[1] B. D. Josephson, Phys. Letters 1, 251 (1962).

[2] B. D. Josephson, Advan. Phys. 14, 419 (1965).

[3] P. W. Anderson, *Lectures on the Many-Body Problem*, edited by E. Caianello (Academic, New York, 1964), Vol. 2, p. 113.

[4] P. W. Anderson, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (North-Holland, Amsterdam, 1967), Vol. 5, p. 1.

[5] P. W. Anderson and J. M. Rowell, Phys. Rev. Letters 10, 230 (1963).

[6] J. M. Rowell, Phys. Rev. Letters 11, 200 (1963).

[7] R. C. Jaklevic, J. Lambe, A. H. Silver, and J. E. Mercereau, Phys. Rev. Letters 12, 159 (1964).

[8] R. C. Jaklevic, J. Lambe, J. E. Mercereau, and A. H. Silver, Phys. Rev. 140, A1628 (1965).

[9] J. E. Zimmerman and A. H. Silver, Phys. Rev. 141, 367 (1966).

[10] T. A. Fulton, Solid State Commun. 8, 1357 (1970).

[11] P. W. Anderson and A. H. Dayem, Phys. Rev. Letters 13, 195 (1964).

[12] T. A. Fulton and R. C. Dynes, Phys. Rev. Letters 25, 794 (1970).

[13] R. A. Ferrell and R. E. Prange, Phys. Rev. Letters 10, 479 (1963).

[14] C. Owen and D. J. Scalapino, Phys. Rev. 164, 538 (1967).

[15] A. Th. A. M. De Waele and R. De Bruyn Ouboter, Physica 41, 225 (1969); 42, 626 (1969).

[16] W. C. Stewart, Appl. Phys. Letters 12, 277 (1968).

[17] D. E. McCumber, J. Appl. Phys. 39, 3113 (1968).

[18] J. Clarke, Proc. Roy. Soc. (London) A308, 447 (1969).

[19] J. Swihart, J. Appl. Phys. 32, 461 (1961).

[20] Multiple I_c's in large-inductance double tunnel junction have been observed by previous workers, e.g., J. E. Mercereau, Proceedings of the U. S.-Japan Seminar on Low Temperature Physics, 1967 (unpublished); A. M. Goldman (private communication).

[21] J. Clarke and T. A. Fulton, J. Appl. Phys. 40, 4470 (1969).

[22] These authors have independently suggested the mechanical analog of Sec. III. D. B. Sullivan and J. E. Zimmerman, Am. J. Phys. 39, 1504 (1971).

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Electron Correlations at Metallic Densities. V [*]

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In this paper we present a modification of an earlier theory of Singwi *et al.* of electron correlations at metallic densities. The modification consists in allowing for the change of the pair correlation function in an external weak field via the density derivative of the equilibrium pair correlation function. This results in a new expression for the local-field correction. The present theory has the merit of satisfying *almost* exactly the compressibility sum rule and of giving a satisfactory pair correlation function. Results of self-consistent numerical calculations for the static pair correlation function, correlation energy, compressibility, and plasmon dispersion relation for the electron liquid in the metallic-density range are presented. For those interested in the application of the results of the present paper, numerical values of the local-field correction as a function of wave number have been tabulated in the density range $r_s = 1-6$.

I. INTRODUCTION

In a series[1,2] of recent papers Singwi *et al.* have presented a theory of wave-number and frequency-dependent dielectric function $\epsilon(\vec{q}, \omega)$ of an electron liquid in the metallic-density range $(1 \leq r_s \leq 6)$. This theory attempts to take into account in an approximate manner both the exchange and Coulomb correlations through a local-field correction (as defined by Nozières and Pines[3]) which depends on the pair correlation function. The latter is related to the imaginary part of the inverse dielectric function through the fluctuation-dissipation theorem. Thus, it is a self-consistent theory. The first version of the theory,[1] hereafter referred to as I, yielded a physically acceptable pair distribution function $g(r)$, but the compressibility sum rule was only poorly satisfied. Although this deficiency was rectified to a considerable extent in a latter version[2] of the theory, hereafter referred to as II, by screening the Coulomb potential entering the local-field correction, the compressibility was not very satisfactory. The theory has since been applied to a variety of calculations[4-7] for free-electron-like metals with a fair degree of success. Results for the generalized paramagnetic susceptibility derived on the basis of this theory have been no less encouraging.[8-10]

Although the local-field correction in the theory of Singwi *et al.* is static, it will in general depend on frequency. The importance of the frequency dependence of the local-field correction in the dielectric response function will show up in phenomena such as the optical absorption and plasma dispersion. If the present discrepancy between the calculated and observed plasma dispersion (see Fig. 5) is any indication of the magnitude of the frequency-dependent correction to the local field, the latter could be as large as 30%. Unfortunately, at present it does not seem too easy to take into account in any satisfactory manner the frequency dependence of the local-field correction, since it will involve consideration of relaxation mechanism of an interacting electron gas. On the other hand, there is a large class of phenomena where the frequency dependence is not so important, and in that case one would like to have a satisfactory expression for the response function.

In this paper we present a modification of the theory of Singwi *et al.* which has the merit of satisfying *almost exactly* the compressibility sum rule and of giving a pair correlation function $g(r)$ of the same quality as in I. In brief, this modification consists in allowing for the change in the pair correlation function in an external weak field via the density derivative of the equilibrium pair correlation function $g^e(r)$. This then results in an additional term involving the density derivative of $g^e(r)$ in the local-field correction of Singwi *et al.*[1] Since the density derivative of $g^e(r)$ is related to the three-particle equilibrium correlation function, it is in this sense that three-particle correlations are built into our new local-field expression. It is this later feature which we believe to be very important and which will have significant consequences, as we shall show in a separate paper, on the calculated annihilation rate of positrons in heavier alkali metals in which Coulomb correlations are very important. We shall see in the sequel that the new term in the local field correction, as anticipated, gives an important contribution to the $\vec{q} \to 0$ behavior of the static dielectric function $\epsilon(\vec{q}, 0)$ and at the same time has an almost insignificant effect on the very-large-$\vec{q}$ behavior of $\epsilon(\vec{q}, \omega)$. In all calculations of lattice dynamics, it is imperative that the dielectric response function satisfies the compressibility sum rule. Since one is concerned in this and other calculations with frequencies much lower than the plasma frequency, the present static approximation should indeed be very good.

In Sec. II the theory of an effective field felt by an electron is given. In Sec. III the compressibility sum rule is discussed, and in Sec. IV the compressibility in the Hartree-Fock approximation is derived. Section V deals with sum rules. In Sec. VI results of our self-consistent numerical calculations for the static pair correlation function, correlation energy, compressibility, and plasma dispersion relation for the electron liquid in the metallic-density range are presented. A simple analytic expression for the correlation energy is also given. In Sec. VII, for the benefit of those wishing to apply these results to the calculation of other physical properties for free-electron-like metals, numerical values of the local field $G(q)$ have been tabulated for $r_s = 1-6$.

II. THEORY

A. Classical Case

In this section we shall follow the derivation given in I closely, omitting some of the details. The equation of motion for the classical one-particle distribution function $f(\vec{x}, \vec{p}; t)$ in the presence of an external potential $V_{\text{ext}}(\vec{x}, t)$ is

$$\left(\frac{\partial}{\partial t}+\vec{v}\cdot\vec{\nabla}_x\right) f(\vec{x},\vec{p};t)-\vec{\nabla}_x V_{\text{ext}}(\vec{x},t)\cdot\vec{\nabla}_p f(\vec{x},\vec{p};t) - \int \vec{\nabla}_x \phi(|\vec{x}-\vec{x}'|)\cdot\vec{\nabla}_p f(\vec{x},\vec{p};\vec{x}',\vec{p}'\,|\,t)\,d\vec{x}'\,d\vec{p}'=0\,, \qquad (1)$$

where $\phi(x)$ is the Coulomb potential and $f(\vec{x}, \vec{p}; \vec{x}', \vec{p}'\,|\,t)$ is the two-particle distribution function. The equation of motion for the two-particle distribution function involves, in turn, the three-particle distribution function and so on. Singwi *et al.* in I truncated this hierarchy of equations by using the following ansatz for the two-particle distribution function:

$$f(\vec{x},\vec{p};\vec{x}'\vec{p}'\,|\,t)=f(\vec{x},\vec{p};t)f(\vec{x}',\vec{p}';t)g(\vec{x},\vec{x}';t)\,, \qquad (2)$$

where for $g(\vec{x}, \vec{x}'; t)$ they took the equilibrium static pair correlation function $g^e(|\vec{x}-\vec{x}'|)$. They thus introduced correlations between particles through a physical function, and tacitly assumed that in the presence of a weak external field, $g(\vec{x}, \vec{x}'; t)$ is not different from $g^e(|\vec{x}-\vec{x}'|)$, which, however, is not the case.

