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Theory of the Local Field Correction in an Electron Gas

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The wave-vector- and frequency-dependent dielectric function $\epsilon(\mathbf{k}, \omega)$ of an electron gas can be expressed in terms of Lindhard's function and a complex local field correction $G(\mathbf{k}, \omega)$ which incorporates all the effects of dynamic exchange and correlation in the system. The general properties of $G(\mathbf{k}, \omega)$ are discussed, in particular the static and high-frequency limits. It is shown that for small k, both $G(\mathbf{k}, 0)$ and $G(\mathbf{k}, \infty)$ vary as k^2, with different coefficients, but both determined by the average kinetic and potential energies per particle. For large k, $G(\mathbf{k}, \infty)$ varies again as k^2 and it is argued that the same holds true for $G(\mathbf{k}, 0)$, with both coefficients (though different) determined by the average kinetic energy per particle. General formulas for the plasma dispersion relation and damping, involving, respectively, the real and imaginary parts of $G(\mathbf{k}, \omega)$, are given. The term in the plasma frequency which is proportional to k^2 is given directly in terms of the average kinetic and potential energies per particle, a result true at all temperatures. A calculation of the frequency dependence of $G(\mathbf{k}, \omega)$, starting from the exact equation of motion for the particle–hole operator and employing a decoupling approximation introduced previously by Toigo and Woodruff, is presented. Explicit results for $G(\mathbf{k}, \omega)$ are obtained for small k and all ω. The complete expressions for $G(\mathbf{k}, 0)$ and $G(\mathbf{k}, \infty)$ in this approximation have been obtained and are plotted.

KEY WORDS: Dielectric function ; generalized mean-field representation; dynamic local field correction; plasma dispersion and damping; particle–hole operator; equation of motion; moment-conserving decoupling; static mean-field approximations.

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1. INTRODUCTION

A quantity which is the key to understanding many of the properties of metals that are due to the effects of electron–electron interactions is the wave-vector- and frequency-dependent dielectric function $\epsilon(\mathbf{k}, \omega)$. Knowledge of this quantity allows one to describe and calculate such properties as the density fluctuation excitation spectrum, the ground state energy, the screening of external charges, the longitudinal electrical conductivity, etc. The model which one usually employs in the calculation of $\epsilon(\mathbf{k}, \omega)$ is one in which the ions are replaced by a uniform, neutralizing background of positive charge, the assumption being that $\epsilon(\mathbf{k}, \omega)$ is not essentially altered by the replacement of the discrete ion lattice with a uniform background.

Following the pioneering work of Bohm and Pines,[1] which led to the development of the random phase approximation (RPA), an expression for $\epsilon(\mathbf{k}, \omega)$ corresponding to the RPA was first obtained by Lindhard.[2] This has since been applied in many calculations and is discussed in detail in several books and review articles.[3–9] The RPA provides a good description of long-wavelength plasma oscillations and screening phenomena but leads to some unphysical features of the pair distribution function in the range of metallic densities ($2 \leqslant r_s \leqslant 6$). This arises from the failure of the RPA to take account of short-range correlations in the motions of the electrons. A first improvement upon the RPA was introduced by Hubbard[10] in the form of a function $G(\mathbf{k})$, which has come to be called the local field correction, to take into account exchange and correlation effects neglected in RPA. The function $G(\mathbf{k})$ has since been extensively used in calculations of metallic properties[11–13] and many forms of $G(\mathbf{k})$ have been proposed (for a review see Shaw[14] and Appendix A of this work). The importance of $G(\mathbf{k})$ for the calculation of metallic properties has been thoroughly discussed and emphasized by Shaw.[14]

More recently it has been recognized that the local field correction should also be a function of frequency and a general expression for $\epsilon(\mathbf{k}, \omega)$ in terms of Lindhard's function and the dynamic local field correction $G(\mathbf{k}, \omega)$ has been given.[15,16] However, thus far calculations have been restricted to the static limit $\omega = 0$.

In this work we discuss some general properties of the complex function $G(\mathbf{k}, \omega)$ and present a calculation of the frequency dependence within a well-defined approximation. In Section 2 we first review some general relations involving the density–density response function $\chi(\mathbf{k}, \omega)$,[17] which is linked directly to the dielectric function $\epsilon(\mathbf{k}, \omega)$.[6] In Section 3 we introduce a formally exact representation for $\chi(\mathbf{k}, \omega)$ which may be termed a generalized mean field representation[18] since it is of the same form as the one used in all mean field approximations (MFA) (reviewed in Appendix A) except that the effective potential is a complex quantity which is both wave number and frequency dependent; the latter is identified with $v(k)[1 - G(\mathbf{k}, \omega)]$, where $v(k) = 4\pi e^2/k^2$. We also discuss in Section 3 another dielectric function frequently employed in the calculation of metallic properties, namely the one corresponding to the effective interaction between an electron and a test charge and denoted by $\tilde{\epsilon}_e(\mathbf{k}, \omega)$.[14] Both $\epsilon(\mathbf{k}, \omega)$ and $\tilde{\epsilon}_e(\mathbf{k}, \omega)$ are expressed in terms of $G(\mathbf{k}, \omega)$, which can thus be considered the basic unknown quantity of the theory. Some basic properties of $G(\mathbf{k}, \omega)$ are discussed in Section 4, in particular the static and high-frequency limits, and it is pointed out that the real and imaginary parts of $G(\mathbf{k}, \omega)$ are connected by a Kramers–Kronig relation. The real part of $G(\mathbf{k}, \omega)$ enters into the plasma dispersion relation while the imaginary part of $G(\mathbf{k}, \omega)$ occurs in the damping; the general formulas are given in Eqs. (56a)–(56c) and (57).

In Section 5 we present a calculation of $G(\mathbf{k}, \omega)$ using a decoupling method employed by Toigo and Woodruff[15] on the equation of motion for the particle–hole operator. Their decoupling has the virtue that it conserves the third frequency moment of the imaginary part of $\chi(\mathbf{k}, \omega)$ as well as the f-sum rule.[6] A simple "trick" allows us to obtain results which are much simpler than those of Toigo and Woodruff,[15] who restricted calculations to the static limit $\omega = 0$ because of the complexity involved.

In Section 6 we briefly discuss a formula for the ground state energy of the electron gas corresponding to the Toigo–Woodruff decoupling followed by the Hartree–Fock factorization. The calculation of the ground state energy on the basis of this formula is, however, not a simple undertaking and has not been carried out here.

2. DEFINITIONS AND GENERAL RELATIONS

As a means of introducing the notation, we shall here list the basic quantities, relations, and properties defining our system. We consider a system of N electrons in a cubical box of volume Ω (with periodic boundary conditions), immersed in a uniform, neutralizing background of positive charge of density $|e|N/\Omega \equiv |e|\rho$. The Hamiltonian of this system is given by[4]

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2\Omega} \sum_{\mathbf{k}\neq 0} v(k)[\rho(\mathbf{k})\rho(-\mathbf{k}) - N] \tag{1a}$$

where $\rho(\mathbf{k})$ is the density fluctuation operator defined as

$$\rho(\mathbf{k}) = \sum_{i=1}^{N} \exp(-i\mathbf{k}\cdot\mathbf{r}_i) \tag{2a}$$

and $v(k) = 4\pi e^2/k^2$ is the Fourier transform of the Coulomb potential,

$v(r) = e^2/r$. For our purposes later on it will be useful to write the Hamiltonian also in second quantized form, involving the creation and annihilation operators $a^+_{\mathbf{k}\sigma}$ and $a_{\mathbf{k}\sigma}$, respectively, for a particle of momentum $\hbar\mathbf{k}$ and spin orientation σ. In second quantized form the Hamiltonian is

$$H = \sum_{\mathbf{k}\sigma} \hbar\omega_0(k) a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \frac{1}{2\Omega} \sum_{\mathbf{k}\neq 0} v(k)[\rho(\mathbf{k})\rho(-\mathbf{k}) - N] \tag{1b}$$

where $\omega_0(k) = \hbar k^2/2m$, and the density fluctuation operator $\rho(\mathbf{k})$ is given by

$$\rho(\mathbf{k}) = \sum_{\mathbf{q}\sigma} a^+_{\mathbf{q}\sigma} a_{\mathbf{q}+\mathbf{k}\sigma} \tag{2b}$$

$N = \rho(\mathbf{k} = 0)$ is the total number of particles operator.

As usual, we shall work in the Heisenberg picture with time-dependent operators $A(t)$ defined by $A(t) = [\exp(itH/\hbar)]A(0)[\exp(-itH/\hbar)]$.

The basic correlation function, which contains all the information about the density fluctuations in the system, is the time-dependent density–density commutator $\tilde{\chi}''(k, t - t')$, defined by[17]

$$\tilde{\chi}''(k, t - t') = (1/2\hbar\Omega)\langle[\rho(\mathbf{k}, t), \rho(-\mathbf{k}, t')]\rangle \tag{3}$$

where the angular brackets denote an equilibrium thermal ensemble average appropriate to the system Hamiltonian (1). We are considering a homogeneous electron gas, i.e., we are assuming our system to have translational and rotational invariance; thus $\tilde{\chi}''$ depends only on the absolute value of k. We observe that $\tilde{\chi}''(k, t - t')$ is a purely imaginary function and an odd function of $t - t'$. Its Fourier transform, the spectral function

$$\tilde{\chi}''(k, \omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega(t-t')} \tilde{\chi}''(k, t - t') \tag{4}$$

is a real, odd function of ω with the important property[17]

$$\omega\tilde{\chi}''(k, \omega) \geqslant 0 \tag{5}$$

which, as we shall see, has an important consequence and bearing for this work. The above property is closely connected with the fact that the energy transfer per unit time from an external probe to a stable system in thermodynamic equilibrium is a nonnegative quantity.[6,17]

In addition to $\tilde{\chi}''(k, t - t')$, we shall also introduce the retarded density–density response function $\tilde{\chi}(k, t - t')$, a real function defined as[17]

$$\tilde{\chi}(k, t - t') = 2i\,\theta(t - t')\tilde{\chi}''(k, t - t') \tag{6}$$

where $\theta(t - t')$ is the unit step function (which vanishes for negative values of its argument). Although the above function contains no more information than $\tilde{\chi}''(k, t - t')$, it is a useful quantity to define since it describes the linear response of the system to an external probe or potential which couples to the density fluctuations in the system. Specifically, the Fourier transform of the quantity (6), $\chi(k, \omega)$, gives the linear response $\langle\rho(\mathbf{k}, \omega)\rangle$ of the number density fluctuation to an external potential $U_{\text{ext}}(\mathbf{k}, \omega)$ or test charge of density $z\rho_{\text{ext}}(\mathbf{k}, \omega)$ via the relations

$$\langle\rho(\mathbf{k}, \omega)\rangle = -\chi(k, \omega)eU_{\text{ext}}(k, \omega) \tag{7a}$$

$$= -\chi(k, \omega)(4\pi ez/k^2)\rho_{\text{ext}}(\mathbf{k}, \omega) \tag{7b}$$

We note that the definition (6) implies that $\chi(k, \omega)$ can be expressed entirely in terms of its imaginary part, the spectral function $\chi''(k, \omega)$:

$$\chi(k, \omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega(t-t')}2i\theta(t - t')\tilde{\chi}''(k, t - t') \tag{8a}$$

$$= P\int_{-\infty}^{\infty} \frac{d\omega'}{\pi}\frac{\chi''(k, \omega)}{\omega' - \omega} + i\chi''(k, \omega) \tag{8b}$$

The first term on the right of (8b) is a principal value (P) integral, which we shall also denote by $\chi'(k, \omega)$; it is the real part of the complex function $\chi(k, \omega)$ and is an even function of ω.

The function $\chi(k, \omega)$ is directly related to some dielectric functions that play an important role in the theory of metals. In particular, these dielectric functions enter directly into calculations of screening effects and charge distributions around impurities and the calculation of phonon frequencies in metals.[4,6] The ordinary longitudinal dielectric function or dielectric function for a test charge (appropriate to test-charge–test-charge interactions), which we have denoted by $\epsilon(k, \omega)$, is derived using Poisson's equation for an electron system and is defined as follows[6]:

$$\frac{1}{\epsilon(k, \omega)} = 1 + \frac{e\langle\rho(\mathbf{k}, \omega)\rangle}{z\rho_{\text{ext}}(\mathbf{k}, \omega)} = \frac{U(\mathbf{k}, \omega)}{U_{\text{ext}}(\mathbf{k}, \omega)} \tag{9}$$

where

$$U(\mathbf{k}, \omega) = U_{\text{ext}}(\mathbf{k}, \omega) + (4\pi e/k^2)\langle\rho(\mathbf{k}, \omega)\rangle \tag{10}$$

is the total effective potential acting on a test-charge particle in the system; the total effective electric field $\mathbf{E}(\mathbf{k}, \omega)$ acting on this particle is $\mathbf{E}(\mathbf{k}, \omega) = -i\mathbf{k}U(\mathbf{k}, \omega)$. From Eq. (7) one then obtains in linear response theory the following relation[6] between $\epsilon(k, \omega)$ and $\chi(k, \omega)$:

$$1/\epsilon(k, \omega) = 1 - v(k)\chi(k, \omega) \tag{11}$$

3. AN EXACT GENERALIZED MEAN FIELD REPRESENTATION

It is somewhat more convenient to use complex frequencies z and to deal with the complex density–density response function $\chi(k, z)$ defined in terms of the spectral function $\chi''(k, \omega)$ by[17]

$$\chi(k, z) = \int_0^\infty dt\, e^{izt}\tilde{\chi}(k, t), \qquad \operatorname{Im} z > 0 \tag{12a}$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''(k, \omega)}{\omega - z} \tag{12b}$$

The integral (12b) serves to define $\chi(k, z)$ in both the upper and lower halves of the complex z plane as an analytic function off the real axis. The physical response function, which we have denoted $\chi(k, \omega)$, represents the boundary value as z approaches ω on the real axis from above, i.e.,

$$\chi(k, \omega) \equiv \lim \ \chi(k, \omega + i\epsilon) = \chi'(k, \omega) + i\chi''(k, \omega) \tag{13}$$

We consider in this section a formally exact representation for $\chi(k, z)$ and $\epsilon(k, \omega)$. This representation has been introduced in previous work[18] where it was applied to the calculation of scattering functions and to the description of collective modes and their damping in classical liquids. For the electron gas this representation will be given in the form

$$\chi(k, z) = \frac{\chi_0(k, z)}{1 + [v(k) + \phi(k, z)]\chi_0(k, z)} \tag{14}$$

or equivalently,

$$\chi^{-1}(k, z) = \chi_0^{-1}(k, z) + v(k) + \phi(k, z) \tag{15}$$

This equation has the form of the Dyson equation well known in the theory of Green's functions.[19–21] $\chi_0(k, z)$ is the density–density response function for a system of noninteracting particles; the general expression is

$$\chi_0(k, z) = \frac{1}{\hbar\Omega} \sum_{\mathbf{q}\sigma} \frac{n_\sigma^{(0)}(\mathbf{q} + \frac{1}{2}\mathbf{k}) - n_\sigma^{(0)}(\mathbf{q} - \frac{1}{2}\mathbf{k})}{z - (\hbar\mathbf{q}\cdot\mathbf{k}/m)} \tag{16}$$

where $n_\sigma^{(0)}(q)$ is the Fermi distribution function. The complex, frequency- and wave-number-dependent potential $\phi(k, z)$ here plays the role of the self-energy. When $\phi(k, z)$ is replaced by zero, (14) gives the expression for the response function in the RPA. In the case when $\phi(k, z)$ is approximated by a real, frequency-independent function $\phi(k)$, (14) reduces to the expression for the response function obtained in static mean field approximations (MFA), which are reviewed in Appendix A. We shall therefore refer to (14) as an exact generalized mean field representation.[18] This is not to be confused with the generalized RPA discussed in Refs. 6 and 9, which is also a static MFA type of theory. Note that the long-range correlations characteristic of the electron system have been taken into account explicitly by separating off the Coulomb interaction $v(k)$. Thus $\phi(k, z)$ represents the collisional part of the total effective interaction between density fluctuations.

