbar\frac{\delta\langle\psi_\sigma^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x}',t)\rangle}{\delta V_e(\mathbf{x}'',t'')} =\langle T\{\psi_\sigma^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x}',t)\rho(\mathbf{x}'',t'')\}\rangle -\langle\psi_\sigma^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x}',t)\rangle\langle\rho(\mathbf{x}'',t'')\rangle, \tag{A3}$$

Eq. (A2) may be rewritten as

$$\left\{i\hbar(\partial/\partial t)-h(\mathbf{x})+h(\mathbf{x}')-V_e(\mathbf{x},t)+V_e(\mathbf{x}',t)-\int d\mathbf{x}''[\Phi(\mathbf{x}-\mathbf{x}'')-\Phi(\mathbf{x}'-\mathbf{x}'')]\langle\rho(\mathbf{x}'',t)\rangle\right\}\langle\psi_\sigma^\dagger(\mathbf{x},t)\psi_\sigma(x',t)\rangle$$
$$=i\hbar\int d\mathbf{x}''\left[\Phi(\mathbf{x}-\mathbf{x}'')\frac{\delta\langle\psi_\sigma^\dagger(\mathbf{x},t^+)\psi_\sigma(\mathbf{x}',t^+)\rangle}{\delta V_e(\mathbf{x}'',t)}-\Phi(\mathbf{x}'-\mathbf{x}'')\frac{\delta\langle\psi_\sigma^\dagger(\mathbf{x},t^-)\psi_\sigma(\mathbf{x}',t^-)\rangle}{\delta V_e(\mathbf{x}'',t)}\right], \tag{A4}$$

where $t^\pm=t\pm 0$. We have thereby isolated the RPA term. Instead of asking how the density matrix varies with

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[28] R. A. Wolf, Phys. Rev. **137**, B1634 (1965).

[29] See, for instance, L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962).

respect to the external potential we consider its variation relative to the average density $\langle\rho_\sigma(\mathbf{x},t)\rangle$, using the relation

$$\frac{\delta\langle\psi_\sigma^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x}',t)\rangle}{\delta V_e(\mathbf{x}'',t)}=\sum_{\sigma'}\int d\mathbf{x}_1dt_1\frac{\delta\langle\psi_\sigma^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x}',t)\rangle}{\delta\langle\rho_{\sigma'}(\mathbf{x}_1,t_1)\rangle}\frac{\delta\langle\rho_{\sigma'}(\mathbf{x}_1,t_1)\rangle}{\delta V_e(\mathbf{x}'',t)}. \tag{A5}$$

Here we assume, as is conventional, that there exists a one-to-one correspondence between the variation in the external potential and the induced average density. Using Eq. (A3) for $\mathbf{x}=\mathbf{x}'$ in Eq. (A5), and substituting the result in Eq. (A4), the latter becomes

$$[-i\hbar(\partial/\partial t)-h(\mathbf{x})+h(\mathbf{x}')-V_{\mathrm{eff}}(\mathbf{x},\mathbf{x}',\sigma;t^+)+V_{\mathrm{eff}}(\mathbf{x}',\mathbf{x},\sigma;t^-)]\langle\psi_\sigma^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x}',t)\rangle=0, \tag{A6}$$

where

$$\begin{aligned}V_{\mathrm{eff}}(\mathbf{x},\mathbf{x}',\sigma;t^\pm)&=V_e(\mathbf{x},t)+\sum_{\sigma''}\int d\mathbf{x}''\Phi(\mathbf{x}-\mathbf{x}'')\langle\rho_{\sigma''}(\mathbf{x}'',t)\rangle\\&\quad\times\left\{1+\sum_{\sigma'}\int d\mathbf{x}_1dt_1\frac{\delta\ln\langle\psi_\sigma^\dagger(\mathbf{x},t^\pm)\psi_\sigma(\mathbf{x}',t^\pm)\rangle}{\delta\ln\langle\rho_{\sigma'}(\mathbf{x}_1,t_1)\rangle}[g_{\sigma'\sigma''}(\mathbf{x}_1t_1;\mathbf{x}''t)-1]\right\},\end{aligned} \tag{A7}$$

with

$$g_{\sigma'\sigma''}(\mathbf{x}_1t_1;\mathbf{x}''t)=\frac{\langle T\{\rho_{\sigma'}(\mathbf{x}_1,t_1)\rho_{\sigma''}(\mathbf{x}'',t)\}\rangle}{\langle\rho_{\sigma'}(\mathbf{x}_1,t_1)\rangle\langle\rho_{\sigma''}(\mathbf{x}'',t)\rangle}. \tag{A8}$$

The effective potential obtained in Eq. (A7) is nonlocal in character and depends on time, as one would expect. It is important to notice, however, that it contains the normalized density-density correlation function defined in Eq. (A8), which reduces, in the absence of the external field and when $t_1=t$, to the usual equilibrium static pair-correlation function.

The simplest approximation for the functional derivative entering Eq. (A7) consists in assuming that

$$\frac{\delta\langle\psi_\sigma^\dagger(\mathbf{R}+\frac{1}{2}\mathbf{r},t)\psi_\sigma(\mathbf{R}-\frac{1}{2}\mathbf{r},t)\rangle}{\delta\langle\rho_{\sigma'}(\mathbf{x}_1,t_1)\rangle}=\delta_{\sigma\sigma'}\delta(\mathbf{R}-\mathbf{x}_1)\delta(t-t_1). \tag{A9}$$

This assumption makes the effective potential local and reduces the density-density correlation function in Eq. (A7) to the pair-correlation function. From the definition of the Wigner distribution $f_\sigma(\mathbf{R},\mathbf{p};t)$,

$$\begin{aligned}&{}_\sigma(\mathbf{R},\mathbf{p};t)\\&=\int\exp(i\mathbf{p}\cdot\mathbf{r})\langle\psi_\sigma^\dagger(\mathbf{R}+\tfrac{1}{2}\mathbf{r},t)\psi_\sigma(\mathbf{R}-\tfrac{1}{2}\mathbf{r},t)\rangle d\mathbf{r},\end{aligned} \tag{A10}$$

it is apparent that the above assumption amounts to neglecting the change in the velocity distribution as the mean density is varying. If one further replaces the pair-correlation function by its equilibrium value in the absence of the external field, the effective field goes over to that given in Eq. (8) of the text.

Mathematically, the assumptions discussed above are equivalent to a truncation of hierarchy of Green's-function equations, which, in the notation of Baym and Kadanoff,[29] may be expressed as

$$V(1-3)G_2(13^-,23^+)=\psi(1-3)G(3,3^+)G(1,2). \tag{A11}$$

Here, G and G_2 are the one-particle and the two-particle Green's functions in the presence of the external potential, V is the bare interaction potential, and ψ is the Fourier transform of $\psi(\mathbf{q})$. It can be shown that this approximation confirms to the criteria[29] which guarantee that the conservation laws are satisfied.

A possible improvement of the present theory would consist in adopting the free-electron value for the functional derivative entering Eq. (A7). We hope to take up this question in a later paper.