In the zero-frequency and infinite-wavelength limit, $g(\vec{x}, \vec{x}'; t)$ can be written as

$$g(\vec{x},\vec{x}';t)=g^e(|\vec{x}-\vec{x}'|)+\delta n\,\frac{\partial}{\partial n}\,g^e(|\vec{x}-\vec{x}'|)\,, \qquad (3)$$

where n is the number density of electrons and δn is the static density response. Since the external field can be arbitrarily weak, in the linear-response case, terms higher than first order in δn in Eq. (3) do not contribute. For finite wave vector $\vec{q}$, we shall *assume* (in the spirit of linear response) the following symmetric form[11] for $g(\vec{x}, \vec{x}'; t)$:

$$g(\vec{x},\vec{x}';t)=g^e(|\vec{x}-\vec{x}'|)+\tfrac{1}{2}[\delta n(\vec{x},t)+\delta n(\vec{x}',t)] \times\frac{\partial}{\partial n}\,g^e(|\vec{x}-\vec{x}'|)\,, \qquad (4)$$

where $n+\delta n(\vec{x}, t)$ and $n+\delta n(\vec{x}', t)$ are the local densities at $\vec{x}$ and $\vec{x}'$, respectively. The above choice of $g(\vec{x}, \vec{x}'; t)$ for a one-component classical plasma exactly satisfies the compressibility sum rule, that is to say, the isothermal compressibility derived from the limiting behavior $\vec{q}\to 0$, $\omega=0$ of the dielectric function $\epsilon(\vec{q},\omega)$ is the same as that obtained from differentiating the pressure.

For a weak external potential one can write

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

where $f_0(\vec{p})$ is the equilibrium distribution function and $f_1(\vec{x},\vec{p};t)$ is the small deviation induced by the external potential. Using Eqs. (2), (4), and (5) in Eq. (1) and linearizing the latter, one obtains

$$\left(\frac{\partial}{\partial t}+\vec{v}\cdot\vec{\nabla}_x\right)f_1(\vec{x},\vec{p};t)-\left(\vec{\nabla}_x V_{\text{ext}}(\vec{x},t)+\int d\vec{x}'\,\vec{\nabla}_x\psi(|\vec{x}-\vec{x}'|)\delta n(\vec{x}',t)\right)\cdot\vec{\nabla}_{\vec{p}}f_0(\vec{p})=0\,, \tag{6}$$

where

$$\delta n(\vec{x},t)=\int f_1(\vec{x},\vec{p};t)\,d\vec{p}\,, \tag{7}$$

$$\vec{\nabla}_x\psi(\vec{x})=g^e(\vec{x})\vec{\nabla}_x\phi(\vec{x})+\frac{n}{2}\,\frac{\partial}{\partial n}\,g^e(\vec{x})\vec{\nabla}_x\phi(\vec{x})\,. \tag{8}$$

The effective field felt by a particle can therefore be written from Eq. (6) as

$$\begin{aligned}\vec{E}_{\text{eff}}(\vec{x},t)&=-\vec{\nabla}_x V_{\text{ext}}(\vec{x},t)-\int\vec{\nabla}_x\phi(|\vec{x}-\vec{x}'|)\,\delta n(\vec{x}',t)\,d\vec{x}'\\&\quad-\int[g^e(|\vec{x}-\vec{x}'|)-1]\vec{\nabla}_x\phi(|\vec{x}-\vec{x}'|)\delta n(\vec{x}',t)\,d\vec{x}'\\&\quad-\frac{1}{2}\int n\,\frac{\partial}{\partial n}[g^e(|\vec{x}-\vec{x}'|)-1]\\&\qquad\times\vec{\nabla}_x\phi(|\vec{x}-\vec{x}'|)\,\delta n(\vec{x}',t)\,d\vec{x}'\,.\end{aligned} \tag{9}$$

The first two terms on the right-hand side of Eq. (9) correspond to the usual macroscopic electric field [random-phase approximation (RPA)] and the third and the fourth terms correspond to what one calls local-field correction. The third term is the same as in the theory of I. The fourth term is new and takes into account the adjustment of the pair correlation function in the presence of an external potential. Since the density derivative of the equilibrium $g^e(\vec{x})$ is related to the three-particle correlation function, the fourth term in Eq. (9) does contain effects arising out of three-particle correlations.

Proceeding now as in paper I, we can find the solution of Eq. (6) by considering a single Fourier component of the external potential $V_{\text{ext}}(\vec{q},\omega)$. The induced charge density is then

$$\delta n(\vec{q},\omega)=-\frac{Q_0(\vec{q},\omega)}{\phi(\vec{q})+\psi(\vec{q})Q_0(\vec{q},\omega)}\,V_{\text{ext}}(\vec{q},\omega)\,, \tag{10}$$

where

$$\begin{aligned}\phi(\vec{q})&=4\pi e^2/q^2\,,\\\psi(\vec{q})&=\phi(\vec{q})+\phi(\vec{q})\left(1+\frac{n}{2}\,\frac{\partial}{\partial n}\right)\\&\quad\times\left(-\frac{1}{n}\int\frac{d\vec{q}'}{(2\pi)^3}\,\frac{\vec{q}\cdot\vec{q}'}{q'^2}\,[S(\vec{q}-\vec{q}')-1]\right),\end{aligned} \tag{11}$$

and

$$Q_0(\vec{q},\omega)=-\,\phi(\vec{q})\chi_0(\vec{q},\omega)\,, \tag{12}$$

$\chi_0(\vec{q},\omega)$ being the usual free-electron polarizability The dielectric function is therefore given by

$$\epsilon_{\text{cl}}(\vec{q},\omega)=1+\frac{Q_0(\vec{q},\omega)}{1-G_{\text{cl}}(\vec{q})Q_0(\vec{q},\omega)}\,, \tag{13}$$

where

$$G_{\text{cl}}(\vec{q})=\left(1+\frac{n}{2}\,\frac{\partial}{\partial n}\right)\left(-\frac{1}{n}\int\frac{d\vec{q}'}{(2\pi)^3}\,\frac{\vec{q}\cdot\vec{q}'}{q'^2}\,[S(\vec{q}-\vec{q}')-1]\right), \tag{14}$$

where the term in the right large parenthesis was designated as $G(\vec{q})$ in I.

B. Quantum Mechanical Case

So far our analysis of the dielectric function has been purely in classical terms. It is straightforward to show that the compressibility as obtained from the limit $\omega=0$, as $\vec{q}\to 0$ of $\epsilon(\vec{q},\omega)$ of Eq. (13) is the same as one would obtain from the classical virial. This will not be the case if the density derivative term were absent in Eq. (14) as was the case in I. Following the arguments advanced in I, we assert that Eq. (13) is valid in the quantum mechanical case too with the proviso that the classical free-electron polarizability is replaced by its quantum mechanical analog, i.e., by the usual Lindhard function. In the present case we make an additional assumption that the local-field correction $G(\vec{q})$ in the quantum mechanical case is, instead of Eq. (14), given by

$$G(\vec{q})=\left(1+an\,\frac{\partial}{\partial n}\right)\left(-\frac{1}{n}\int\frac{d\vec{q}'}{(2\pi)^3}\,\frac{\vec{q}\cdot\vec{q}'}{q'^2}\,[S(\vec{q}-\vec{q}')-1]\right), \tag{15}$$

where a for the moment is to be treated as a parameter. Undoubtedly, the precise form of $G(\vec{q})$ in the quantum mechanical case, which corresponds to some effective particle-hole interaction, will be extremely complicated and has hitherto not been possible to calculate. We have here not only lumped all quantum correction to $G_{\text{cl}}(\vec{q})$ in a single parameter a, but have also tacitly assumed that $G(\vec{q})$ has the same structure as $G_{\text{cl}}(\vec{q})$. These assumptions are hard to justify in any rigorous manner. The only justification we can give at present is that they seem to work very well. It is a fortunate circumstance that a single value of the parameter a in the entire metallic-density range is adequate. This we believe is not accidental, and one should look for a better understanding of $G(\vec{q})$. To avoid any confusion, we shall write in the quantum mechanical case the expression for the dielectric function as

$$\epsilon(\vec{q}, \omega) = 1 + \frac{Q_0(\vec{q}, \omega)}{1 - G(\vec{q}) Q_0(\vec{q}, \omega)} , \tag{16}$$

where $G(\vec{q})$ is given by Eq. (15) and $Q_0(\vec{q}, \omega)$ by Eq. (12), with $\chi_0(\vec{q}, \omega)$ being the usual Lindhard function.