Before going on to show this in more detail and giving the precise physical meaning conveyed by $\phi(k, z)$, we first note the following important fact. Not only $\chi(k, z)$ but also $\chi^{-1}(k, z)$ is an analytic function of z off the real axis; for $\chi^{-1}(k, z)$ this fact can be proved[17] from the property (5). It therefore follows from (15) that $\phi(k, z)$ is also analytic off the real axis.

We define

$$\phi(k, \omega) \equiv \lim_{\epsilon \to 0+} \phi(k, \omega + i\epsilon) = \phi'(k, \omega) + i\phi''(k, \omega) \tag{17}$$

In terms of $\phi(k, \omega)$ the dielectric function $\epsilon(k, \omega)$ defined by (11) is given by

$$\epsilon(k, \omega) = 1 + \frac{v(k)\chi_0(k, \omega)}{1 + \phi(k, \omega)\chi_0(k, \omega)} \tag{18a}$$

$$= 1 + \frac{v(k)\chi_0(k, \omega)}{1 - G(k, \omega)v(k)\chi_0(k, \omega)} \tag{18b}$$

where we have defined $\phi(k, \omega) = -v(k)G(k, \omega)$ to bring (18a) into the form suggested by the work of Hubbard.[10] $\chi_0(k, \omega)$ is the density response function for a noninteracting electron gas, or free electron polarizability, and $G(k, \omega)$ is a complex function describing all the dynamic exchange and short-range correlation effects due to the Coulomb interaction of the electrons. If the function $G(k, \omega)$ is replaced by zero, Eq. (18b) gives the dielectric function in the RPA first obtained by Lindhard[2] and discussed extensively in Ref. 6. In Hubbard's original work,[10,22] as well as in the static MFA expressions considered since (and discussed in Appendix A), the complex function $G(k, \omega)$ was replaced by a real, frequency-independent function $G(k)$. The expression (18b) for $\epsilon(k, \omega)$ has since appeared in the work of several authors[15,16]; however, calculations thus far have only been done for the static case $\omega = 0$.

In addition, and closely related to $\epsilon(k, \omega)$, there is another dielectric function frequently employed in the calculation of some metallic properties.[23] This latter function, which we shall denote by $\tilde{\epsilon}_e(k, \omega)$, is in fact just a useful construct to enable one to describe an effective interaction between an electron and a test charge. Thus the function $\tilde{\epsilon}_e(k, \omega)$ relates the total potential which acts on an electron in the conduction band to the bare crystalline potential. A derivation of the function $\tilde{\epsilon}_e(k, \omega)$ has recently been given by Shaw,[14] to whom we refer for further details and earlier references. Since the notation chosen by Shaw might lead to some confusion,[3] we shall briefly

[3] In particular, Shaw's function $\chi(q, \omega)$ (see Ref. 14) is not the same as ours, which is defined by Eqs. (7) and (8), in accordance with the notation of Kadanoff and Martin[17] and Pines and Nozières.[6] The function in Shaw's notation which corresponds to our function $\chi(q, \omega)$ is $-R(q, \omega)$ [Eq. (2.11) of Ref. 14].

indicate the relations in our notation. First, one defines an effective potential $V(\mathbf{k}, \omega)$ [different from $U(\mathbf{k}, \omega)$] to describe the electronic density response in the presence of the external potential $U_{\text{ext}}(\mathbf{k}, \omega)$ by the relation [compare Eq. (7)]

$$\langle \rho(\mathbf{k}, \omega) \rangle = -\chi_0(k, \omega) e V(\mathbf{k}, \omega) \tag{19}$$

and, analogously to Eq. (9), one defines $\tilde{\epsilon}_e(k, \omega)$ by setting

$$1/\tilde{\epsilon}_e(k, \omega) = V(\mathbf{k}, \omega)/U_{\text{ext}}(\mathbf{k}, \omega) \tag{20}$$

Notice that in defining $V(\mathbf{k}, \omega)$ by (19) we have lumped all the effects of the interaction, i.e., all contributions due to exchange and correlations, into $V(\mathbf{k}, \omega)$. In the RPA where exchange and short-range correlations are neglected, the effective potential $V(\mathbf{k}, \omega)$ is the same as $U(\mathbf{k}, \omega)$, the effective potential seen by a test charge in the presence of $U_{\text{ext}}(\mathbf{k}, \omega)$ [cf. Eq. (10)]. Comparison of Eqs. (7) and (19) results in the expression

$$1/\tilde{\epsilon}_e(k, \omega) = \chi(k, \omega)/\chi_0(k, \omega) \tag{21}$$

Using (11), one obtains the relation between $\tilde{\epsilon}_e(k, \omega)$ and $\epsilon(k, \omega)$:

$$\tilde{\epsilon}_e(k, \omega) = \frac{v(k)\chi_0(k, \omega)\epsilon(k, \omega)}{\epsilon(k, \omega) - 1} \tag{22}$$

By substituting expression (18b) for $\epsilon(k, \omega)$ we obtain a formally exact expression for $\tilde{\epsilon}_e(k, \omega)$ in terms of the basic unknown function $G(k, \omega)$:

$$\tilde{\epsilon}_e(k, \omega) = 1 + v(k)[1 - G(k, \omega)]\chi_0(k, \omega) \tag{23}$$

Note that in RPA, $\tilde{\epsilon}_e(k, \omega)$ is the same as $\epsilon(k, \omega)$.

From Eqs. (19), (20), (7), and (10) it follows that the effective potential $V(\mathbf{k}, \omega)$ acting on an electron in the presence of $U_{\text{ext}}(\mathbf{k}, \omega)$ is given by

$$\begin{aligned} eV(\mathbf{k}, \omega) &= eU_{\text{ext}}(\mathbf{k}, \omega) + v(k)[1 - G(k, \omega)]\langle \rho(\mathbf{k}, \omega) \rangle \\ &= eU(\mathbf{k}, \omega) - v(k)G(k, \omega)\langle \rho(\mathbf{k}, \omega) \rangle \end{aligned} \tag{24}$$

where $U(\mathbf{k}, \omega)$ has been defined in (10) as the effective potential which would act on a test charge particle in the presence of $U_{\text{ext}}(\mathbf{k}, \omega)$. The quantity $V_{xc}(\mathbf{k}, \omega) \equiv V(\mathbf{k}, \omega) - U(\mathbf{k}, \omega)$, which describes the difference in the effective potentials acting on an electron and on a test charge in the presence of an external test charge, is thus linked directly to $G(k, \omega)$:

$$eV_{xc}(\mathbf{k}, \omega) = -v(k)G(k, \omega)\langle \rho(\mathbf{k}, \omega) \rangle \tag{25}$$

which is a natural generalization of the result obtained by Shaw.[14] In the RPA where $G(k, \omega)$ is replaced by zero, the above quantity vanishes. The quantities $V_{xc}(\mathbf{k}, \omega)$ and $G(k, \omega)$ thus describe in an exact fashion the extent to which the behavior of an electron is influenced by dynamic exchange and correlation effects arising from the interaction of the particles.

In treatments concerned with the application of the dielectric functions to calculations of metallic properties, the relation (19) is usually obtained or quoted as a first-order perturbation result. By adopting (19) as the definition of $V(\mathbf{k}, \omega)$ we obtain a formally exact framework in which the two dielectric functions $\epsilon(k, \omega)$ and $\tilde{\epsilon}_e(k, \omega)$ can both be expressed in terms of a single unknown function, $G(k, \omega)$.

It is of some interest to note also the expression for the effective electric field acting on an electron, $E_{\text{eff}}(\mathbf{k}, \omega) = -i\mathbf{k}V(\mathbf{k}, \omega)$. In real space–time this effective electric field is given by

$$e\mathbf{E}_{\text{eff}}(\mathbf{r}, t) = -\nabla[eU_{\text{ext}}(\mathbf{r}, t)] + \int d^3r' \int_{-\infty}^{\infty} dt' \, [\nabla v(\mathbf{r} - \mathbf{r}')\, \delta(t - t') + \nabla\Phi(\mathbf{r} - \mathbf{r}', t - t')][\langle\rho(\mathbf{r}', t')\rangle - \rho] \tag{26a}$$

where $\Phi(r, t)$ is the real, spherically symmetric potential defined by

$$\Phi(r, t) = \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \phi(k, \omega) \exp(i\mathbf{k}\cdot\mathbf{r} - i\omega t)$$
$$= -\int \frac{d^3k}{(2\pi)^3}\, v(k) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, G(k, \omega) \exp(i\mathbf{k}\cdot\mathbf{r} - i\omega t) \tag{27}$$

Because of the analytic properties of $\phi(k, z)$ discussed above, it follows that $\Phi(r, t) = 0$ for $t < 0$, i.e., $\Phi(r, t)$ is a "retarded" function like $\tilde{\chi}(k, t)$. Hence (26a) can be rewritten

$$e\mathbf{E}_{\text{eff}}(\mathbf{r}, t) = -\nabla[eU_{\text{ext}}(\mathbf{r}, t)] + \int d^3r' \, \nabla v(\mathbf{r} - \mathbf{r}')[\langle\rho(\mathbf{r}', t)\rangle - \rho] + \int d^3r' \int_{-\infty}^{t} dt' \, \nabla\Phi(\mathbf{r} - \mathbf{r}', t - t')[\langle\rho(\mathbf{r}', t')\rangle - \rho] \tag{26b}$$

Here it has been assumed that the external potential has been switched on adiabatically at $t = -\infty$. From (26) we clearly see why $\Phi(r, t)$ represents a local field correction to the RPA where the last term is absent. If there is an electron at the position $(\mathbf{r}, t)$ where we are calculating the effective electric field, then the electron density in the neighborhood of $(\mathbf{r}, t)$ is decreased by dynamic correlation effects. The RPA overestimates the charge displacement because it takes no account of the local reduction in density. Note that $\Phi(r, t)$ can be termed a memory function. The last term in (26b) says that in establishing an effective field at $(\mathbf{r}, t)$, the system has a memory for the effect of the average density at a point $\mathbf{r}'$ at some prior time t'. This is precisely what one expects for short-range effects which are mediated by the collisions between the particles.

4. GENERAL PROPERTIES OF $G(k, \omega)$

First let us note explicitly the relation in the static limit $\omega = 0$ between the static dielectric function $\epsilon(k, 0)$ and $G(k, 0)$:

$$\epsilon(k, 0) - 1 = \frac{v(k)\chi_0(k)}{1 - G(k, 0)v(k)\chi_0(k)} \tag{28}$$

In the long-wavelength limit $\epsilon(k, 0)$ is related to the isothermal compressibility K_T by the compressibility relation or sum rule[6]:

$$\lim_{k \to 0} \epsilon(k, 0) = 1 + \frac{4\pi e^2 \rho^2 K_T}{k^2} = 1 + \frac{k_{FT}^2 K_T}{k^2 K_T^{(0)}} \tag{29}$$

where $K_T^{(0)}$ is the free particle compressibility and k_{FT} is defined by $k_{FT}^2 = 4\pi e^2 \rho^2 K_T^{(0)}$; at zero temperature this reduces to the Fermi–Thomas value[4]: $k_{FT}^{(2)} = 6\pi\rho e^2/\epsilon_F{}^0 = 3\omega_p{}^2/V_F{}^2$ ($V_F = \hbar k_F/m$ is the free particle velocity at the Fermi surface). It is an important requirement for all calculations of the lattice dynamics of metals that the static dielectric function satisfies the above relation.[13]

Equations (28) and (29) imply that the static local field correction at long wavelengths is given by

$$\lim_{k \to 0} G(k, 0) = \gamma_0 k^2/k_F{}^2 \tag{30}$$

where γ_0 is the dimensionless factor

$$\gamma_0 = \frac{k_F{}^2}{m\omega_p{}^2}\left(\frac{1}{\rho K_T^{(0)}} - \frac{1}{\rho K_T}\right) \tag{31}$$

and we have used the fact that $\lim_{k \to 0} \chi_0(k) = \rho^2 K_T^{(0)}$. The fact that for small k, $G(k, 0)$ is related to the compressibility in the above manner seems to have first been emphasized by Geldart and Vosko.[24]

At this point it is useful to recall the virial theorem and its connection with the compressibility. These have played an important role in some recent treatments of electron correlations at metallic densities.[25,26] The general form of the virial theorem for a system of particles interacting only via Coulomb forces is given by Landau and Lifshitz[27]; it has also been the subject of a thorough quantum mechanical investigation by Argyres.[28] For the homogeneous electron gas the virial form for the pressure reads[25]

$$\begin{aligned} p &= \tfrac{2}{3}\rho\langle \mathrm{KE}\rangle - \tfrac{1}{6}\rho^2 \int d^3r\, [g(r) - 1] r v'(r) \\ &= \tfrac{2}{3}\rho\langle \mathrm{KE}\rangle + \tfrac{1}{6}\rho^2 \int d^3r\, [g(r) - 1] v(r) \end{aligned} \tag{32a}$$

where $\langle \mathrm{KE}\rangle$ is the average kinetic energy per particle and $g(r)$ is the radial distribution function. The last term is proportional to the average potential energy per particle $\langle V\rangle$, and hence

$$p = \tfrac{1}{3}\rho[2\langle \mathrm{KE}\rangle + \langle V\rangle] \tag{32b}$$

which is the general form found in Ref. 27.

From the above equation one obtains the following expression for $K_T^{(25)}$:

$$\frac{1}{\rho K_T} = \left.\frac{\partial p}{\partial \rho}\right|_T = \frac{2}{3}\frac{\partial}{\partial \rho}[\rho\langle \mathrm{KE}\rangle] + \frac{1}{3}\frac{\partial}{\partial \rho}[\rho\langle V\rangle] \tag{33}$$

Substituting (33) into (31), we can write γ_0 as

$$\gamma_0 = \gamma_0^{(\mathrm{KE})} + \gamma_0^{(V)} \tag{34}$$

where

$$\gamma_0^{(\mathrm{KE})} = -\frac{2k_{\mathrm{F}}^2}{3m\omega_p^2}\frac{\partial}{\partial \rho}[\rho(\langle \mathrm{KE}\rangle - \langle \mathrm{KE}\rangle_0)] \tag{35}$$

$$\gamma_0^{(V)} = -\frac{k_{\mathrm{F}}^2}{3}\int_0^\infty dr\, r\left[g(r) - 1 + \frac{1}{2}\rho\frac{\partial g(r)}{\partial \rho}\right] \tag{36}$$

The quantity $\langle \mathrm{KE}\rangle_0$ is the average kinetic energy per particle for the noninteracting system. Thus the static local field correction and static dielectric function in the long-wavelength limit are related directly to the average kinetic and potential energies per particle. The relations (32)–(36) for the ground state system are discussed further in Appendix B.

Next let us note that $\chi^{-1}(k, z)$ has the following asymptotic expansion for large z:

$$\chi^{-1}(k, z) \sim -\frac{1}{M_1}\left[z^2 - \frac{M_3}{M_1} + \frac{(M_3/M_1)^2 - M_5/M_1}{z^2} + \cdots\right] \tag{37}$$

where the quantities $M_n(k)$ are the frequency moments of the spectral function $\chi''(k, \omega)$. These can be obtained as equal time commutators using the defining equations (3) and (4):

$$M_n(k) = \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\,\omega^n\chi''(k,\omega) = \frac{1}{\hbar\Omega}\left\langle\left[\left(i\frac{\partial}{\partial t}\right)^n\rho(\mathbf{k},t),\,\rho(-\mathbf{k},t)\right]\right\rangle \tag{38a}$$

$$= \frac{1}{\hbar\Omega}\left\langle\left[\left(i\frac{\partial}{\partial t}\right)^{n-m}\rho(\mathbf{k},t),\,\left(-i\frac{\partial}{\partial t'}\right)^m\rho(-\mathbf{k},t')\right]_{t'=t}\right\rangle \tag{38b}$$

where m is an integer between zero and n. Only the odd n frequency moments survive, and because of (5) the $M_n(k)$ are nonnegative quantities. The right-hand sides of (38a) and (38b) can be evaluated by making repeated use of the Heisenberg equation of motion and the equal time commutation relations. Making use of (38b) with an appropriate integer m, rather than (38a), usually results in considerable simplification and time-saving in working out the equal time commutators, a fact which is sometimes overlooked (cf. Section 5).

The moments which have thus far been obtained are $M_1(k)$ and $M_3(k)$.[17,30] The first-moment sum rule is

$$M_1(k) = \rho k^2/m \tag{39}$$

and the third-moment sum rule is[30,31]

$$\begin{aligned} M_3(k) &= (\rho k^2/m)[\omega_0^2(k) + 4\omega_0(k)\langle \text{KE}\rangle/\hbar + Q(k)] \\ &\equiv (\rho k^2/m)\omega_3^2(k) \end{aligned} \tag{40}$$

where $Q(k)$ is a function defined below. Equations (39) and (40) are consequences and expressions of the local conservation laws for the particle density and longitudinal momentum density. This will be seen in the discussion of Section 5.

The general expression for $Q(k)$ can be found in Refs. 30 and 31. For an electron gas moving in a uniform positive background, $Q(k)$ is given by[32]

$$\begin{aligned} Q(k) &= (1/m\Omega) \sum_{\mathbf{q}\neq 0} (\hat{\mathbf{k}}\cdot\mathbf{q})^2[S(\mathbf{k}+\mathbf{q}) - S(q)] \\ &= \omega_p^2 + I(k) \end{aligned} \tag{41}$$

where $S(q)$ is the static structure factor and $\omega_p^2 = 4\pi\rho e^2/m$ is the square of the plasma frequency.

The quantity $I(k)$ can be expressed as

$$I(k) = (e^2/m\pi) \int_0^\infty dq\, q^2[S(q) - 1]J(q, k) \tag{42}$$

with

$$J(q, k) = \frac{5}{6} - \frac{q^2}{2k^2} + \frac{k}{4q}\left(\frac{q^2}{k^2} - 1\right)^2 \ln\left|\frac{q+k}{q-k}\right| \tag{43}$$

a function only of the ratio q/k, positive for all values of this ratio and monotonically decreasing. In the limits $k \to 0$ and $k \to \infty$, the function $I(k)$ behaves as[32]

$$I(k) = (4k^2/15m)\langle V\rangle, \qquad k \to 0 \tag{44}$$

$$I(k) = \tfrac{2}{3}\,\omega_p^2[g(0) - 1], \qquad k \to \infty \tag{45}$$

where $\langle V\rangle$ is the potential energy per particle, expressed here as

$$\langle V\rangle = \frac{1}{2}\int \frac{d^3q}{(2\pi)^3}\, v(q)[S(q) - 1] \tag{46}$$

and $g(0)$ is the radial distribution function evaluated at $r = 0$; in Appendix A we argue that $g(0)$ should be zero. However, we shall continue to use $g(0)$ in the corresponding formulas to serve as a reminder of the origin of this term.

Since an asymptotic expansion similar to (37) holds also for $\chi_0^{-1}(k, z)$ [with the $M_n(k)$ replaced by the corresponding noninteracting moments $M_n^{(0)}(k)$], it follows from (15) that the quantity $\phi(k, z)$ has the following asymptotic expansion for large z:

$$\phi(k, z) \sim \phi_\infty(k) - [a_1(k)/z^2] + \cdots \tag{47}$$

where

$$\phi_\infty(k) \equiv \phi(k, \infty) \equiv -v(k)G(k, \infty)$$

$$G(k, \infty) = -\frac{2k^2}{m\omega_p^2}(\langle\mathrm{KE}\rangle - \langle\mathrm{KE}\rangle_0) - \frac{3}{4k_\mathrm{F}^3}\int_0^\infty dq\, q^2[S(q) - 1]J(q, k) \tag{48}$$

is the expression for the local field correction in the limit of very large frequencies. The quantity $a_1(k)$ involves the interaction parts of both $M_3(k)$ and $M_5(k)$.

It is useful to note explicitly the limiting forms of $G(k, \infty)$ for both small and large k. In the limit $k \to 0$ one has, using (44),

$$\lim_{k\to 0} G(k, \infty) = \gamma_\infty k^2/k_\mathrm{F}^2 \tag{49}$$

where γ_∞ is given by

$$\gamma_\infty = -\frac{k_\mathrm{F}^2}{m\omega_p^2}\left[2(\langle\mathrm{KE}\rangle - \langle\mathrm{KE}\rangle_0) + \frac{4}{15}\langle V\rangle\right] \tag{50}$$

Thus for small k both the static and high-frequency limits of the local field correction are determined by the average kinetic and potential energies per particle.

In the limit of large k one has, using (45),

$$\lim_{k\to\infty} G(k, \infty) = -\frac{2k^2}{m\omega_p^2}(\langle\mathrm{KE}\rangle - \langle\mathrm{KE}\rangle_0) + \frac{2}{3}[1 - g(0)] \tag{51}$$

At this point it is well to recall the inequality[32] $\langle\mathrm{KE}\rangle \geqslant \langle\mathrm{KE}\rangle_0$, which holds rigorously for the ground state (and probably for all temperatures). Hence the high-frequency limit $G(k, \infty)$ varies with k^2 for both $k \to 0$ and $k \to \infty$.

Because $\phi(k, z) - \phi_\infty(k)$ is analytic off the real axis and vanishes for large z as $1/z^2$, we can write a spectral representation[18]

$$\phi(k, z) - \phi_\infty(k) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\phi''(k, \omega)}{\omega - z} \tag{52}$$

where $\phi''(k, \omega) = \operatorname{Im} \phi(k, \omega)$ is a real, odd function of ω. We shall see below that $\phi''(k, \omega)$ gives essentially the collisional damping of the density fluctuations in the electron gas.

Equation (52) implies the following Kramers–Kronig relation between the real and imaginary parts of $G(k, \omega)$, denoted respectively by $G'(k, \omega)$ and $G''(k, \omega)$:

$$G'(k, \omega) - G(k, \infty) = P \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{G''(k, \omega')}{\omega' - \omega} \tag{53}$$

An immediate consequence of (53) is obtained by taking $\omega = 0$, resulting in the sum rule

$$G(k, 0) - G(k, \infty) = P \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{G''(k, \omega)}{\omega} \tag{54}$$

This is a fundamental sum rule satisfied by $G''(k, \omega)$. For small k it immediately follows from (30) and (49) that

$$\lim_{k \to 0} P \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{G''(k, \omega)}{\omega} = (\gamma_0 - \gamma_\infty) \frac{k^2}{k_F^2} \tag{55}$$

The real and imaginary parts of $G(k, \omega)$ enter directly into the dispersion relation and damping of the plasma oscillations. Since in general only the long-wavelength plasma oscillations satisfy the condition of small damping, we give here only the relations valid for the limit $k \to 0$. The real part of the plasma frequency $\omega_p(k)$ can be shown to be given by

$$\omega_p^2(k) = \omega_p^2[1 - G'(k, \omega_p(k))] + \omega_{30}^2(k) + \cdots \tag{56a}$$

$$= \omega_p^2 \left(1 - \gamma_\infty \frac{k^2}{k_F^2}\right) + 2 \frac{k^2 \langle \mathrm{KE} \rangle_0}{m} + \cdots \tag{56b}$$

where we have kept only the terms of order k^2. Here $\omega_{30}^2(k)$ is the quantity defined by the third frequency moment (40) corresponding to the non-interacting system. Using Eq. (50) for γ_∞, we can rewrite (56b) as

$$\omega_p^2(k) = \omega_p^2 + \frac{k^2}{m} \left(2\langle \mathrm{KE} \rangle + \frac{4}{15} \langle V \rangle\right) + \cdots \tag{56c}$$

Thus $\omega_p(k)$ is related directly to the average kinetic and potential energies per particle. The imaginary part $\omega_I(k)$, which describes the damping of the plasma oscillations, is given by

$$\omega_I(k) = -\frac{\omega_p}{2}\left[\frac{m\omega_p{}^2}{\rho k^2}\chi_0''(k, \omega_p) + G''(k, \omega_p)\right] \tag{57}$$

The above expressions are entirely general. They apply to the classical limit as well as to the ground state of the electron gas. The last term in (56b) gives the RPA contribution, while the term $\gamma_\infty k^2/k_F{}^2$ gives the effect of the local field correction in the high-frequency limit under consideration. The first term on the right of (57) describes in general the Landau damping. In the ground state this term vanishes for wave numbers up to a critical value k_c given by the equation $\omega_p(k_c) = k_c v_F + \omega_0(k_c)$ and hence gives no contribution to the damping. The physical reason for this, as well as the nature of Landau type damping, are discussed fully in the book by Pines and Nozières (PN).[6] In the classical limit, on the other hand, the Landau damping term is no longer zero but exponentially small for $k \to 0$. The other term $G''(k, \omega_p)$, will in general always lead to a damping for $k \neq 0$. Since it arises from the imaginary part of the dynamic local field correction and since the latter describes the short-range and memory effects associated with collisions, one can call the damping to which it gives rise "collisional damping."

The relations discussed thus far are all rigorous consequences of the formalism introduced in this section. For the remainder of this section, however, we wish to add some remarks of a nonrigorous, speculative character concerning the static local field correction $G(k, 0)$ and thereby also the static dielectric function $\epsilon(k, 0)$. We have already seen that for small k, both $G(k, 0)$ and $G(k, \infty)$ vary with k^2. Also, we have found that for large k, $G(k, \infty)$ varies with k^2, with a coefficient determined by the difference $\langle KE\rangle - \langle KE\rangle_0$. Now this latter quantity also enters the static local field correction factor γ_0 [Eqs. (34), (35)]. By analogy with the corresponding kinetic energy contribution to $G(k, \infty)$ it is perhaps not unreasonable to suppose that the kinetic energy contribution to $G(k, 0)$ is $\gamma_0^{(KE)}k^2/k_F{}^2$ for all k. This is perhaps made more plausible by noting that the factor $\gamma_0^{(KE)}$ reflects the difference between the true momentum distribution function and the noninteracting, Fermi distribution function. Since we have written the Dyson-like equation (15) in terms of $\chi_0^{-1}(k, z)$ rather than an unknown function describing the propagation in the interacting system, it should not be surprising to find that difference reflected in a corresponding contribution to the local field correction.

For the potential energy contribution to $G(k, 0)$ one can take a form derived by Schneider[25] and Vashishta and Singwi[26] and discussed in more detail in Appendix A. This would lead to the following expression for $G(k, 0)$:

$$G(k, 0) = \gamma_0^{(\mathrm{KE})} \frac{k^2}{k_F{}^2} - k \int_0^\infty dr \left[g(r) - 1 + \frac{1}{2} \rho \frac{\partial g(r)}{\partial \rho} \right] j_1(kr)$$

$$= \gamma_0^{(\mathrm{KE})} \frac{k^2}{k_F{}^2} - \frac{1}{2\rho} \int \frac{d^3q}{(2\pi)^3} \frac{\mathbf{k}\cdot\mathbf{q}}{q^2} \left[S(\mathbf{k} - \mathbf{q}) - 1 + \rho \frac{\partial S(\mathbf{k} - \mathbf{q})}{\partial \rho} \right] \tag{58}$$

where $j_1(x)$ is the first-order spherical Bessel function. It is easily verified that for $k \to 0$, (58) is consistent with Eqs. (30)–(36). On the other hand, for large k, (58) predicts

$$\lim_{k \to \infty} G(k, 0) = \gamma_0^{(\mathrm{KE})} \frac{k^2}{k_F{}^2} + 1 - g(0) - \frac{1}{2} \rho \frac{\partial g(0)}{\partial \rho} \tag{59}$$

which should be compared with a similar expression for the large -k limit of $G(k, \infty)$ [Eq. (51)].