It is worth pointing out the approximations that go into deriving Eq. (16) from an exact set of equations.[12] These approximations have been discussed by Langreth,[13] and we shall refer the reader to his paper for details. The dielectric function $\epsilon(\vec{q}, \omega)$ can be expressed in terms of a vertex function $\tilde{\Lambda}_p(\vec{q}, \omega)$, which in general depends on the energy and momentum of the electron (here denoted by the suffix p). The vertex function is given by an integral equation involving the effective particle-hole interaction $\tilde{I}(\vec{q}, \omega; p, p')$ which is frequency as well as momentum dependent. If we assume that the interaction $\tilde{I}$ is static and depends only on the momentum transfer $\vec{q}$, an approximation first introduced by Hubbard,[14] Eq. (16) for $\epsilon(\vec{q}, \omega)$ follows. In the present context, $\tilde{I}(\vec{q})$ corresponds to $-2\phi(\vec{q})G(\vec{q})$, and $\tilde{\Lambda}(\vec{q}, \omega)$ is

$$\tilde{\Lambda}(\vec{q}, \omega) = [1 + G(\vec{q})\phi(\vec{q})\chi_0(\vec{q}, \omega)]^{-1} ,$$

where $\tilde{\Lambda}(\vec{q}, \omega) = \epsilon(\vec{q}, \omega)\Lambda(\vec{q}, \omega)$.

III. COMPRESSIBILITY SUM RULE

The ratio κ/κ_f of the compressibility of an interacting to a free-electron gas is given by the formula[15]

$$\lim_{\vec{q} \to 0} \epsilon(\vec{q}, 0) = 1 + \frac{q_{\mathrm{TF}}^2}{q^2} \frac{\kappa}{\kappa_f} , \tag{17}$$

where q_{TF} is the Thomas-Fermi wave vector. In the RPA, $\kappa/\kappa_f = 1$.

From the expression for the quantum mechanical virial theorem, it follows [see Appendix, Eq. (A3)] that the ratio of the compressibility of the free- to the interacting-electron gas is

$$\left(\frac{\kappa_f}{\kappa}\right)_V = \frac{1}{n\epsilon_F} \left[n \frac{\partial}{\partial n} (n \langle \mathrm{ke} \rangle) + \frac{n^2}{2} \int d\vec{x}\, \phi(\vec{x}) \right.$$
$$\left. \times \left([g(\vec{x}, n) - 1] + \frac{n}{2} \frac{\partial}{\partial n} [g(\vec{x}, n) - 1] \right) \right] ; \tag{18a}$$

whereas the corresponding expression, as derived from the $\lim \epsilon(\vec{q}, 0)$ as $\vec{q} \to 0$ of Eq. (16) with $G(\vec{q})$ of Eq. (15), can be written as

$$\left(\frac{\kappa_f}{\kappa}\right)_D = \frac{1}{n\epsilon_F} \left[n \frac{\partial}{\partial n} (n \langle \mathrm{ke} \rangle_f) + \frac{n^2}{2} \int d\vec{x}\, \phi(\vec{x}) \right.$$
$$\left. \times \left([g(\vec{x}, n) - 1] + an \frac{\partial}{\partial n} [g(\vec{x}, n) - 1] \right) \right] . \tag{18b}$$

In the above equations, $\langle \mathrm{ke} \rangle$ denotes the expectation value of the kinetic energy per particle in the ground state of the interacting system, $\langle \mathrm{ke} \rangle_f$ is the corresponding quantity for a noninteracting case, and ϵ_F is the Fermi energy. The suffixes V and D stand, respectively, for virial theorem and dielectric function.

Obviously, if $\langle \mathrm{ke} \rangle = \langle \mathrm{ke} \rangle_f$, Eqs. (18a) and (18b) would be identical for $a = \frac{1}{2}$ and hence the two ratios of the compressibility will be the same. But we know that $\langle \mathrm{ke} \rangle \neq \langle \mathrm{ke} \rangle_f$. However, one may take into account in a phonomenological way the difference between $\langle \mathrm{ke} \rangle$ and $\langle \mathrm{ke} \rangle_f$ by choosing a suitable value for the parameter a such that $(\kappa_f/\kappa)_D = (\kappa_f/\kappa)_V$. In the Appendix we have pursued such an analysis and have shown that a is a very slowly varying function of r_s and obeys the inequality

$$1 \gtrsim a \geq \tfrac{1}{2} . \tag{19}$$

Note that the upper bound of a is subject to some uncertainty as discussed in the Appendix. Equation (18b) can also be alternatively written as

$$\left(\frac{\kappa_f}{\kappa}\right)_D = 1 - \lim_{\vec{q} \to 0} \frac{G(\vec{q})}{(q/q_F)^2} \left(\frac{q_{\mathrm{TF}}}{q_F}\right)^2 . \tag{20}$$

IV. COMPRESSIBILITY IN HARTREE-FOCK APPROXIMATION

In the Hartree-Fock (HF) approximation $\langle \mathrm{ke} \rangle = \langle \mathrm{ke} \rangle_f$, and hence for $a = \frac{1}{2}$, $(\kappa_f/\kappa)_D = (\kappa_f/\kappa)_V$. In the HF approximation the structure factor $S(q)$ is given by

$$S(\vec{q}) = 1 - \frac{2}{(2\pi)^3} \frac{1}{n} \int_{|\vec{k}| \leq q_F} d\vec{k} \int_{|\vec{k}'| \leq q_F} d\vec{k}'\, \delta(\vec{k} - \vec{k}' + \vec{q}) . \tag{21}$$

Using this value of $S(\vec{q})$ in Eq. (15) and with $a = \frac{1}{2}$, it is straightforward to show that

$$\lim_{\vec{q} \to 0} G(\vec{q}) = \left(1 + \frac{n}{2} \frac{n}{\partial n}\right) \frac{3}{8} \frac{q^2}{q_F^2} = \frac{1}{4} \left(\frac{q}{q_F}\right)^2 . \tag{22}$$

(For the evaluation of the integral, see Eq. (22) of I.) Using Eq. (22) in Eq. (20), we have

$$(\kappa_f/\kappa)_D = 1 - \tfrac{1}{4}(q_{\mathrm{TF}}/q_F)^2 , \tag{23}$$

which is the same as one would obtain by differentiating the ground-state energy in the HF approximation. It is interesting to note that the result of Eq. (23) is the same as obtained recently by Toigo and Woodruff,[16] who used a very different method. The present derivation is much simpler; besides, it is also apparent from it that the compressibility ratio as given by Eq. (23) has no effect of Coulomb correlations in it.

V. SUM RULES

It is easy to show that in the limit of large frequencies Eq. (16) reduces to

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

where ω_p is the plasma frequency. From the analytical properties of $\epsilon(\vec{q}, \omega)$ and the above asymptotic behavior, it follows that

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

and

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

Equation (16) also satisfies the "perfect"-screening requirement

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

The compressibility sum rule is *almost* exactly satisfied as will be discussed in Sec. VI.

The theories of I and II as well as the present one satisfy particle-number conservation. This follows from very general arguments. Particle conservation states that

$$\int d\vec{x} \, [g(\vec{x}) - 1] = -1/n , \tag{24a}$$

which implies that

$$\lim_{\vec{q} \to 0} S(\vec{q}) \to 0 . \tag{24b}$$

From the fluctuation-dissipation theorem, we have

$$S(\vec{q}) = -(\hbar q^2/4\pi e^2 n) \int_0^\infty d\omega \, \mathrm{Im}[1/\epsilon(\vec{q}, \omega)] . \tag{25}$$

Using Eq. (16) for $\epsilon(\vec{q}, \omega)$ in Eq. (25) and remembering the fact that

$$\lim_{\vec{q} \to 0} G(q) \to \gamma q^2 , \tag{26}$$

it follows straightforwardly that $\lim S(\vec{q}) \to 0$ as $\vec{q} \to 0$. Equation (26) is valid in I, II, and the present theory, and in fact in all theories of the Hubbard-type,[16] and hence number conservation is satisfied in all these theories. The contention of Geldart and Taylor[17] that the number conservation is violated by the theories of I and II is therefore invalid.[18]

It may be noted that the relation[5]

$$G(\infty) = 1 - g(0) , \tag{27}$$

which is valid in I and II, does not hold in the present case. Here Eq. (27) is replaced by

$$G(\infty) = \left(1 + an \frac{\partial}{\partial n}\right) [1 - g(0)] . \tag{28}$$

It is, therefore, no longer possible to determine $g(0)$ simply by knowing $G(\infty)$ for one value of r_s.