This brings us to the work of Kleinman[33] and Langreth.[34] Kleinman[33] has obtained a result for the static local field correction $G(k, 0)$ which also varies with k^2 for both small and large k, a result which was verified by Langreth.[34] An objection to the Kleinman–Langreth theories has been raised by Singwi *et al.*,[35,36] who pointed out that a k^2 behavior of $G(k, 0)$ for large k would lead to an unphysical result in that $g(r)$ would have a $1/r$ singularity at the origin. However, their objection is based on the assumption that $G(k, \omega)$ is independent of ω, and can therefore be only maintained for the static mean field approximations discussed in Appendix A.

5. A CALCULATION OF $G(k, \omega)$

In the first part of this section we follow to some extent the calculation of Toigo and Woodruff (TW),[15] who have used a method for decoupling the equation of motion for the density response function $\chi(k, t)$ which conserves the third frequency moment $M_3(k)$ [cf. Eqs. (40)–(43)] in addition to $M_1(k)$. A general method of moment conserving approximations was previously introduced by Tahir-Kehli and Jarret.[37] At a key point in the calculation we employ a simple "trick" which leads to simpler formulas and show that a term neglected by Toigo and Woodruff because of the complexity of the formulas involved in fact leads to no additional contribution. The results we obtain will be seen to be simpler than those obtained by the latter authors, who restricted calculations to the static limit $\omega = 0$.

We work with the particle–hole operator $\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t)$ defined by[6]

$$\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t) = a_{\mathbf{q}\sigma}^+(t) a_{\mathbf{q}+\mathbf{k}\sigma}(t) \tag{60}$$

For $\mathbf{k} = 0$ this is the operator for the number of particles with momentum $\hbar\mathbf{q}$ and spin orientation σ. The density fluctuation operator $\rho(\mathbf{k}, t)$ [(2b)] is

$$\rho(\mathbf{k}, t) = \sum_{\mathbf{q}\sigma} \hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t) \tag{61}$$

The particle–hole operator obeys the exact equation of motion[6]

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t) &= [\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t), H] \\ &= \hbar\omega_0(\mathbf{q}, \mathbf{k})\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t) \\ &\quad + \frac{1}{\Omega}\sum_{\mathbf{q}'} v(q')[a^+_{\mathbf{q}\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}-\mathbf{q}'\sigma} - a^+_{\mathbf{q}+\mathbf{q}'\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}\sigma}] \end{aligned} \tag{62}$$

where

$$\omega_0(\mathbf{q}, \mathbf{k}) = \omega_0(\mathbf{q} + \mathbf{k}) - \omega_0(q) = (\hbar\mathbf{q}\cdot\mathbf{k}/m) + \omega_0(\mathbf{k})$$

is the excitation frequency for a free particle–hole pair. For brevity we have not indicated the time argument in some of the operators above; we shall often omit writing (t) after long expressions involving operators when the time argument is clear from the context. By summing both sides of (62) over $\mathbf{q}\sigma$ we obtain the continuity equation for particle conservation,

$$\partial\rho(\mathbf{k}, t)/\partial t = -i\mathbf{k}\cdot\mathbf{j}(\mathbf{k}, t) \tag{63}$$

where

$$\mathbf{j}(\mathbf{k}, t) = (\hbar/m)\sum_{\mathbf{q}\sigma} (\mathbf{q} + \tfrac{1}{2}\mathbf{k})\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t) \tag{64}$$

is the current density fluctuation operator.

Multiplying Eq. (62) by $\mathbf{k}\cdot(\mathbf{q} + \mathbf{k}/2)/m$ and summing over $\mathbf{q}\sigma$, we obtain the equation

$$\begin{aligned} i\frac{\partial}{\partial t}\mathbf{k}\cdot\mathbf{j}(\mathbf{k}, t) &= \frac{1}{\hbar}[\mathbf{k}\cdot\mathbf{j}(\mathbf{k}, t), H] \\ &= \sum_{\mathbf{q}\sigma}\left[\frac{\hbar\mathbf{k}\cdot(\mathbf{q} + \frac{1}{2}\mathbf{k})}{m}\right]^2 \hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t) \\ &\quad + \frac{1}{\Omega}\sum_{\mathbf{q}\mathbf{q}'\sigma} v(q')\frac{\mathbf{k}\cdot\mathbf{q}}{m}[a^+_{\mathbf{q}\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}-\mathbf{q}'\sigma} - a^+_{\mathbf{q}+\mathbf{q}'\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}\sigma}] \end{aligned} \tag{65}$$

which expresses the continuity equation for the longitudinal current fluctuation $\hat{\mathbf{k}}\cdot\mathbf{j}(\mathbf{k}, t)$. This is the equation which goes into the derivation of the third-moment sum rule $M_3(k)$, as seen by using Eq. (38b) with $n = 3$, $m = 1$. In obtaining the above equation we have used the fact that the sum over $\mathbf{q}$

of the operators in the last square bracket vanishes identically. Equation (65) will be used below.

Next we define the retarded response function

$$\tilde{\chi}_{\mathbf{q}\sigma}(\mathbf{k}, t) = i\,\theta(t)(1/\hbar)\langle[\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t), \rho(-\mathbf{k}, 0)]\rangle \tag{66}$$

in terms of which the density–density response function $\tilde{\chi}(k, t)$ defined by (3) and (6) is given by

$$\tilde{\chi}(k, t) = (1/\Omega) \sum_{\mathbf{q}\sigma} \tilde{\chi}_{\mathbf{q}\sigma}(\mathbf{k}, t) \tag{67}$$

From Eq. (62) we obtain the following equation for $\tilde{\chi}_{\mathbf{q}\sigma}(\mathbf{k}, t)$:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \tilde{\chi}_{\mathbf{q}\sigma}(\mathbf{k}, t) &= -\delta(t)\langle[\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, 0), \rho(-\mathbf{k}, 0)]\rangle \\ &\quad + \hbar\omega_0(\mathbf{q}, \mathbf{k})\tilde{\chi}_{\mathbf{q}\sigma}(\mathbf{k}, t) + i\,\theta(t)\frac{1}{\hbar\Omega}\sum_{\mathbf{q}'} v(q') \\ &\quad \times \langle[a^+_{\mathbf{q}\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}-\mathbf{q}'\sigma}(t) - a^+_{\mathbf{q}+\mathbf{q}'\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}\sigma}(t), \rho(-\mathbf{k}, 0)]\rangle \end{aligned} \tag{68}$$

Now, the first term on the right of (68) involves an equal time commutator,

$$[a^+_{\mathbf{q}\sigma}a_{\mathbf{q}+\mathbf{k}\sigma}, \rho(-\mathbf{k})] = \hat{n}_{\mathbf{q}\sigma} - \hat{n}_{\mathbf{q}+\mathbf{k}\sigma} \tag{69}$$

where $\hat{n}_{\mathbf{q}\sigma} = a^+_{\mathbf{q}\sigma}a_{\mathbf{q}\sigma}$. Hence the exact equation of motion (68) can be written

$$\begin{aligned} \left[i\hbar\frac{\partial}{\partial t} - \hbar\omega_0(\mathbf{q}, \mathbf{k})\right]&\tilde{\chi}_{\mathbf{q}\sigma}(\mathbf{k}, t) \\ &= \delta(t)[n_\sigma(\mathbf{q} + \mathbf{k}) - n_\sigma(q)] \\ &\quad + \frac{1}{\Omega}\sum_{\mathbf{q}'} v(q')\tilde{\chi}^{(3)}_{\mathbf{q}\sigma}(\mathbf{q}', \mathbf{k}, t) \end{aligned} \tag{70}$$

where $n_\sigma(q) = \langle\hat{n}_{\mathbf{q}\sigma}\rangle$ is the average number of particles of momentum $\hbar\mathbf{q}$ and spin σ, and $\tilde{\chi}^{(3)}_{\mathbf{q}\sigma}(\mathbf{q}', \mathbf{k}, t)$ is a three particle–hole response function defined as

$$\tilde{\chi}^{(3)}_{\mathbf{q}\sigma}(\mathbf{q}', \mathbf{k}, t - t') = 2i\,\theta(t - t')\tilde{\chi}^{(3)''}_{\mathbf{q}\sigma}(\mathbf{q}', \mathbf{k}, t - t') \tag{71a}$$

$$\begin{aligned} \tilde{\chi}^{(3)''}_{\mathbf{q}\sigma}(\mathbf{q}', \mathbf{k}, t - t') = \frac{1}{2\hbar}&\langle[a^+_{\mathbf{q}\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}-\mathbf{q}\sigma}(t) \\ &- a^+_{\mathbf{q}+\mathbf{q}'\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}\sigma}(t), \rho(-\mathbf{k}, t')]\rangle \end{aligned} \tag{71b}$$

Taking the Fourier transform of (70) with respect to time, we have

$$\begin{aligned} \hbar[\omega - \omega_0(\mathbf{q}, \mathbf{k}) + i\epsilon]\chi_{\mathbf{q}\sigma}(\mathbf{k}, \omega) &= n_\sigma(\mathbf{q} + \mathbf{k}) - n_\sigma(q) \\ &\quad + \frac{1}{\Omega}\sum_{\mathbf{q}'} v(q')\chi^{(3)}_{\mathbf{q}\sigma}(\mathbf{q}', \mathbf{k}, \omega) \end{aligned} \tag{72}$$

where the positive infinitesimal ϵ is to serve as a reminder that we are dealing with retarded response functions.

At this point we use the decoupling procedure of TW,[15] which is equivalent to making the following operator ansatz:

$$\sum_{\mathbf{q}'} v(q')[a^+_{\mathbf{q}\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}-\mathbf{q}'\sigma} - a^+_{\mathbf{q}+\mathbf{q}'\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}\sigma}] = A_{\mathbf{q}\sigma}(\mathbf{k})\rho(\mathbf{k}) \tag{73}$$

where $A_{\mathbf{q}\sigma}(\mathbf{k})$ is a c-number function to be determined below. The above implies the following decoupling approximation for the corresponding response functions:

$$(1/\Omega)\sum_{\mathbf{q}'} v(q')\tilde{\chi}^{(3)}_{\mathbf{q}\sigma}(\mathbf{q}', \mathbf{k}, t) = A_{\mathbf{q}\sigma}(\mathbf{k})\tilde{\chi}(k, t) \tag{74}$$

where we have used the definitions (6) and (71). Inserting the Fourier transform of (74) into the last term on the right of (72), we obtain

$$\chi_{\mathbf{q}\sigma}(\mathbf{k}, \omega) = \frac{n_\sigma(\mathbf{q}+\mathbf{k}) - n_\sigma(q)}{\hbar[\omega - \omega_0(\mathbf{q}, \mathbf{k}) + i\epsilon)} + \frac{A_{\mathbf{q}\sigma}(\mathbf{k})\chi(k, \omega)}{\hbar[\omega - \omega_0(\mathbf{q}, \mathbf{k}) + i\epsilon]} \tag{75}$$

Using (67), we then obtain

$$\chi(k, \omega) = X_0(k, \omega) + \chi(k, \omega)\frac{1}{\hbar\Omega}\sum_{\mathbf{q}\sigma}\frac{A_{\mathbf{q}\sigma}(\mathbf{k})}{\omega - \omega_0(\mathbf{q}, \mathbf{k}) + i\epsilon} \tag{76a}$$

or

$$\chi(k, \omega) = X_0(k, \omega)\left[1 - \frac{1}{\hbar\Omega}\sum_{\mathbf{q}\sigma}\frac{A_{\mathbf{q}\sigma}(\mathbf{k})}{\omega - \omega_0(\mathbf{q}, \mathbf{k}) + i\epsilon}\right]^{-1} \tag{76b}$$

where

$$X_0(k, \omega) = \frac{1}{\hbar\Omega}\sum_{\mathbf{q}\sigma}\frac{n_\sigma(\mathbf{q}+\mathbf{k}) - n_\sigma(q)}{\omega - \omega_0(\mathbf{q}, \mathbf{k}) + i\epsilon} \tag{77}$$

is of the form of a free-particle-type density–density response function corresponding to the true momentum distribution function $n_\sigma(q)$. In order to perform calculations and obtain explicit formulas, we shall eventually replace $n_\sigma(q)$ by the Fermi distribution $n^{(0)}_\sigma(q)$, so that $X_0(k, \omega)$ will then describe the free-electron polarizability $\chi_0(k, \omega)$. However, for the moment we continue to use $n_\sigma(q)$ in the formulas. Comparison of (76b) with the general expression

$$\chi(k, \omega) = \frac{\chi_0(k, \omega)}{1 + [v(k) + \phi(k, \omega)]\chi_0(k, \omega)} \tag{78}$$

will then yield an approximation for the local field correction $\phi(k, \omega) = -v(k)G(k, \omega)$.

The function $A_{\mathbf{q}\sigma}(k)$ is to be chosen so that

$$\frac{1}{\Omega}\sum_{\mathbf{q}'} v(q')\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega\chi_{\mathbf{q}\sigma}^{(3)''}(\mathbf{q}', \mathbf{k}, \omega) = A_{\mathbf{q}\sigma}(\mathbf{k})\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega\chi''(k, \omega) \quad (79a)$$

where $\chi_{\mathbf{q}}^{(3)''}(\mathbf{q}', \mathbf{k}, \omega)$ is the Fourier transform of the function defined in (71b). The above condition determining $A_{\mathbf{q}\sigma}(\mathbf{k})$ can be rewritten as

$$\frac{1}{\Omega}\sum_{\mathbf{q}'} v(q')\left(-i\frac{\partial}{\partial t'}\right)\tilde{\chi}_{\mathbf{q}\sigma}^{(3)''}(\mathbf{q}', \mathbf{k}, t - t')\bigg|_{t=t'} = A_{\mathbf{q}\sigma}(\mathbf{k})\left(-i\frac{\partial}{\partial t'}\right)\tilde{\chi}''(k, t - t')\bigg|_{t=t'} \quad (79b)$$

or, using the definitions (3) and (71) as well as the continuity equation (63),

$$\frac{1}{\Omega}\sum_{\mathbf{q}'} v(q')\frac{1}{2\hbar}\langle[a_{\mathbf{q}\sigma}^{+}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}-\mathbf{q}'\sigma} - a_{\mathbf{q}+\mathbf{q}'\sigma}^{+}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}\sigma}, \mathbf{k}\cdot\mathbf{j}(-\mathbf{k})]\rangle$$

$$= A_{\mathbf{q}\sigma}(\mathbf{k})\frac{1}{2\hbar\Omega}\langle[\rho(\mathbf{k}), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k})]\rangle = A_{\mathbf{q}\sigma}(\mathbf{k})\frac{\rho k^2}{2m} \quad (79c)$$

In the above equation the time argument of all the operators is the same, so that we have equal time commutators on both sides which can be evaluated. It is in choosing to differentiate both sides of (79b) with respect to t' rather than t which is the "trick" we have alluded to above. For, by differentiating with respect to t in (79b) as did TW, the commutator on the left side of (79c) would be replaced by a much more complicated commutator involving four a^+ and four a operators, rather than the three a^+ and a operators occurring on the left of (79c). This prompted TW to neglect the interaction Hamiltonian in working out the commutators, due to the complexity involved. However, because the local conservation law for the particle number, Eq. (63), is independent of the interaction between the particles, the interaction term neglected by TW[15] leads in fact to no additional contribution.

Before evaluating $A_{\mathbf{q}\sigma}(\mathbf{k})$ explicitly we now show that the TW decoupling (73), together with the condition (79) on $A_{\mathbf{q}\sigma}(\mathbf{k})$, conserves the third-moment sum rule for $\chi''(k, \omega)$, i.e., $M_3(k)$. Inserting the decoupling (73) into (65), the continuity equation for the longitudinal momentum operator is approximated by

$$i\frac{\partial}{\partial t}\mathbf{k}\cdot\mathbf{j}(\mathbf{k}, t) \simeq \sum_{\mathbf{q}\sigma}\left[\frac{\hbar\mathbf{k}\cdot(\mathbf{q} + \frac{1}{2}\mathbf{k})}{m}\right]^2\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t)$$

$$+ \frac{1}{\Omega}\sum_{\mathbf{q}\sigma}\frac{\mathbf{k}\cdot\mathbf{q}}{m}A_{\mathbf{q}\sigma}(\mathbf{k})\rho(\mathbf{k}, t) \quad (80)$$

Hence the commutator with $\mathbf{k}\cdot\mathbf{j}(-\mathbf{k}, t)$ gives

$$\frac{1}{\hbar\Omega}\left\langle\left[i\frac{\partial}{\partial t}\mathbf{k}\cdot\mathbf{j}(\mathbf{k}, t), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k}, t)\right]\right\rangle$$
$$= \frac{1}{\hbar\Omega}\left\{\sum_{\mathbf{q}\sigma}\left[\frac{\hbar\mathbf{k}\cdot(\mathbf{q}+\frac{1}{2}\mathbf{k})}{m}\right]^2\langle[\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k}, t)]\rangle\right.$$
$$\left. + \frac{1}{\Omega}\sum_{\mathbf{q}\sigma}\frac{\mathbf{k}\cdot\mathbf{q}}{m}A_{\mathbf{q}\sigma}(\mathbf{k})\langle[\rho(\mathbf{k}, t), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k}, t)]\rangle\right\} \tag{81a}$$

However, because of (79c) the right side can be rewritten as

$$\frac{1}{\hbar\Omega}\left\{\sum_{\mathbf{q}\sigma}\left[\frac{\hbar\mathbf{k}\cdot(\mathbf{q}+\frac{1}{2}\mathbf{k})}{m}\right]^2\langle[\hat{n}_\sigma(\mathbf{q}, \mathbf{k}, t), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k}, t)]\rangle\right.$$
$$+ \frac{1}{\Omega}\sum_{\mathbf{q}\mathbf{q}'\sigma} v(q')\frac{\mathbf{k}\cdot\mathbf{q}}{m}$$
$$\left.\times\langle[a^+_{\mathbf{q}\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}-\mathbf{q}'\sigma} - a^+_{\mathbf{q}+\mathbf{q}'\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}\sigma}, \mathbf{k}\cdot\mathbf{j}(-\mathbf{k})]\rangle\right\} \tag{81b}$$

which is in fact the exact expression for $M_3(k)$ obtained from (38b) and (65).

The calculation of $A_{\mathbf{q}\sigma}(\mathbf{k})$ amounts to calculating the equal time commutators

$$[\hat{A}(\mathbf{q}), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k})] - [\hat{A}(\mathbf{q}+\mathbf{q}'), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k})] \tag{82}$$

where $\hat{A}(\mathbf{q})$ is the operator [cf. Eq. (79c)]

$$\hat{A}(\mathbf{q}) = a^+_{\mathbf{q}\sigma}\rho(\mathbf{q}')a_{\mathbf{q}+\mathbf{k}-\mathbf{q}'\sigma} \tag{83}$$

Using (64), we have

$$[\hat{A}(\mathbf{q}), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k})] = \sum_{\mathbf{q}_1\sigma_1}\frac{\hbar\mathbf{k}\cdot\mathbf{q}_1}{m}[\hat{A}(\mathbf{q}), a^+_{\mathbf{q}_1\sigma_1}a_{\mathbf{q}_1-\mathbf{k}\sigma_1}] - \omega_0(k)[\hat{A}(\mathbf{q}), \rho(-\mathbf{k})] \tag{84}$$

The above commutators can be worked out and lead to the result

$$\langle[\hat{A}(\mathbf{q}) - \hat{A}(\mathbf{q}+\mathbf{q}'), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k})]\rangle$$
$$= \left[\omega_0(k) + \frac{\hbar\mathbf{k}\cdot\mathbf{q}}{m}\right][n_\sigma(q) - n_\sigma(\mathbf{q}+\mathbf{k}) + n_\sigma(\mathbf{q}+\mathbf{k}-\mathbf{q}') - n_\sigma(\mathbf{q}-\mathbf{q}')]$$
$$- \frac{\hbar\mathbf{k}\cdot\mathbf{q}'}{m}[n_\sigma(\mathbf{q}+\mathbf{k}-\mathbf{q}') - n_\sigma(\mathbf{q}-\mathbf{q}')]$$
$$+ \left[\omega_0(k) + \frac{\hbar\mathbf{k}\cdot\mathbf{q}}{m}\right]\{\langle\rho(\mathbf{q}')(a^+_{\mathbf{q}\sigma}a_{\mathbf{q}-\mathbf{q}'\sigma} - a^+_{\mathbf{q}+\mathbf{q}'\sigma}a_{\mathbf{q}\sigma})\rangle$$
$$+ \langle\rho(\mathbf{q}')(a^+_{\mathbf{q}+\mathbf{k}+\mathbf{q}'\sigma}a_{\mathbf{q}+\mathbf{k}\sigma} - a^+_{\mathbf{q}+\mathbf{k}\sigma}a_{\mathbf{q}+\mathbf{k}-\mathbf{q}'\sigma})\rangle\}$$
$$+ \frac{\hbar\mathbf{k}\cdot\mathbf{q}'}{m}\{\langle\rho(\mathbf{q}'-\mathbf{k})(a^+_{\mathbf{q}\sigma}a_{\mathbf{q}+\mathbf{k}-\mathbf{q}'\sigma} - a^+_{\mathbf{q}+\mathbf{q}'\sigma}a_{\mathbf{q}+\mathbf{k}\sigma})\rangle$$
$$- \langle\rho(\mathbf{q}')(a^+_{\mathbf{q}\sigma}a_{\mathbf{q}-\mathbf{q}'\sigma} - a^+_{\mathbf{q}+\mathbf{k}+\mathbf{q}'\sigma}a_{\mathbf{q}+\mathbf{k}\sigma})\rangle\} \tag{85}$$

In terms of the above quantities, the expression for $A_{\mathbf{q}\sigma}(\mathbf{k})$, (79c), becomes

$$A_{\mathbf{q}\sigma}(k)\frac{\rho k^2}{m} = \frac{1}{\hbar\Omega}\sum_{\mathbf{q}'} v(q')\langle[\hat{A}(\mathbf{q}) - \hat{A}(\mathbf{q}+\mathbf{q}'), \mathbf{k}\cdot\mathbf{j}(-\mathbf{k})]\rangle \tag{86}$$

At this point, because of the unknown two-particle density matrices of the type $\langle\rho(\mathbf{q}')a^+_{\mathbf{q}\sigma}a_{\mathbf{q}-\mathbf{q}'\sigma}\rangle$, etc., occurring on the right-hand side of (85) it is necessary to introduce an additional approximation. In order to carry the calculation further we therefore resort to the usual Hartree–Fock factorization of the type

$$\langle a_1{}^+a_2{}^+a_3a_4\rangle = \langle a_1{}^+a_4\rangle\langle a_2{}^+a_3\rangle - \langle a_1{}^+a_3\rangle\langle a_2{}^+a_4\rangle \tag{87a}$$

Thus one has, for example,

$$\langle\rho(\mathbf{q}')a^+_{\mathbf{q}\sigma}a_{\mathbf{q}-\mathbf{q}'\sigma}\rangle = \langle N\rangle\,\delta_{\mathbf{q}',0}n_\sigma(q) + n_\sigma(\mathbf{q}-\mathbf{q}')[1 - n_\sigma(q)] \tag{87b}$$

When this factorization is employed in the terms on the right-hand side of (85) there occurs a huge cancellation of terms, with the result

$$\begin{aligned} A_{\mathbf{q}\sigma}(\mathbf{k})\frac{\rho k^2}{m} = &-\frac{\rho k^2}{m}v(k)[n_\sigma(\mathbf{q}+\mathbf{k}) - n_\sigma(q)] \\ &+ [n_\sigma(\mathbf{q}+\mathbf{k}) - n_\sigma(q)] \\ &\times \frac{1}{\Omega}\sum_{\mathbf{q}'} v(q')\frac{\mathbf{k}\cdot\mathbf{q}'}{m}[n_\sigma(\mathbf{q}+\mathbf{q}') - n_\sigma(\mathbf{q}+\mathbf{k}+\mathbf{q}')] \end{aligned} \tag{88}$$

The first term on the right is precisely the RPA term, which when substituted into (76) leads immediately to the RPA expression for $\chi(k, \omega)$. The result (88) is much simpler than that of TW.[15] Thus far the above expression for $A_{\mathbf{q}\sigma}(\mathbf{k})$ applies to all potentials with a Fourier transform $v(k)$. For the Coulomb potential we can write the result (88) as

$$A_{\mathbf{q}\sigma}(\mathbf{k}) = -v(k)[n_\sigma(\mathbf{q}+\mathbf{k}) - n_\sigma(q)][1 - \tilde{f}(\mathbf{q}, \mathbf{k})] \tag{89}$$

where the dimensionless quantity $\tilde{f}(\mathbf{q}, \mathbf{k})$ is given by

$$\tilde{f}(\mathbf{q}, \mathbf{k}) = \frac{1}{\rho\Omega}\sum_{\mathbf{q}'\neq 0}\frac{\mathbf{k}\cdot\mathbf{q}'}{q'^2}[n_\sigma(\mathbf{q}+\mathbf{q}') - n_\sigma(\mathbf{q}+\mathbf{k}+\mathbf{q}')] \tag{90}$$

Substituting (89) into the expression occurring in (76b) and replacing $n_\sigma(q)$ by the Fermi distribution $n_\sigma^{(0)}(q)$, one identifies

$$\frac{1}{\hbar\Omega}\sum_{\mathbf{q}\sigma}\frac{A_{\mathbf{q}\sigma}(\mathbf{k})}{\omega - \omega_0(\mathbf{q}, \mathbf{k}) + i\epsilon} \equiv -v(k)\chi_0(k, \omega)[1 - G(k, \omega)] \tag{91}$$

where

$$G(k, \omega) = \frac{P(k, \omega)}{\chi_0(k, \omega)} \tag{92}$$

$$P(k, \omega) = \frac{1}{\hbar\Omega} \sum_{\mathbf{q}\sigma} \frac{n_\sigma^{(0)}(\mathbf{q} + \mathbf{k}) - n_\sigma^{(0)}(q)}{\omega - \omega_0(\mathbf{qk}) + i\epsilon} \tilde{f}(\mathbf{q}, \mathbf{k})$$
$$= \frac{1}{\hbar\Omega} \sum_{\mathbf{q}\sigma} \frac{n_\sigma^{(0)}(\mathbf{q} + \frac{1}{2}\mathbf{k}) - n_\sigma^{(0)}(\mathbf{q} - \frac{1}{2}\mathbf{k})}{\omega - (\hbar\mathbf{k}\cdot\mathbf{q}/m) + i\epsilon} f(\mathbf{q}, \mathbf{k}) \tag{93}$$

$$f(\mathbf{q}, \mathbf{k}) \equiv \tilde{f}^{(0)}(\mathbf{q} - \tfrac{1}{2}\mathbf{k}, \mathbf{k})$$
$$= \frac{1}{\rho\Omega} \sum_{\mathbf{q}'\neq 0} \frac{\mathbf{k}\cdot\mathbf{q}'}{q'^2} \left[n_\sigma^{(0)}\left(\mathbf{q} - \frac{\mathbf{k}}{2} + \mathbf{q}'\right) - n_\sigma^{(0)}\left(\mathbf{q} + \frac{\mathbf{k}}{2} + \mathbf{q}'\right)\right] \tag{94}$$

It is useful to note that $f(\mathbf{q}, \mathbf{k}) = f(\mathbf{q}, -\mathbf{k}) = f(-\mathbf{q}, \mathbf{k}) = f(-\mathbf{q}, -\mathbf{k})$. We note that $P(k, \omega)$ is analytic in the upper half ω plane, as is also $\chi_0^{-1}(k, \omega)$; hence the local field correction $G(k, \omega)$ as given by (92)–(94) is also analytic there, in agreement with the general analytic properties of the function $\phi(k, z)$ discussed in Section 3.

From (92) we obtain for the real and imaginary parts of $G(k, \omega)$

$$G'(k, \omega) = \frac{P'\chi_0' + P''\chi_0''}{|\chi_0(k, \omega)|^2}, \qquad G''(k, \omega) = \frac{P''\chi_0' - P'\chi_0''}{|\chi_0(k, \omega)|^2} \tag{95}$$

where

$$P''(k, \omega) = -\frac{\pi}{\hbar\Omega} \sum_{\mathbf{q}\sigma} \left[n_\sigma^{(0)}\left(\mathbf{q} + \frac{\mathbf{k}}{2}\right) - n_\sigma^{(0)}\left(\mathbf{q} - \frac{\mathbf{k}}{2}\right)\right] f(\mathbf{q}, \mathbf{k})\, \delta\left[\omega - \frac{\hbar\mathbf{q}\cdot\mathbf{k}}{m}\right] \tag{96}$$

$$P'(k, \omega) = P\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{P''(k, \omega')}{\omega' - \omega} \tag{97}$$

The expressions for $\chi_0''(k, \omega)$ and $\chi_0'(k, \omega)$ are the same as those for $P''(k, \omega)$ and $P'(k, \omega)$ with $f(\mathbf{q}, \mathbf{k})$ replaced by unity. Both $P''(k, \omega)$ and $\chi_0''(k, \omega)$ are odd functions of ω, while $P'(k, \omega)$ and $\chi_0'(k, \omega)$ are even functions of ω.