VI. CALCULATIONS

Equations (15), (16), and (25) constitute the basic equations of this paper. They have to be solved self-consistently with a as a parameter, the value of which is limited by the inequality (19). One could determine the value of a for each value of r_s such that the compressibility sum rule is *exactly* satisfied. However, a self-consistent numerical calculation in such a scheme would be very time consuming. In practice it turns out that a is an extremely slowly varying function of r_s in the entire metallic-density range. Calculations were made for $r_s = 4$ for different values of a lying between $\frac{1}{2}$ and 1, and it was found that for the choice of $a = \frac{2}{3}$ the compressibility sum rule was almost exactly satisfied. This value of a was then chosen for calculations for all values of r_s ranging from 0.5 to 7. In order to illustrate the sensitivity of various calculated quantities to the choice of a, we have summarized in the table in the Appendix some results for $r_s = 4$. For present numerical calculation we have chosen a to be $\frac{2}{3}$. Since the bounds on a were derived by considering the long-wavelength situation, there is no *a priori* reason to believe that the above choice for the value of a would also give a pair correlation function which is good for small interparticle separation. Again it turns out that the value of the pair correlation function for small interparticle separation is not sensitive to the choice of the value of a. This is, indeed, a fortunate circumstance.

Equation (15) after angular integrations can be written as

$$G(\vec{q}) = G_I(q, r_s) + \frac{2}{3}\left(-\frac{q}{3}\frac{\partial}{\partial q} G_I(q, r_s) - \frac{r_s}{3}\frac{\partial}{\partial r_s} G_I(q, r_s)\right) , \tag{29}$$

where

$$G_I(q, r_s) = -\frac{3}{4}\int_0^\infty q'^2 [S(q', r_s) - 1] \left(1 + \frac{q^2 - q'^2}{2qq'} \ln\left|\frac{q + q'}{q - q'}\right|\right) dq' , \tag{30}$$

where q is in units of q_F. Equations (16), (25), and (29) were solved self-consistently on a digital computer. The computational time involved in the present calculations was about twice that in I but much less than that involved in II. To evaluate the derivative of $G_I(q, r_s)$ with respect to r_s, self-consistent calculations were done for two neighboring values of r_s, say, $r_s = 3.96$ and 4.00, thus giving us the derivative for $r_s = 3.98$. This was also taken to be the value of the derivative for $r_s = 3.96$ and 4.00. To establish the accuracy of such a procedure calculations were performed at several neighboring densities (say 3.94, 3.96, 3.98, and 4.00), and it was found that the value of the derivative did not change within our prescribed accuracy. The derivative in (29) with respect to q can be evaluated with any desired accuracy. It is this derivative which gives a dominant contribution. Approximately ten to twelve iterations were needed to obtain a self-consistency in $G(\vec{q})$ of better than 0.1%. This in turn meant a much higher accuracy in $S(\vec{q})$.

In the remaining subsections we shall present the results for the pair correlation function, correlation energy, and compressibility for values of r_s ranging from 1 to 6.

A. Pair Correlation Function

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

$$g(r) = 1 + (3/2r)\int_0^\infty q \sin(qr)[S(q)-1]\,dq\ , \qquad (31)$$

where q is units of q_F and r in units of q_F^{-1}. Self-consistent values of $S(q)$ were used in Eq. (31) to calculate $g(r)$. The results are shown in Figs. 1–3 for various values of r_s. For the sake of comparison, corresponding curves in the theories of I and II are shown along with $g(r)$ of Toigo and Woodruff,[19] in the original Hubbard approximation and in RPA. It is clear from these figures that in the present case $g(r)$ for large values of r_s and small interparticle separation is slightly better than that in II and definitely much better than that in Ref. 19. The $g(r)$ of paper I is slightly less negative than the present one for $r_s > 4$. The negative values of $g(0)$ are indeed so small in the present theory that for all practical purposes they may be considered to be zero.

B. Correlation Energy

As in I, correlation energy per particle can be written as

$$\epsilon_{\text{corr}} = \frac{1}{r_s^2}\int_0^{r_s}\left[-\frac{4}{\pi}\left(\frac{9\pi}{4}\right)^{1/3}\bar{\gamma}(r_s') + 0.9163\right]dr_s'\ \text{Ry}, \qquad (32)$$

where

$$\bar{\gamma}(r_s) = -\tfrac{1}{2}\int_0^\infty [S(q)-1]\,dq\ , \qquad (33)$$

where q is in units of q_F. The Ferrel condition[20] on the ground-state energy, which is equivalent to

$$\frac{d}{dr_s}\bar{\gamma}(r_s) \geq 0\ ,$$

is satisfied for the values of $\bar{\gamma}$ given in Table I. Values of the correlation energy per particle are given in Table II, together with the values based on previous approximate schemes.

Values of the correlation energy for $r_s = 1-6$ can be fitted to the following analytic expression to within half a percent accuracy:

$$\epsilon_{\text{corr}} = -0.112 + 0.0335 \ln r_s\ \text{Ry}\ . \qquad (34)$$

The form of Eq. (34) is the same as that of the interpolation formula of Pines and Nozières.[21] The values of ϵ_{corr} in the interpolation scheme of the latter authors could differ from the present calculated values by as much as 15%, depending on r_s.

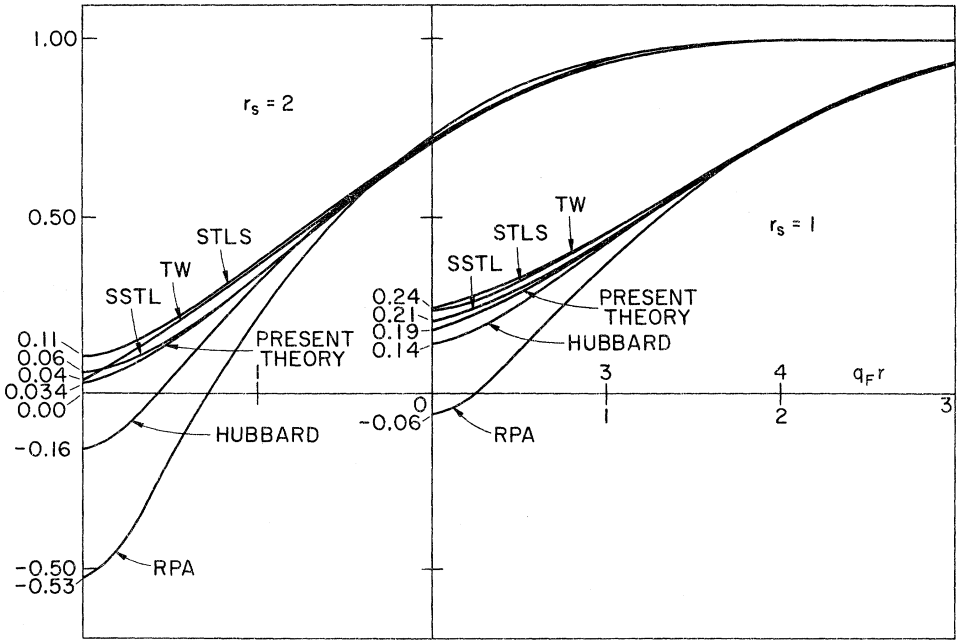

FIG. 1. Pair correlation function $g(r)$ vs $q_F r$ for $r_s = 1$ and 2. The abbrevations STLS, SSTL and TW stand, for Refs. 1, 2, and 19. The same is to be understood in other figures.

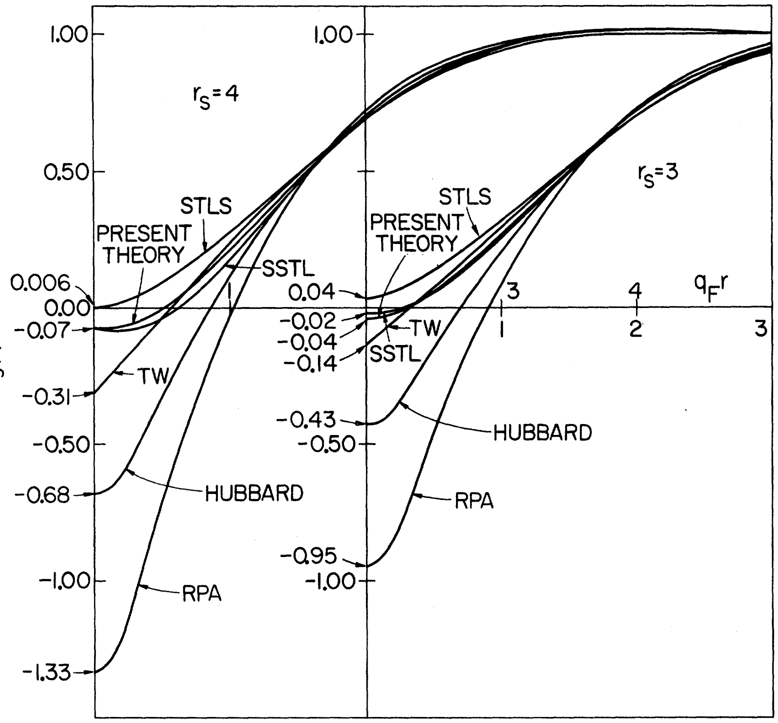

FIG. 2. Pair correlation function $g(r)$ vs q_Fr for $r_s=3$ and 4.

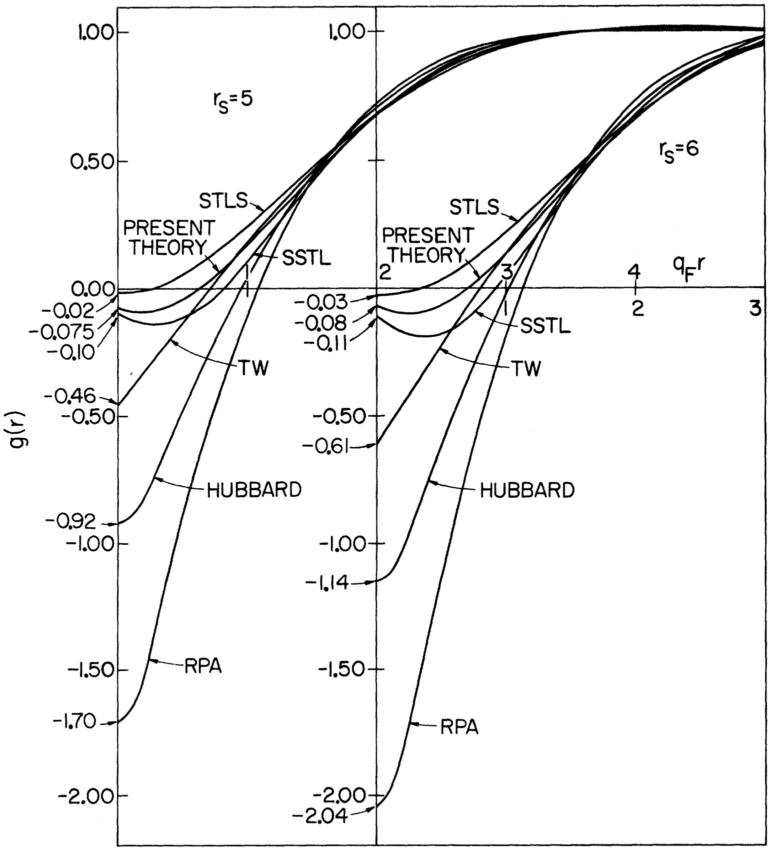

FIG. 3. Pair correlation function $g(r)$ vs q_Fr for $r_s=5$ and 6.

TABLE I. Values of $\bar{\gamma}$.

r_s	1	2	3	4	5	6
$\bar{\gamma}$	0.45388	0.49190	0.51679	0.53478	0.54847	0.55927

TABLE III. Values of γ.

r_s	1	2	3	4	5	6
γ	0.24284	0.26137	0.27433	0.28408	0.29184	0.29816

C. Compressibility

The dielectric function of Eq. (16) in the limit $\vec{q}\to 0$ and $\omega=0$ has the following form:

$$\lim_{\vec{q}\to 0}\epsilon(\vec{q},0)=1+\frac{(q_{\mathrm{TF}}/q)^2}{1-\gamma\,(q_{\mathrm{TF}}/q_F)^2}\ , \tag{35}$$

where

$$\gamma=-\frac{1}{2}\int_0^\infty dq\left[\tfrac{1}{3}[S(q,r_s)-1]\right.$$
$$\left.+\frac{2}{3}\left(-\frac{q}{3}\frac{\partial}{\partial q}S(q,r_s)-\frac{r_s}{3}\frac{\partial}{\partial r_s}S(q,r_s)\right)\right]. \tag{36}$$

Note that γ and $\bar{\gamma}$ are different; the former is related to the slope of the compressibility ratio, and the latter determines the interaction energy per electron.

Using the compressibility sum rule Eq. (17), it follows from (35) that

$$\kappa_f/\kappa=1-\gamma(q_{\mathrm{TF}}/q_F)^2\ . \tag{37}$$

The values of γ for different values of r_s are given in Table III. The values of κ_f/κ as obtained from Eq. (37) are compared in Fig. 4 with those obtained from differentiating the ground-state energy (unmarked continuous curve). It is clear from the figure that *the two results almost coincide in the entire metallic-density range*. This justifies the claim made in the Introduction that the compressibility sum rule is almost exactly satisfied in the present theory. The curve for κ_f/κ obtained from ground-state energy in HF approximation is a continuous straight line which intersects the r_s axis at 6.03. For the sake of comparison, curves for κ_f/κ as obtained from the $\vec{q}\to 0$ limit of $\epsilon(\vec{q},0)$ in different theories are also given in Fig. 4. Note that it is the small Coulomb correlation contribution to the compressibility ratio that gives rise to a curvature which is concave towards the origin. The dashed curve marked present theory is indeed concave towards the origin.

D. Plasmon Dispersion

The dielectric function in the limit $\vec{q}\to 0$ and ω finite has the form

$$\lim_{\vec{q}\to 0}\epsilon(\vec{q},\omega)=1-\frac{\omega_p^2}{\omega^2}\left[1+\frac{9}{5}\left(\frac{q}{q_{\mathrm{TF}}}\right)^2-\gamma\left(\frac{q}{q_F}\right)^2+\cdots\right], \tag{38}$$

where ω_p is the plasma frequency. The plasma dispersion relation is then

$$\omega_p(q)=\omega_p+\alpha(\hbar q^2/m)\ , \tag{39}$$

where

$$\alpha=\frac{\hbar q_F^2}{3m\omega_p}\left[\frac{9}{10}-\frac{1}{2}\gamma\left(\frac{q_{\mathrm{TF}}}{q_F}\right)^2\right], \tag{40}$$

but

$$\alpha_{\mathrm{RPA}}=3\hbar q_F^2/10m\omega_p\ .$$

In Fig. 5 we have plotted $\alpha/\alpha_{\mathrm{RPA}}$ as a function of r_s in various theories. The experimental values

TABLE II. Correlation energy (Ry/electron).

r_s	1	2	3	4	5	6
Present theory	−0.112	−0.089	−0.075	−0.065	−0.058	−0.052
Singwi *et al.* (Ref. 1)	−0.125	−0.097	−0.080	−0.070	−0.063	−0.057
Singwi *et al.* (Ref. 2)	−0.124	−0.092	−0.075	−0.064	−0.056	−0.050
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
Toigo-Woodruff[a]	−0.134 (−0.103)	−0.095 (−0.083)	−0.079 (−0.071)	−0.068 (−0.063)	−0.061 (−0.057)	(−0.052)

[a] The values in parentheses in the last row are those calculated by us using the numerical values of $G(q)$ given by Toigo and Woodruff (Ref. 16). These values are different from those reported by these authors in Ref. 19. The discrepancy seems to be due to the poor numerical accuracy of their computation.

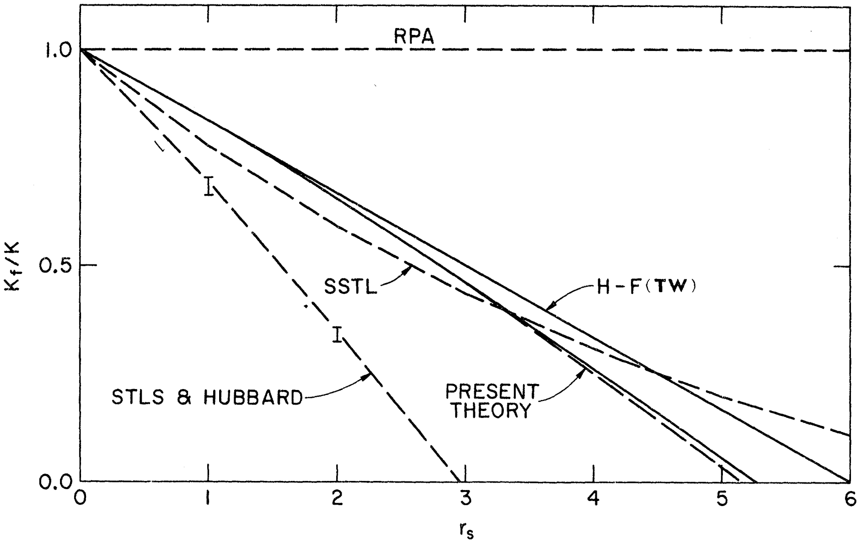

FIG. 4. Ratio between the free-electron compressibility and the compressibility of the electron liquid vs r_s. The unlabelled full curve is obtained by differentiation of the ground-state energy. The broken curve (labelled present theory) is obtained from Eq. (37). The full curve [labelled HF(TW)] is obtained from differentiating the ground-state energy in HF approximation. The same curve is obtained in the theory of Ref. 16.

available for a few metals are also given in the figure. Comparison between theory and experiment may not have much significance, since the influence of ion lattice on the measured values is not known.

VII. SELF-CONSISTENT VALUES OF $G(q)$

Since the dielectric function occurs in the calculation of a variety of metallic properties, we thought it worthwhile to give a table of self-consistent values of $G(q)$ for $r_s = 1-6$. These are given in Table IV. Values of $G(q)$ for $q \leq 2q_F$ can be fitted quite well with a simple function of the form

$$G(q) = A(1 - e^{-B(q/q_F)^2}) , \tag{41}$$

(valid only for $q \leq 2q_F$). Values of the parameters A and B are given in Table V.