Before embarking on an explicit calculation of $P''(k, \omega)$ and $P'(k, \omega)$ it is useful to define the frequency moments of $P''(k, \omega)$:

$$P_n(k) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^n P''(k, \omega)$$
$$= -\frac{1}{\hbar\Omega} \sum_{\mathbf{q}\sigma} \left[n_\sigma^{(0)}\left(\mathbf{q} + \frac{\mathbf{k}}{2}\right) - n_\sigma^{(0)}\left(\mathbf{q} - \frac{\mathbf{k}}{2}\right)\right] f(\mathbf{q}, \mathbf{k}) \left(\frac{\hbar\mathbf{q}\cdot\mathbf{k}}{m}\right)^n \tag{98}$$

Only the odd n moments survive. In terms of $P_n(k)$ one obtains for the asymptotic expansions for large ω of $P(k, \omega)$ and $G(k, \omega)$:

$$P(k, \omega) \sim -\frac{1}{\omega^2}\left[P_1(k) + \frac{P_3(k)}{\omega^2} + \cdots\right] \tag{99}$$

$$G(k, \omega) \sim \frac{P_1(k)}{M_1^{(0)}(k)}\left[1 + \frac{(P_3/P_1) - (M_3^{(0)}/M_1^{(0)})}{\omega^2} + \cdots\right] \tag{100}$$

where the moments $M_n^{(0)}(\mathrm{k})$ are given by the expressions (38)–(40) with $v(r) = 0$, or alternatively by (98) with $f(\mathbf{q}, \mathbf{k})$ replaced by unity. The first term on the right of (100) represents the quantity $G(k, \infty)$ within the approximation under consideration, i.e.,

$$G(k, \infty) = \frac{P_1(k)}{M_1^{(0)}(k)} = \frac{m}{\rho k^2} P_1(k) \tag{101}$$

the exact expression being given by (48). Let us also note the expression for the static limit $\omega = 0$ of $G(k, \omega)$:

$$G(k, 0) = \frac{P(k, 0)}{\chi_0(k, 0)} = \frac{P'(k, 0)}{\chi_0(k)} = \frac{P_{-1}(k)}{\chi_0(k)} \tag{102}$$

We shall come back to the relations (100)–(102) shortly.

One can obtain explicit expressions for the functions $f(\mathbf{q}, \mathbf{k})$ and $P''(k, \omega)$ at zero temperature. In this case $n_\sigma^{(0)}(q)$ is a step function; i.e., $n_\sigma^{(0)}(q) = 1$ for $q \leqslant k_{\mathrm{F}}$, zero otherwise. One obtains

$$f(\mathbf{q}, \mathbf{k}) = \frac{3}{16 k_{\mathrm{F}}^2}\left[\mathbf{k}\cdot\left(\mathbf{q} + \frac{\mathbf{k}}{2}\right) w\left(\mathbf{q} + \frac{\mathbf{k}}{2}\right) - \mathbf{k}\cdot\left(\mathbf{q} - \frac{\mathbf{k}}{2}\right) w\left(\mathbf{q} - \frac{\mathbf{k}}{2}\right)\right]$$

$$w(\mathbf{q}) = 1 + \frac{k_{\mathrm{F}}^2}{q^2} - \frac{q}{2k_{\mathrm{F}}}\left(1 - \frac{k_{\mathrm{F}}^2}{q^2}\right)^2 \ln\left|\frac{q + k_{\mathrm{F}}}{q - k_{\mathrm{F}}}\right|, \qquad q = |\mathbf{q}| \tag{103a}$$

It will be useful to note also the limiting form of the above expression for $k \to 0$. In this limit one has

$$f(\mathbf{q}, \mathbf{k} \to 0) = -\frac{1}{\rho}\int \frac{d^3q'}{(2\pi)^3}\frac{\mathbf{k}\cdot\mathbf{q}'}{q'^2}\,\mathbf{k}\cdot\nabla_{\mathbf{q}'} n_\sigma^{(0)}(\mathbf{q} + \mathbf{q}')$$

$$= \frac{3k^2}{16 k_{\mathrm{F}}^2}\left\{(\hat{\mathbf{k}}\cdot\hat{\mathbf{q}})^2\left[1 - \frac{3k_{\mathrm{F}}^2}{q^2} + \frac{k_{\mathrm{F}}}{q}\left(\frac{3k_{\mathrm{F}}^2}{2q^2} - \frac{q^2}{2k_{\mathrm{F}}^2} - 1\right)\ln\left|\frac{q + k_{\mathrm{F}}}{q - k_{\mathrm{F}}}\right|\right]\right.$$

$$\left. + 1 + \frac{k_{\mathrm{F}}^2}{q^2} + \frac{k_{\mathrm{F}}}{q}\left(1 - \frac{q^2}{2k_{\mathrm{F}}^2} - \frac{k_{\mathrm{F}}^2}{2q^2}\right)\ln\left|\frac{q + k_{\mathrm{F}}}{q - k_{\mathrm{F}}}\right|\right\} \tag{103b}$$

When (103a) is substituted into (96) one finds after a lengthy calculation (for details see Appendix C) the following expression for $P''(k, \omega)$: For $0 < k \leqslant 2k_{\mathrm{F}}$ and $0 \leqslant \omega \leqslant kv_{\mathrm{F}} - \omega_0(k)$

$$P''(k, \omega) = \frac{mk}{64\pi\hbar^2}\left\{2\frac{\omega}{\omega_{\mathrm{F}}} + \left(1 + \frac{\omega}{\omega_{\mathrm{F}}}\right)^{-1/2}\left(4 + 2\frac{\omega}{\omega_{\mathrm{F}}} - \frac{\omega^2}{2\omega_{\mathrm{F}}^2}\right)\right.$$

$$\times \ln\left|\frac{[1 + (\omega/\omega_{\mathrm{F}})]^{1/2} + 1}{[1 + (\omega/\omega_{\mathrm{F}})]^{1/2} - 1}\right|$$

$$- \left(1 - \frac{\omega}{\omega_F}\right)^{-1/2}\left(4 - 2\frac{\omega}{\omega_F} - \frac{\omega^2}{2\omega_F^2}\right) \ln\left|\frac{[1 - (\omega/\omega_F)]^{1/2} + 1}{[1 - (\omega/\omega_F)]^{1/2} - 1}\right|\Bigg\}$$

$$+ \frac{m^2\omega}{32\pi\hbar^3 k}\Bigg\{8 \ln\frac{\omega}{\omega_F} - 16 \ln 2$$

$$+ \left(1 + \frac{\omega}{\omega_F}\right)^{-1/2}\left(4 + 2\frac{\omega}{\omega_F} - \frac{\omega^2}{2\omega_F^2}\right) \ln\left|\frac{[1 + (\omega/\omega_F)]^{1/2} + 1}{[1 + (\omega/\omega_F)]^{1/2} - 1}\right|$$

$$+ \left(1 - \frac{\omega}{\omega_F}\right)^{-1/2}\left(4 - 2\frac{\omega}{\omega_F} - \frac{\omega^2}{2\omega_F^2}\right) \ln\left|\frac{[1 - (\omega/\omega_F)]^{1/2} + 1}{[1 - (\omega/\omega_F)]^{1/2} - 1}\right|\Bigg\} \tag{104a}$$

where $\omega_F = \omega_0(k_F) = \hbar k_F^2/2m$.

For all k and $|kv_F - \omega_0(k)| \leqslant \omega \leqslant kv_F + \omega_0(k)$,

$$P''(k, \omega)$$

$$= \frac{mk_F}{32\pi\hbar^2}\left(\frac{\omega}{kv_F} - \frac{k}{2k_F}\right)\left[\left(\frac{\omega}{kv_F} - \frac{k}{2k_F}\right)^2 - 1 + 4 \ln\left|\left(\frac{\omega}{kv_F} - \frac{k}{2k_F}\right)^2 - 1\right|\right]$$

$$- \frac{mk_F}{32\pi\hbar^2}\left(\frac{\omega}{kv_F} + \frac{k}{2k_F}\right)\left[\left(\frac{\omega}{kv_F} + \frac{k}{2k_F}\right)^2 - 1 + 4 \ln\left|\left(\frac{\omega}{kv_F} + \frac{k}{2k_F}\right)^2 - 1\right|\right]$$

$$+ \frac{mk_F}{32\pi\hbar^2}\Bigg\{\left(\frac{\omega}{kv_F} + \frac{k}{2k_F}\right)\left(\frac{\omega}{\omega_F} + 4 \ln\frac{\omega}{\omega_F}\right) - 8\left(\frac{\omega}{kv_F} - \frac{k}{2k_F}\right) \ln 2$$

$$+ \left(\frac{\omega}{kv_F} + \frac{k}{2k_F}\right)\left(1 + \frac{\omega}{\omega_F}\right)^{-1/2}\left(4 + 2\frac{\omega}{\omega_F} - \frac{\omega^2}{2\omega_F^2}\right)$$

$$\times \ln\left|\frac{[1 + (\omega/\omega_F)]^{1/2} + 1}{[1 + (\omega/\omega_F)]^{1/2} - 1}\right|$$

$$+ \frac{3}{2}\left[1 + 2\left(\frac{\omega}{kv_F} - \frac{k}{2k_F}\right)^2 - \frac{1}{3}\left(\frac{\omega}{kv_F} - \frac{k}{2k_F}\right)^4\right] \ln\left|\frac{\omega - \omega_0(k) + kv_F}{\omega - \omega_0(k) - kv_F}\right|$$

$$- \frac{3}{2}\left[1 + 2\left(\frac{\omega}{kv_F} + \frac{k}{2k_F}\right)^2 - \frac{1}{3}\left(\frac{\omega}{kv_F} + \frac{k}{2k_F}\right)^4\right] \ln\left|\frac{\omega + \omega_0(k) + kv_F}{\omega + \omega_0(k) - kv_F}\right|\Bigg\} \tag{104b}$$

$$\begin{aligned} P''(k, \omega) &= 0 \quad \text{for} \quad kv_F + \omega_0(k) \leqslant \omega \\ &= 0 \quad \text{for} \quad 0 \leqslant \omega \leqslant \omega_0(k) - kv_F, \\ & \qquad\qquad\; k \geqslant 2k_F \end{aligned} \tag{104c}$$

The function $P''(k, \omega)$ is shown in Figs. 1–3 as a function of ω for several values of k.

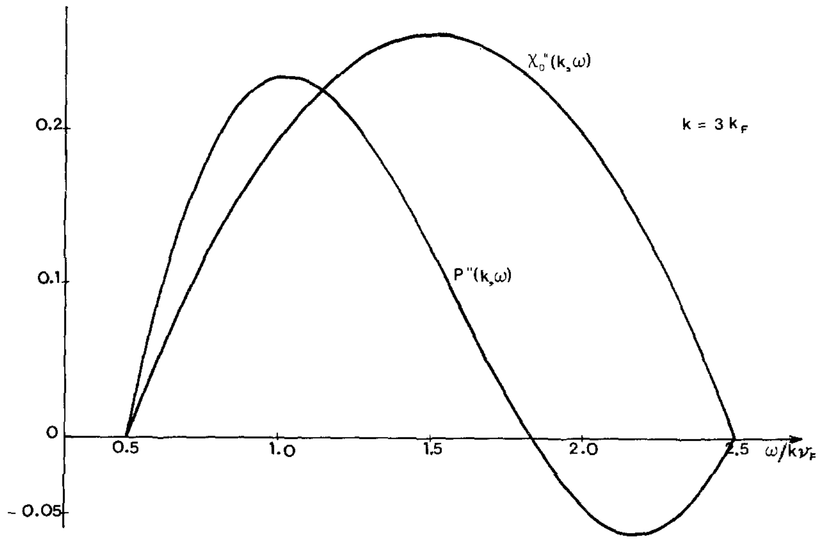

Fig. 1. The functions $P''(k, \omega)$ and $\chi_0''(k, \omega)$ vs. ω/kv_F for $k = 3k_F$. The vertical scale is in units of $mk_F/\pi^2\hbar^2$; the same is to be understood for Figs. 2 and 3.

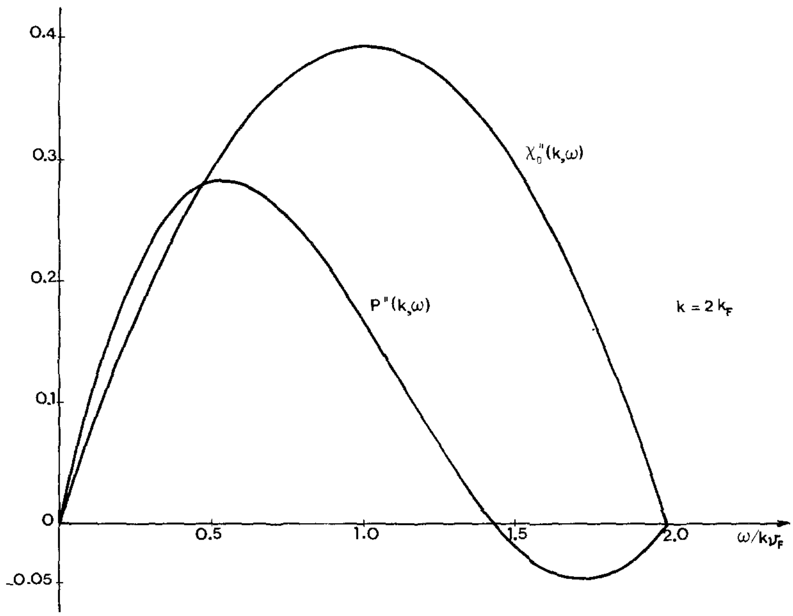

Fig. 2. $P''(k, \omega)$ and $\chi_0''(k, \omega)$ vs. ω/kv_F for $k = 2k_F$.