VIII. CONCLUDING REMARKS

The basic result of this paper is the expression (15) for the local-field correction $G(q)$. It represents our approximation to the effective particle-hole interaction which occurs in the kernel of the integral equation for the vertex function. The expression for dielectric function is such that in the classical case, the compressibility sum rule is *exactly* satisfied; whereas in the quantum mechanical case it is *almost exactly* satisfied. The theory also yields a satisfactory pair correlation function.

A few comments concerning the new term in the local-field correction are worth reiterating. It might appear to a cursory reader that it is the choice of the value of the parameter a which is responsible for giving the correct compressibility.

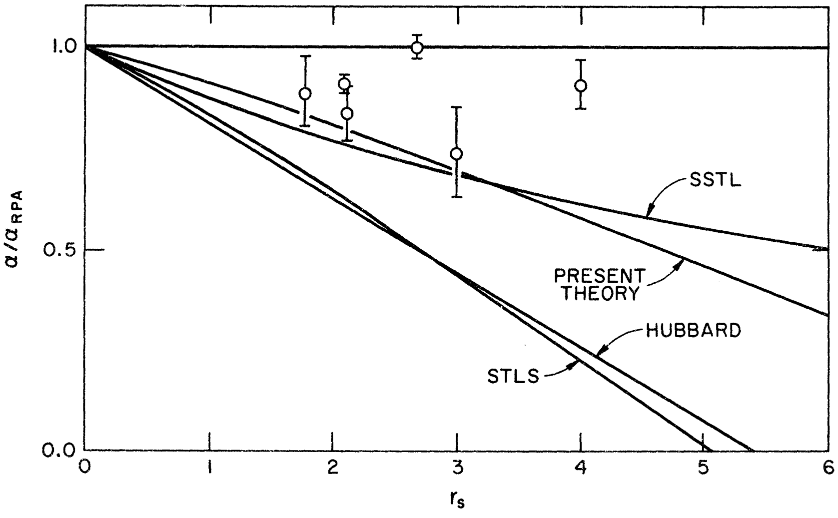

FIG. 5. Coefficient of the leading term in the plasmon dispersion relation (in units of its RPA value) vs r_s. The experimental values (for Be, Al, Sb, Mg, Li, and Na, in order of increasing r_s) are taken from H. Raether, in *Springer Tracts in Modern Physics* (Springer-Verlag, Berlin, 1965), Vol. 38.

TABLE IV. Self-consistent values of $G(q)$.

q/q_F r_s	1	2	3	4	5	6
0.1	0.0024	0.0026	0.0027	0.0028	0.0029	0.0030
0.2	0.0098	0.0105	0.0110	0.0114	0.0117	0.0120
0.3	0.0219	0.0236	0.0247	0.0256	0.0263	0.0269
0.4	0.0386	0.0416	0.0437	0.0453	0.0466	0.0476
0.5	0.0597	0.0645	0.0679	0.0704	0.0724	0.0740
0.6	0.0848	0.0919	0.0968	0.1005	0.1034	0.1058
0.7	0.1135	0.1234	0.1303	0.1354	0.1394	0.1427
0.8	0.1454	0.1586	0.1678	0.1746	0.1800	0.1844
0.9	0.1799	0.1970	0.2089	0.2178	0.2248	0.2305
1.0	0.2164	0.2380	0.2530	0.2642	0.2732	0.2804
1.1	0.2542	0.2808	0.2994	0.3134	0.3245	0.3336
1.2	0.2926	0.3246	0.3472	0.3643	0.3780	0.3891
1.3	0.3309	0.3687	0.3957	0.4163	0.4327	0.4462
1.4	0.3684	0.4123	0.4439	0.4682	0.4877	0.5038
1.5	0.4043	0.4544	0.4908	0.5190	0.5418	0.5608
1.6	0.4378	0.4941	0.5355	0.5677	0.5940	0.6159
1.7	0.4684	0.5309	0.5772	0.6134	0.6430	0.6679
1.8	0.4956	0.5640	0.6150	0.6551	0.6880	0.7157
1.9	0.5189	0.5930	0.6485	0.6922	0.7282	0.7584
2.0	0.5384	0.6179	0.6775	0.7245	0.7632	0.7958
2.1	0.5548	0.6392	0.7025	0.7525	0.7937	0.8282
2.2	0.5690	0.6578	0.7245	0.7771	0.8203	0.8564
2.3	0.5814	0.6743	0.7440	0.7989	0.8438	0.8812
2.4	0.5924	0.6890	0.7614	0.8182	0.8645	0.9029
2.5	0.6022	0.7022	0.7770	0.8355	0.8829	0.9220
2.6	0.6110	0.7141	0.7910	0.8509	0.8993	0.9389
2.8	0.6262	0.7347	0.8151	0.8772	0.9269	0.9670
3.0	0.6387	0.7518	0.8350	0.8987	0.9491	0.9893
3.5	0.6625	0.7839	0.8719	0.9378	0.9884	1.0274
4.0	0.6790	0.8062	0.8970	0.9634	1.0130	1.0501
5.0	0.7003	0.8347	0.9279	0.9936	1.0403	1.0732
6.0	0.7134	0.8519	0.9458	1.0100	1.0536	1.0829
8.0	0.7285	0.8711	0.9647	1.0259	1.0648	1.0887
10.0	0.7368	0.8814	0.9742	1.0330	1.0685	1.0890
20.0	0.7519	0.8992	0.9888	1.0415	1.0694	1.0826
50.0	0.7597	0.9077	0.9945	1.0428	1.0659	1.0750
100.0	0.7619	0.9099	0.9958	1.0428	1.0644	1.0724

This is true to some extent, but what is of great significance here is the mathematical structure of this new term. As mentioned before, it involves the density derivative of $g^e(r)$ which in turn is related[22] to the three-particle correlation function. And hence the local-field correction has in it the effects of three-particle correlations. Remember that the density-derivative term in (15) which represents the effect of three-particle correlations is here evaluated numerically in our self-consistent calculations without any approximations. The effect of this new term in the local field manifests in a dramatic fashion in the calculation of positron annihilation rates in heavier alkalis. In the nonlinear theory of positron annihilation in metals of Sjölander and Stott,[23] in which no account is taken of this derivative term in the local field, one obtains for Cs metal ($r_s \simeq 6$) an annihilation rate which is three times larger than the experimental value. This is due to the fact that too much polarization charge mounts on the positron. But when one takes into account[24] the derivative term in $G(\vec{q})$ in the theory of Sjölander and Stott, one obtains annihilation rates in agreement with experiment. This agreement is due to the reduction in the polarization charge on the positron which in turn is brought about by the derivative term in $G(\vec{q})$. The weakness of the present theory lies in the fact that we have been unable to estimate the value of the parameter a from first principles, although we have been able to put fairly narrow bounds on it in the limit of long wavelength. The difficulty is further compounded by the fact that our correction term is in general nonlocal, and we have made here a local approximation. The parameter a in general will also depend on the wave number q. The burden of nonlocality and of q dependence has been absorbed in the choice of the value of a. From the practical point of view what is remarkable is that a single value of this parameter suffices in the entire metallic-density range.

We have also been able to extend the considerations of this paper to spin correlations in the paramagnetic state. At present we do not have numerical results for the Stoner enhancement factor. As far as the use of the dielectric function in the calculation of metallic properties of simple metals is concerned, the present results do offer a satisfactory solution. However, for the study of optical properties of these metals, a static approximation for the local field correction may not be very satisfactory.

APPENDIX

For a system of electrons interacting via Coulomb potential in the presence of a uniform rigid positive background, an expression for the compressibility ratio κ_f/κ can be easily derived starting from the quantum mechanical virial theorem. The pressure for the system can be written as

$$P = \tfrac{2}{3}\left(n\langle \mathrm{ke}\rangle + \tfrac{1}{2}n\langle \mathrm{pe}\rangle\right), \tag{A1}$$

where $\langle \mathrm{ke}\rangle$ and $\langle \mathrm{pe}\rangle$ are, respectively, the expectation values of the kinetic and potential energies per particle in the ground state, and n is the number density. Compressibility is defined as

$$\frac{1}{\kappa} = n\,\frac{\partial P}{\partial n}\ . \tag{A2}$$

Expressing $\langle \mathrm{pe}\rangle$ in terms of the equilibrium pair correlation function $g(\vec{x})$ and differentiating Eq. (A1) with respect to the number density n, one easily obtains for the compressibility ratio

$$\left(\frac{\kappa_f}{\kappa}\right)_V = \frac{1}{n\epsilon_F}\left[n\,\frac{\partial}{\partial n}\left(n\langle \mathrm{ke}\rangle\right) + \frac{n^2}{2}\int d\vec{x}\,\phi(\vec{x})\right.$$

TABLE V. Values of parameters A and B in Eq. (41).

r_s	1	2	3	4	5	6
A	0.70853	0.85509	0.97805	1.08482	1.17987	1.26569
B	0.36940	0.33117	0.30440	0.28430	0.26850	0.25561

$$\times\left(\left[g(\vec{x},n)-1\right]+\frac{n}{2}\frac{\partial}{\partial n}\left[g(\vec{x},n)-1\right]\right)\Bigg], \quad \text{(A3)}$$

where

$$\langle \text{pe}\rangle = \tfrac{1}{2}n\int d\vec{x}\,\phi(\vec{x})\left[g(\vec{x},n)-1\right]$$

$$= -\frac{4}{\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{\bar{\gamma}(r_s)}{r_s}\ \text{Ry} \quad \text{(A4)}$$

and

$$\bar{\gamma}(r_s) = -(2q_F)^{-1}\int_0^\infty dq\left[S(q,n)-1\right], \quad \text{(A5)}$$

where ϵ_F is the Fermi energy. On the other hand, an expression for $(\kappa_f/\kappa)_D$ can also be obtained from the limit $\vec{q}\to 0$ of the dielectric function $\epsilon(\vec{q},0)$. Now we have

$$\lim_{\vec{q}\to 0} G(\vec{q}) = \left(1+an\frac{\partial}{\partial n}\right)\left(-\frac{q^2}{6\pi^2 n}\int_0^\infty dq\left[S(q,n)-1\right]\right). \quad \text{(A6)}$$

Using the Fourier transform

$$\int d\vec{x}\,e^{i\vec{q}\cdot\vec{x}}\left[g(\vec{x},n)-1\right] = (1/n)\left[S(\vec{q},n)-1\right] \quad \text{(A7)}$$

in (A6), then substituting Eq. (A6) into $\vec{q}\to 0$ and $\omega=0$ limit of $\epsilon(\vec{q},\omega)$ of Eq. (16), and then comparing it with Eq. (17) of the text, one obtains

$$\left(\frac{\kappa_f}{\kappa}\right)_D = \frac{1}{n\epsilon_F}\left[n\frac{\partial}{\partial n}\left(n\langle\text{ke}\rangle_f\right)+\frac{n^2}{2}\int d\vec{x}\,\phi(\vec{x})\right.$$

$$\left.\times\left(\left[g(\vec{x},n)-1\right]+an\frac{\partial}{\partial n}\left[g(\vec{x},n)-1\right]\right)\right], \quad \text{(A8)}$$

where $\langle\text{ke}\rangle_f$ is the kinetic energy per electron for the noninteracting case.

The condition that the two compressibility ratios be the same is obtained by equating Eqs. (A3) and (A8), thus giving

$$n\frac{\partial}{\partial n}\left(n\langle\text{ke}\rangle - n\langle\text{ke}\rangle_f\right)$$

$$-\left(a-\tfrac{1}{2}\right)\frac{n^2}{2}n\frac{\partial}{\partial n}\int d\vec{x}\,\phi(\vec{x})\left[g(\vec{x},n)-1\right]=0\,. \quad \text{(A9)}$$

The first term on the left-hand side of Eq. (A9) can be written in terms of the interaction energy if one writes the ground-state energy per particle E_0 as

$$E_0 = \langle\text{ke}\rangle_f + \int_0^1 (d\lambda/\lambda)\,\langle\text{pe}(\lambda)\rangle\,, \quad \text{(A10)}$$

where λ is a parameter representing the strength of the interaction. Also we have

$$E_0 = \langle\text{ke}\rangle + \langle\text{pe}\rangle\,. \quad \text{(A11)}$$

From Eqs. (A10), (A11), and (A4) and remembering that

$$\int_0^1 \frac{d\lambda}{\lambda}\langle\text{pe}(\lambda)\rangle = -\frac{4}{\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s^2}\int_0^{r_s}\bar{\gamma}(x)\,dx\ \text{Ry}\,,$$

one can write

$$\langle\text{ke}\rangle - \langle\text{ke}\rangle_f = -\frac{4}{\pi}\left(\frac{9\pi}{4}\right)^{1/3}\left(\frac{1}{r_s^2}\int_0^{r_s}\bar{\gamma}(x)\,dx - \frac{\bar{\gamma}(r_s)}{r_s}\right)\text{Ry}\,. \quad \text{(A12)}$$

Substituting Eq. (A12) into Eq. (A9) and using Eq. (A4), we get

$$(1/r_s)\int_0^{r_s}\bar{\gamma}(x)\,dx + \tfrac{1}{10}(2a+1)\,r_s\bar{\gamma}'(r_s) = \tfrac{1}{5}(6-2a)\,\bar{\gamma}(r_s)\,, \quad \text{(A13)}$$

$\bar{\gamma}'(r_s)$ being the derivative of $\bar{\gamma}(r_s)$.

It is easily seen that Ferrell condition[20] on the

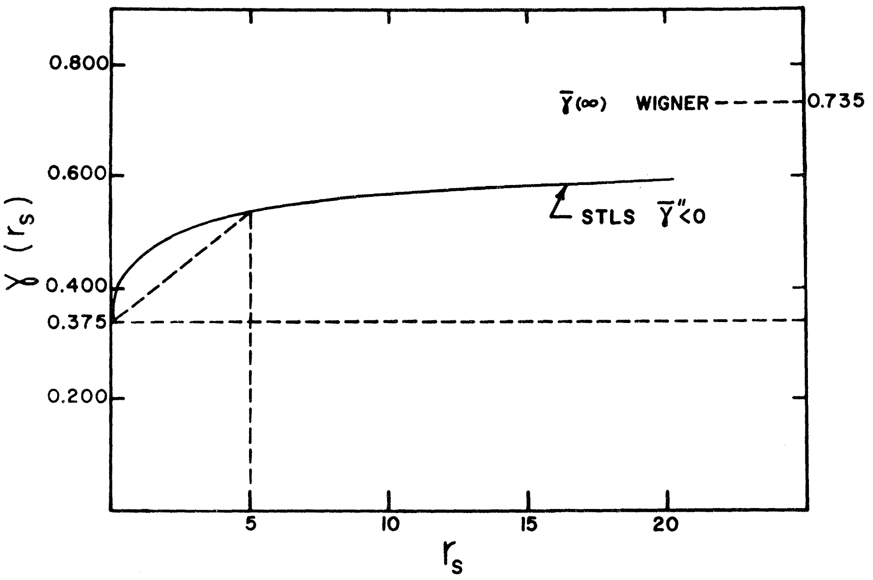

FIG. 6. Function $\bar{\gamma}(r_s)$ vs r_s. Solid curve gives the values of $\bar{\gamma}$ (γ in their notation) of I.

ground-state energy, which is equivalent to

$$\frac{d}{dr_s}\,\bar{\gamma}(r_s) \geq 0 \,, \tag{A14}$$

requires that $\bar{\gamma}(r_s)$ be an increasing function of r_s. Using the fact that $\bar{\gamma}(r_s)$ is positive and so also its first derivative $\bar{\gamma}'(r_s)$ [from Eq. (A14)], we shall establish the bounds for the parameter a in Eq. (A13).

In the high-density limit an exact value for the parameter a can be obtained, where one knows that the Gell-Mann and Brueckner (GB)[25] result for the ground-state energy per particle becomes exact. Using the GB expression for the correlation energy, one has

$$\lim_{r_s \to 0} \bar{\gamma}(r_s) = 0.375 \,, \tag{A15}$$

$$\lim_{r_s \to 0} r_s\, \bar{\gamma}'(r_s) = O(-r_s \ln r_s) \,. \tag{A16}$$

Hence, in the limit $r_s \to 0$, Eq. (A13) leads to

$$\bar{\gamma}(0) = \tfrac{1}{5}(6 - 2a)\,\bar{\gamma}(0) \,, \tag{A17}$$

which gives

$$a = \tfrac{1}{2} \,. \tag{A18}$$

Also from Wigner's low-density calculation[26] we have

$$\lim_{r_s \to \infty} \bar{\gamma}'(r_s) = O(1/r_s^3)$$

and

$$\bar{\gamma}''(r_s) < 0 \,.$$

It then follows that for $r_s \to \infty$,

$$(1/r_s) \int_0^{r_s} \bar{\gamma}(y)\, dy = \bar{\gamma}(\infty) \,.$$

Using the above relations in Eq. (A13), we have

$$a(\infty) = \tfrac{1}{2} \,. \tag{A19}$$

Clearly $a = \frac{1}{2}$ does not satisfy Eq. (A13) for all values of r_s; the parameter a is thus a function of r_s. A bound for $a(r_s)$ can be obtained by noting that the Ferrell condition in Eq. (A14) implies that

$$\bar{\gamma}(0) \leq (1/r_s) \int_0^{r_s} \bar{\gamma}(x)\, dx \,. \tag{A20}$$

TABLE VI. Effect of variation of a.