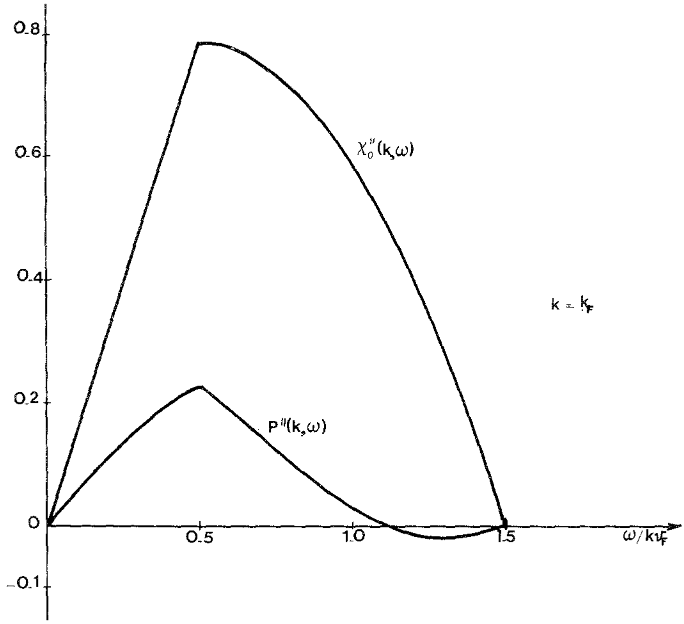

Fig. 3. $P''(k, \omega)$ and $\chi_0''(k, \omega)$ vs. ω/kv_F for $k = k_F$.

The expression for the real part $P'(k, \omega)$ for arbitrary k and given by (97) has not been determined. It will contain integrals of the type given in Appendix D, where the expression obtained for $\omega = 0$, i.e., for the quantity $P(k, 0) = P_{-1}(k)$, is given. However, we can obtain $P(k, \omega)$ explicitly in the limit $k \to 0$. First we observe that the expression for $P''(k, \omega)$ [Eq. (96)] in the limit $k \to 0$ becomes

$$P''(k, \omega) = -\frac{2\pi}{\hbar}\int \frac{d^3q}{(2\pi)^3}\,\mathbf{k}\cdot\nabla_q n_\sigma^{(0)}(q) f(\mathbf{q}, \mathbf{k})\,\delta\left[\omega - \frac{\hbar\mathbf{q}\cdot\mathbf{k}}{m}\right]$$

$$= \frac{2\pi}{\hbar k_F}\int \frac{d^3q}{(2\pi)^3}\,\delta(q - k_F)\mathbf{k}\cdot\mathbf{q} f(\mathbf{q}, \mathbf{k})\,\delta\left[\omega - \frac{\hbar\mathbf{q}\cdot\mathbf{k}}{m}\right] \qquad (105)$$

When the angular integration over the δ function is carried out and the form (103b) for $f(\mathbf{q}, \mathbf{k})$ is substituted one finds the simple result

$$P''(k, \omega) = \frac{3m^2\omega k}{16\pi\hbar^3 k_F^2}\left(1 - \frac{\omega^2}{k^2 v_F^2}\right), \qquad |\omega| \leqslant kv_F \qquad (106)$$

$$= 0, \qquad kv_F \leqslant |\omega|$$

which is also obtained from the expansion of (104a) for $k \ll 2k_F$. The complex quantity $P(k, \omega)$ defined by (93) in the limit $k \to 0$ is thus found to be given by

$$P(k, \omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{P''(k, \omega)}{\omega' - \omega - i\epsilon}$$

$$= \frac{mk^2}{4\pi^2\hbar^2 k_F} \left\{ 1 - \frac{3\omega^2}{2k^2 v_F^2} - \frac{3\omega}{4kv_F}\left(1 - \frac{\omega^2}{k^2 v_F^2}\right) \ln\left[\frac{\omega + kv_F + i\epsilon}{\omega - kv_F + i\epsilon}\right]\right\} \tag{107}$$

where the principal branch of the logarithm is to be understood. From this we obtain for the real part

$$P'(k, \omega) = \frac{mk^2}{4\pi^2\hbar^2 k_F} \left\{ 1 - \frac{3\omega^2}{2k^2 v_F^2} - \frac{3\omega}{4kv_F}\left(1 - \frac{\omega^2}{k^2 v_F^2}\right) \ln\left|\frac{\omega + kv_F}{\omega - kv_F}\right|\right\} \tag{108}$$

The functions (106) and (108) are shown in Fig. 4 as a function of ω for $k/k_F = 0.1$. Although the general expression for $P'(k, \omega)$ has not been obtained, the behavior of $P'(k, \omega)$ and $G'(k, \omega)$ for large ω and arbitrary k is given by the asymptotic expansions (99) and (100).

To facilitate comparison with the expressions (104)–(108), we shall recall here the corresponding expressions for the functions $\chi_0''(k, \omega)$ and $\chi_0'(k, \omega)$, which also enter into the expression (95) for the local field correction $G(k, \omega)$:

$$\chi_0''(k, \omega) = \frac{m^2\omega}{2\pi\hbar^3 k} \quad \text{for} \quad 0 < k \leqslant 2k_F, 0 \leqslant \omega \leqslant kv_F - \omega_0(k)$$

$$= \frac{mk_F^2}{4\pi\hbar^2 k}\left[1 - \left(\frac{\omega}{kv_F} - \frac{k}{2k_F}\right)^2\right],$$

$$|kv_F - \omega_0(k)| \leqslant \omega \leqslant kv_F + \omega_0(k)$$

$$= 0 \quad \text{for} \quad kv_F + \omega_0(k) \leqslant \omega$$

$$= 0 \quad \text{for} \quad 0 \leqslant \omega \leqslant \omega_0(k) - kv_F, \quad k \geqslant 2k_F \tag{109}$$

$$\chi_0'(k, \omega) = \frac{mk_F}{2\pi^2\hbar^2}\left\{1 + \frac{k_F}{2k}\left[1 - \left(\frac{\omega}{kv_F} + \frac{k}{2k_F}\right)^2\right] \ln\left|\frac{\omega + \omega_0(k) + kv_F}{\omega + \omega_0(k) - kv_F}\right|\right.$$
$$\left. - \frac{k_F}{2k}\left[1 - \left(\frac{\omega}{kv_F} - \frac{k}{2k_F}\right)^2\right] \ln\left|\frac{\omega - \omega_0(k) + kv_F}{\omega - \omega_0(k) - kv_F}\right|\right\} \tag{110}$$

For $\omega = 0$ one obtains from (110) the static susceptibility of the noninteracting gas ($\eta = k/k_F$):

$$\chi_0(k) \equiv \chi_0'(k, 0) = \frac{mk_F}{2\pi^2\hbar^2}\left[1 + \frac{1}{\eta}\left(1 - \frac{\eta^2}{4}\right) \ln\left|\frac{\eta + 2}{\eta - 2}\right|\right] \tag{111}$$

which enters into the expression (102) for the static limit of the local field correction. The functions (109) and (110) are shown in Fig. 5 for the value

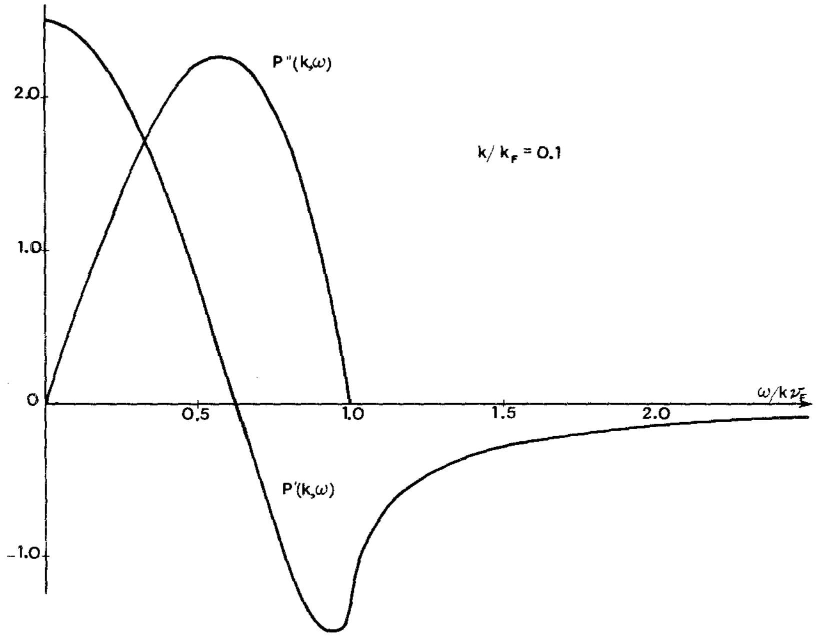

Fig. 4. The functions $P''(k, \omega)$ and $P'(k, \omega)$ defined by Eqs. (106) and (108) vs. ω/kv_F for $k = 0.1k_F$. The vertical scale is in units of $mk_F/\pi^2\hbar^2 \times 10^{-3}$.

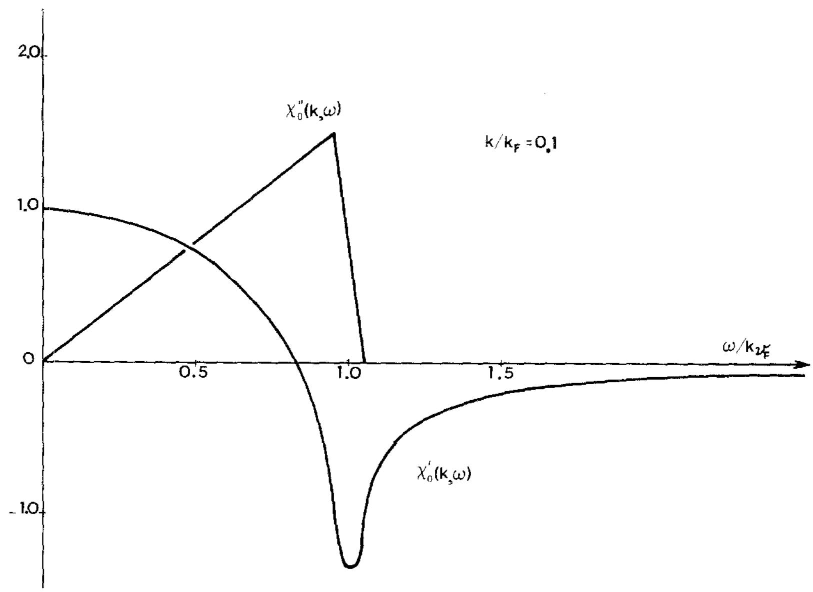

Fig. 5. The functions $\chi_0''(k, \omega)$ and $\chi_0'(k, \omega)$ vs. ω/kv_F for $k = 0.1k_F$. The vertical scale is in units of $mk_F/\pi^2\hbar^2$.

$k/k_F = 0.1$. When the expressions (106) and (108)–(110) are substituted in (95) one obtains explicitly the functions $G'(k, \omega)$ and $G''(k, \omega)$ for $k \ll 2k_F$; the latter are plotted in Fig. 6 as a function of ω for the value $k/k_F = 0.1$.

Having obtained an explicit expression, (104), for $P''(k, \omega)$, one can now calculate the moments $P_1(k)$ and $P_{-1}(k)$ which enter, respectively, the expressions for $G(k, \infty)$ [Eq. (101)] and $G(k, 0)$ [Eq. (102)]. The results are given in Appendix D and are plotted in Fig. 7. It is found that both $G(k, \infty)$ and its derivative with respect to k are continuous at $k = 2k_F$. $G(k, 0)$ is continuous at $k = 2k_F$ but its slope has a logarithmic singularity there. $G(k, 0)$ has a peak at a k value slightly less than $2k_F$ and tends for large k to the limit 2/3.[38] The limiting expressions for $G(k, \infty)$ and $G(k, 0)$ indicated in the figure follow from the expressions given in Appendix D. In particular, it is worthwhile to point out explicitly the values for small k:

$$\lim_{k\to 0} G(k, \infty) = (3/20)k^2/k_F^2 \equiv \gamma_\infty^{(HF)} k^2/k_F^2 \tag{112}$$

$$\lim_{k\to 0} G(k, 0) = \tfrac{1}{4}k^2/k_F^2 \equiv \gamma_0^{(HF)} k^2/k_F^2 \tag{113}$$

Hence the theory presented in this section leads to the value $\gamma_0 = \frac{1}{4}$ for the compressibility factor [cf. Eqs. (30) and (31)], which is the same as obtained

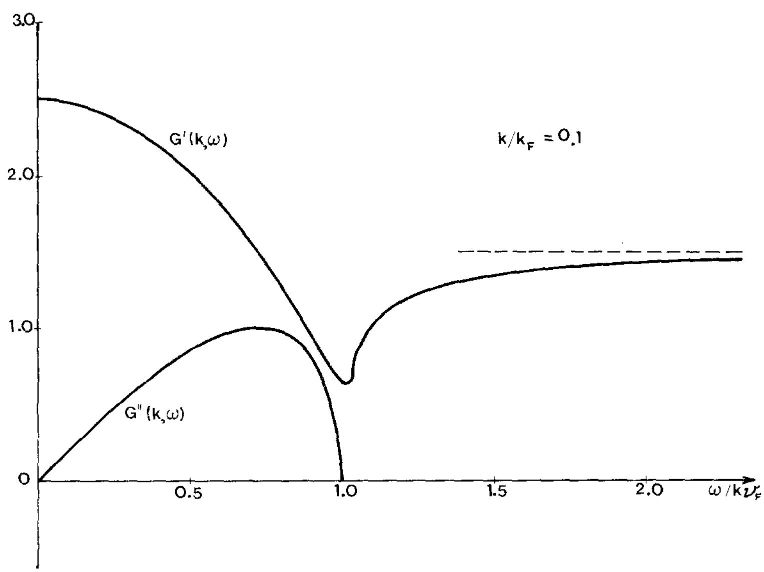

Fig. 6. The functions $G''(k, \omega)$ and $G'(k, \omega)$ vs. ω/kv_F for $k = 0.1k_F$. The vertical scale is in units of 10^{-3}.

from the ground state energy in HF approximation, as shown in Appendix B. The value $\gamma_0 = \frac{1}{4}$ has also been obtained by TW,[15] Hedin and Lundqvist,[7] and Vashishta and Singwi.[26]

At this point it must be pointed out that the above results for $G(k, \infty)$ and $G(k, 0)$ are not consistent for large k with the general properties discussed in Section 4 [Eqs. (51) and (59)]. This is due to the replacement of the momentum distribution $n_\sigma(q)$ by the unit step function, which results in $\langle \mathrm{KE} \rangle = \langle \mathrm{KE} \rangle_0 = 3\epsilon_F{}^0/5$. It represents a serious failure for all calculations which employ the Fermi distribution (corresponding to the use of free particle propagators) instead of the true momentum distribution (corresponding to the renormalized propagator or true one-particle Green's function).[21,39] A calculation of the momentum distribution of the electrons in a metal has recently been made by Overhauser.[40]

The quantity $G(k, \infty)$ enters directly into the dispersion relation for the plasma oscillations [cf. Eqs. (56a)–(56c)]. Thus the above theory predicts

$$\omega_p{}^2(k) = \omega_p{}^2[1 - G(k, \infty)] + \frac{3}{5} k^2 v_F{}^2 + \cdots$$

$$= \omega_p{}^2\left[1 - \frac{3}{20}\frac{k^2}{k_F{}^2} + \cdots\right] + \frac{3}{5} k^2 v_F{}^2 + \cdots \tag{114a}$$

or

$$\omega_p(k) = \omega_p\left[1 + \frac{9}{10}\frac{k^2}{k_{FT}^2} - \frac{3}{40}\frac{k^2}{k_F{}^2} + \cdots\right]$$

$$= \omega_p\left[1 + \left(\frac{9}{10} - \frac{1}{2}\gamma_\infty^{(\mathrm{HF})}\frac{4\alpha r_s}{\pi}\right)\frac{k^2}{k_{FT}^2} + \cdots\right] \tag{114b}$$

where r_s is the dimensionless parameter defined by $k_F = (9\pi/4)^{1/3}/r_s a_0 \equiv 1/\alpha r_s a_0$, a_0 being the Bohr radius. The last term in (114b) represents the correction to the RPA result. This correction has already been obtained by Nozières and Pines[41] (where it has been termed the extra exchange frequency shift of the plasmons), Kanazawa *et al.*,[42] and Pathak and Vashishta[43] (cf. also Appendix A).