a	$g(0)$	γ	$\kappa_f/\kappa = 1 - 0.6634\gamma r_s$
0	+0.006	0.5261	−0.3961
$\frac{1}{2}$	−0.054	0.3282	0.1291
$\frac{2}{3}$	−0.07	0.2841	0.2462
$\frac{3}{4}$	−0.08	0.2685	0.2876

Using Eq. (A20) into Eq. (A13), one gets the inequality

$$a(r_s) \leq \tfrac{1}{2} + \tfrac{5}{2}\,[\bar{\gamma}(r_s) - \gamma(0)]/\bar{\gamma}(r_s) \,. \tag{A21}$$

If one takes $\gamma''(r_s) \leq 0$ (this is the case in all the theories, e.g.,, the GB high-density limit,[25] Wigner's low-density limit,[26] Pines and Nozières's interpolation scheme,[21] Singwi *et al.*,[1,2] and the present theory), one can write

$$\tfrac{1}{2}\,[\bar{\gamma}(0) + \bar{\gamma}(r_s)] \leq (1/r_s) \int_0^{r_s} \bar{\gamma}(x)\, dx \tag{A22}$$

(see Fig. 6), which when substituted in Eq. (A13) gives

$$a(r_s) \leq \tfrac{1}{2} + \tfrac{5}{4}\,[\bar{\gamma}(r_s) - \bar{\gamma}(0)]/\bar{\gamma}(r_s) \,. \tag{A23}$$

One may obtain an estimate for the upper bound of $a(r_s)$ by using the value of $\lim \bar{\gamma}(r_s) = 0.735$ as $r_s \to \infty$ from Wigner's low-density calculation or the value of $\bar{\gamma}(r_s = 20) = 0.5986$ (γ in their notation) from paper I. This leads to the upper bound for $a(r_s) \cong 1$.

Thus we finally obtain the following inequality for the parameter $a(r_s)$:

$$1 \gtrsim a(r_s) \geq \tfrac{1}{2} \,. \tag{A24}$$

It is clear from the foregoing discussion that the upper bound for a has been estimated from the presently available values of $\bar{\gamma}(r_s)$ for large values of r_s. Although the uncertainty in the upper bound for a is related to the uncertainty in the value of $\bar{\gamma}(r_s)$, nonetheless, the former is relatively much less sensitive to the variation in the latter.

In Table VI we give for $r_s = 4$ our self-consistent values of $g(0)$, γ, and κ_f/κ for different values of the parameter a.

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[1] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. 176, 589 (1968); see also J. Hubbard, Phys. Letters 25A, 709 (1967).

[2] K. S. Singwi, A. Sjölander, M. P. Tosi, and R. H. Land, Phys. Rev. B 1, 1044 (1970).

[3] P. Nozières and D. Pines, Nuovo Cimento 9, 470 (1958).

[4] D. L. Price, K. S. Singwi, and M. P. Tosi, Phys. Rev. B 2, 2983 (1970); see also, Wei-Mei Shyu, K. S. Singwi, and M. P. Tosi, Phys. Rev. B 3, 237 (1970).

[5] R. W. Shaw, J. Phys. C 3, 1140 (1970).

[6] Wei-Mei Shyu, J. H. Wehling, M. R. Cordes, and G. D. Gespari, Phys. Rev. B 4, 1802 (1971).

[7] L. Hedin and B. I. Lundqvist, J. Phys. C 4, 2064 (1971).

[8] R. D. Lowde and C. G. Windsor, Advan. Phys. 19, 813 (1970).

[9] G. Pizzimenti, M. P. Tosi, and A. Villari, Nuovo Cimento Letters 81 (1971).

[10] P. Bhattacharyya, K. N. Pathak, and K. S. Singwi, Phys. Rev. B 3, 1568 (1971).

[11] T. Schneider, R. Brout, H. Tomas, and J. Feder, Phys. Rev. Letters 25, 1423 (1970); see also K. S. Singwi, K. Sköld, and M. P. Tosi, Phys. Rev. A 1, 454 (1970).

[12] P. Nozières, *Theory of Interacting Fermi Systems* (Benjamin, New York, 1964).

[13] David C. Langreth, Phys. Rev. 181, 753 (1969).

[14] J. Hubbard, Proc. Roy. Soc. (London) A243, 336 (1957).

[15] J. M. Luttinger and P. Nozières, Phys. Rev. 127, 1423 (1962); 127, 1431 (1962).

[16] F. Toigo and T. O. Woodruff, Phys. Rev. B 2, 3958 (1970).

[17] D. J. W. Geldart and Roger Taylor, Solid State Commun. 9, 7 (1971).

[18] Some more comments on the analysis of Geldart and Taylor (Ref. 17) are appropriate here. These authors use the relation $g(x)=1-(2x^2/\pi)\int_0^\infty d\eta\,\eta\, G(\eta) j_1(\eta x)$, derived by Shaw [see Eq. (4.5) of Ref. 5]. Here $x=q_F r$, $\eta=q/q_F$, $G(\eta)$ is the local field of I, $g(x)$ is the pair correlation function, and $j_1(\eta x)$ is the spherical Bessel function. It should be emphasized that the preceding relation due to Shaw (Ref. 5) is valid only in the theory of I and is a result of the specific form of $G(\eta)$ in that theory. Using the number conservation Eq. (24) of the text, Shaw's relation, and the approximate form of $G(\eta)=A[1-e^{-B\eta^2}]$ of II, Geldart and Taylor (Ref. 17) obtained the relation $AB^{3/2}=\frac{9}{128}\pi^{3/2}$. They then used the values of the parameters A and B as given in II and found that the preceding equation was not satisfied. Hence, they concluded that the number conservation was violated in the theory of Singwi *et al.* (Ref. 1 and 2). This analysis of Geldart and Taylor is manifestly erroneous for two reasons: (i) Shaw's relation connecting $g(x)$ and $G(\eta)$ is *not* valid for the theory of II for which no such simple relation in fact exists, and (ii) in checking the sum rule numerically they used the values of A and B which are valid only for the $G(\eta)$ of II. In fact if Geldart and Taylor (Ref. 17) had used the values of A and B obtained by fitting $G(\eta)$ of I for which Shaw's relation is valid, they would have reached the conclusion that the number conservation is satisfied to the extent of the accuracy of the approximate analytic fit. The number conservation is *exactly* satisfied in I, II, and in the present theory as stated in the text. Geldart and Taylor also point out that the value of $G(\infty)$ in Hartree-Fock (HF) approximation should be equal to $\frac{1}{3}$, whereas our value of $G^{\mathrm{HF}}(\infty)$ is $\frac{1}{2}$. We recognize this deficiency in our theory. Nevertheless, this deficiency in the limiting value of $G(\vec{q})$ in our approximate theory does not seem to affect in any significant manner the value of the pair correlation function $g(r)$ for small r. A very small negative value of $g(0)$ for densities $r_s \geq 4$ may very well be due to this defect in our theory.

[19] F. Toigo and T. O. Woodruff, Phys. Rev. B 4, 371 (1971).

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

[21] D. Pines and P. Nozières, *The Theory of Quantum Fluids* (Benjamin, New York, 1966), p. 360.

[22] P. Schofield, Proc. Phys. Soc. (London) 88, 149 (1966).

[23] A. Sjölander and M. Stott, Phys. Rev. B 5, 2109 (1972).

[24] P. Bhattacharyya and K. S. Singwi, Phys. Rev. Letters (to be published).

[25] M. Gell-Mann and K. A. Brueckner, Phys. Rev. 106, 364 (1957).

[26] E. P. Wigner, Trans. Faraday Soc. 34, 678 (1938); see also Ref. 21, p. 296.

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Phase Reversal and Modulated Flux Motion in Superconducting Thin Films[*]

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It is shown that a small magnetic field alternating at audio frequencies causes an amplitude modulation of the electric field associated with the flux motion oscillating at microwave frequencies in superconducting thin films. The phase of the modulation component of this electric field can be changed almost 180° by reversing the sweep of the external magnetic field. These phenomena can be explained by invoking the influence of boundary currents on the motion of the flux lattice.

I. INTRODUCTION

If a constant homogeneous magnetic field $\vec{H}$ is applied along the normal of a superconducting film carrying a current $\vec{J}$ exceeding a critical value, a flux flow results in the direction perpendicular to both $\vec{J}$ and $\vec{H}$.[1] This critical current is not the critical current for destroying the superconductivity but is related to the pinning of flux in the sample. The vector relation among $\vec{J}$, $\vec{H}$, and the flux-flow velocity $\vec{v}$, is shown in Fig. 1(a). It has been established both experimentally[1] and theoretically[2]