Due to the approximations we have made in obtaining $G(k, \omega)$, it comes as no surprise that we find no damping of the long-wavelength plasma oscillations. For the determination of the "cutoff" wave number k_c where the plasmons are damped out one could employ the expression for $G'(k, \omega)$ given by (95), (106), and (108). The value obtained for k_c is smaller than the one found in RPA.

6. A FORMULA FOR THE GROUND STATE ENERGY

In this brief section we discuss a formula for the ground state energy corresponding to the approximations embodied by Eqs. (92)–(108). Since the local field correction $G(k, \omega)$ as given by Eqs. (92)–(94) is independent of the coupling strength e^2, we can employ the ground state energy theorem of Pines and Nozières.[6] By means of this theorem the Gell-Mann and Brueckner[44] expression for the ground state energy was shown to be equivalent to the result obtained in the RPA. A different looking but equivalent version of the ground state energy theorem was derived independently and applied by Hubbard[10] to the simple static local field correction given in the second row of Table I (Appendix A).

Following Pines and Nozières,[6] one has for the correlation energy per particle (cf. also Appendix B)

$$E_{\text{corr}}(\rho) = \frac{\hbar}{2\rho}\int \frac{d^3k}{(2\pi)^3}\int_0^{e^2} \frac{d\lambda}{\lambda}\, v_\lambda(k)\int_0^\infty \frac{d\omega}{\pi}\,[\chi''_\lambda(k, \omega) - \chi''_0(k, \omega)]$$

$$= \frac{\hbar}{2\rho}\int \frac{d^3k}{(2\pi)^3}\int_0^{e^2} \frac{d\lambda}{\lambda}\, v_\lambda(k)$$

$$\times \int_0^\infty \frac{d\omega}{\pi}\,\text{Im}\left[\frac{\chi_0(k, \omega)}{1 + v_\lambda(k)[1 - G(k, \omega)]\chi_0(k, \omega)} - \chi_0(k, \omega)\right] \tag{115}$$

where $v_\lambda(k) = 4\pi\lambda/k^2$. Employing the steps outlined by Pines,[4] this can be rewritten as

$$E_{\text{corr}}(\rho) = \frac{\hbar}{4\rho}\int \frac{d^3k}{(2\pi)^3}\int_0^{e^2} \frac{d\lambda}{\lambda}\, v_\lambda(k)$$

$$\times \int_{-\infty}^\infty \frac{dw}{\pi}\left[\frac{\chi_0(k, iw)}{1 + v_\lambda(k)[1 - G(k, iw)]\chi_0(k, iw)} - \chi_0(k, iw)\right] \tag{116}$$

The integration over the coupling parameter then yields the expression

$$E_{\text{corr}}(\rho) = \frac{\hbar}{4\rho}\int \frac{d^3k}{(2\pi)^3}\int_{-\infty}^\infty \frac{dw}{\pi}\left\{\frac{1}{1 - G(k, iw)}\right.$$

$$\left.\times \ln\,[1 + v(k)(1 - G(k, iw)\chi_0(k, iw)] - v(k)\chi_0(k, iw)\right\} \tag{117}$$

Setting $G(k, iw) = 0$, one recovers the RPA formula for the correlation energy given by PN.[6]

Following these authors, we now introduce the dimensionless quantities

$$\begin{aligned} x = k/k_{\mathrm{F}}, \qquad u &= w/kv_{\mathrm{F}} \\ v(k)\chi_0(k, iw) &= (\alpha r_s/\pi x^2)Q_x(u) \\ v(k)P(k, iw) &= (\alpha r_s/\pi x^2)P_x(u) \end{aligned} \tag{118}$$

where the real quantity $P_x(u)$ is defined by

$$P_x(u) = \int_{|\mathbf{q}|<1} d^3q\, f(q + \tfrac{1}{2}\mathbf{x}, \mathbf{x}) \int_{-\infty}^{\infty} dt\, e^{itux} \exp[-|t|(\mathbf{q}\cdot\mathbf{x} + \tfrac{1}{2}x^2)] \tag{119}$$

with [cf. Eq. (103a)]

$$\begin{aligned} f\left(\mathbf{q} + \frac{\mathbf{x}}{2}, \mathbf{x}\right) = \frac{3}{16}\mathbf{x}\cdot(\mathbf{q}+\mathbf{x})&\left\{1 + \frac{1}{(\mathbf{q}+\mathbf{x})^2} - \frac{|\mathbf{q}+\mathbf{x}|}{2}\left[1 - \frac{1}{(\mathbf{q}+\mathbf{x})^2}\right]^2 \ln\left|\frac{|\mathbf{q}+\mathbf{x}|+1}{|\mathbf{q}+\mathbf{x}|-1}\right|\right\} \\ &- \frac{3}{16}\mathbf{x}\cdot\mathbf{q}\left\{1 + \frac{1}{q^2} - \frac{q}{2}\left(1 - \frac{1}{q^2}\right)^2 \ln\left|\frac{q+1}{q-1}\right|\right\} \end{aligned} \tag{120}$$

The quantity $Q_x(u)$ is defined the same way as $P_x(u)$ but with $f(\mathbf{q} + \frac{1}{2}\mathbf{x}, \mathbf{x})$ replaced by unity. We note that for $x \ll 1$ the functions $Q_x(u)$ and $P_x(u)$ are given by

$$\begin{aligned} Q_x(u) &= 4\pi R(u), \qquad R(u) = 1 - u\arctan(1/u) \\ P_x(u) &= \pi x^2 P(u), \qquad P(u) = 1 + \tfrac{3}{2}u^2 - \tfrac{3}{2}(1+u^2)u\arctan(1/u) \end{aligned} \tag{121}$$

where the last expression was obtained from (107).

Expressed in Rydbergs, the formula (117) for the correlation energy per particle then reads

$$\begin{aligned} E_{\mathrm{corr}}(r_s) = \frac{3}{4\pi\alpha^2 r_s^2}\int_0^{\infty} dx\, x^3 \int_{-\infty}^{\infty} du &\left\{\left[1 - \frac{P_x(u)}{Q_x(u)}\right]^{-1} \right. \\ &\left. \times \ln\left[1 + \frac{\alpha r_s}{\pi x^2}(Q_x(u) - P_x(u))\right] - \frac{\alpha r_s}{\pi x^2} Q_x(u)\right\} \end{aligned} \tag{122}$$

Here we shall not pursue the calculation of the correlation energy on the basis of this expression any further. Such a calculation would in fact be lengthy. It would entail finding first a more suitable general expression for the quantity $P(k, i\omega)$ or $P_x(u)$ valid for arbitrary x and u. Only the static limit $P(k, 0)$ has been obtained explicitly and is given in Appendix D; the latter itself contains integrals which in general must be evaluated numerically.

A calculation of the correlation energy using an expression similar to (117) but with a simple, static local field correction was first carried out by Hubbard.[10] Using the expression for $G(k)$ given in the second row of Table I, Hubbard has calculated the correlation energy in the range of metallic densities $2 \leqslant r_s \leqslant 5$.

APPENDIX A: STATIC MEAN FIELD APPROXIMATIONS

Here we briefly review a large class of approximations which have been devised in the past for calculating $\epsilon(k, \omega)$, of which the RPA is the simplest case. These can all be termed mean field approximations (MFA) since they are characterized by an expression for $\chi(k, z)$ of the form

$$\chi_{\mathrm{MF}}(k, z) = \frac{\chi_0(k, z)}{1 + \psi(k)\chi_0(k, z)} \tag{A.1}$$

where $\psi(k)$ is an effective static mean field potential, which is written in the form

$$\psi(k) = v(k)[1 - G(k)] \tag{A.2}$$

$G(k)$ being the static local field correction. The form (A.1) results from the general expression (14) if the complex potential $\phi(k, z)$ is approximated by the real, frequency-independent potential $-v(k)G(k)$. The $G(k)$ in (A.2) is usually identified with the static limit $G(k, 0)$, although in Ref. 43, the $G(k)$ is the same as the infinite-frequency limit $G(k, \infty)$ given in Eq. (48) (if the difference between $\langle \mathrm{KE} \rangle$ and $\langle \mathrm{KE} \rangle_0$ is neglected).

A list of expressions for $G(k)$ and corresponding references is given in Table I. Note that all of these expressions have in common the fact that for large k, $G(k)$ tends toward a constant (which may depend on the density), in contrast to the general properties discussed in Section 4. This property of the $G(k)$ in MFA, as pointed out by Singwi *et al.*,[36] results from the assumption that the local field correction is independent of ω and from the corresponding form of the spectral function $\chi''(k, \omega)$ in MFA:

$$\chi''_{\mathrm{MF}}(k, \omega) = \frac{\chi''_0(k, \omega)}{[1 + \psi(k)\chi_0'(k, \omega)]^2 + [\psi(k)\chi''_0(k, \omega)]^2} \tag{A.3}$$

This should be compared with the general expression for $\chi''(k, \omega)$ following from (14):

$$\chi''(k, \omega) = \frac{\chi''_0(k, \omega) - \phi''(k, \omega)|\chi_0(k, \omega)|^2}{\{1 + [v(k) + \phi']\chi_0' - \phi''\chi''_0\}^2 + \{\phi''\chi_0' + [v(k) + \phi']\chi''_0\}^2} \tag{A.4}$$

where $\phi'(k, \omega) = -v(k)G'(k, \omega)$ and $\phi''(k, \omega) = -v(k)G''(k, \omega)$.

Many of the expressions for $G(k)$ given in Table I can be found plotted in Ref. 43 as a function of k for various r_s. Note that in some of these expressions $G(k)$ is given as a functional of the static structure factor $S(q)$, or pair correlation function $g(r)$. Let us discuss in particular the form derived by Singwi *et al.* (STLS)[35] and its extensions by Shaw,[14] Schneider,[25] and Vashishta and Singwi (VS).[26] Since the STLS form for $G(k)$ is just a simpler version of the more general expression obtained by Schneider[25] and VS,[26] we start with the latter. Their expression for $G(k)$ is obtained by taking for the effective mean field potential $\psi(r)$ [the Fourier transform of $\psi(k)$] the form [compare Eqs. (26a) and (26b)]

$$\begin{aligned}\nabla\psi(r) &= \nabla v(r)[1 + a\rho(\partial/\partial\rho)]g(r)\\ &= \nabla v(r) + \{g(r) - 1 + a\rho[\partial g(r)/\partial\rho]\}\nabla v(r)\end{aligned} \tag{A.5}$$

In this manner the short-range correlations are taken into account via $g(r)$, while the long-range correlations are described as in RPA [the latter corresponds to taking $g(r) = 1$]. If the density derivative of $g(r)$ is neglected, one obtains the STLS[35] expression for $\nabla\psi(r)$. In Schneider's theory the parameter a has the "classical" value $\frac{1}{2}$ (the meaning of this will become clear shortly) while in the theory of VS, $1 \gtrsim a \geqslant \frac{1}{2}$, the upper bound being subject to some uncertainty. For numerical calculation VS have chosen a to be $\frac{2}{3}$.

From (A.5) we obtain by Fourier transforming and comparing with (A.2)

$$\begin{aligned}G(k) &= -k\int_0^\infty dr\,\{g(r) - 1 + a\rho[\partial g(r)/\partial\rho]\}j_1(kr)\\ j_1(x) &= (\sin x - x\cos x)/x^2\end{aligned} \tag{A.6a}$$

Alternatively, $G(k)$ can be written in terms of $S(q)$ as

$$G(k) = -\frac{1}{\rho}\int\frac{d^3q}{(2\pi)^3}\frac{\mathbf{k}\cdot\mathbf{q}}{q^2}\left\{(1 - a)[S(\mathbf{k} - \mathbf{q}) - 1] + a\rho\frac{\partial S(\mathbf{k} - \mathbf{q})}{\partial\rho}\right\} \tag{A.6b}$$

A simpler way of writing the above expressions is

$$G(k) = \left(1 + a\rho\frac{\partial}{\partial\rho}\right)G_{\mathrm{STLS}}(k) \tag{A.6c}$$

where

$$\begin{aligned}G_{\mathrm{STLS}}(k) &= -k\int_0^\infty dr\,[g(r) - 1]j_1(kr)\\ &= -\frac{1}{\rho}\int\frac{d^3q}{(2\pi)^3}\frac{\mathbf{k}\cdot\mathbf{q}}{q^2}[S(\mathbf{k} - \mathbf{q}) - 1]\\ &= -\frac{3}{4k_{\mathrm{F}}^3}\int_0^\infty dq\,q^2[S(q) - 1]\left[1 + \frac{k^2 - q^2}{2kq}\ln\left|\frac{k + q}{k - q}\right|\right]\end{aligned} \tag{A.7}$$

Table I. Expressions for the Static Local Field Correction $G(k)$ Employed in Static Mean Field Approximations (MFA)[a]

Ref.	$G(k)$	γ	$\lim_{k\to\infty} G(k)$	$\psi(r)$
1, 4[b]	0	0	0	$v(r)$
10	$\frac{k^2}{2(k^2 + k_F^2)}$	$\frac{1}{2}$	$\frac{1}{2}$	$v(r)[1 - \frac{1}{2}\exp(-k_F r)]$
10–12, 29	$\frac{k^2}{2(k^2 + k_F^2 + k_{FT}^2)}$	$\frac{1}{2(1 + k_{FT}^2/k_F^2)}$	$\frac{1}{2}$	$v(r)[\{1 - \frac{1}{2}\exp[-r(k_F^2 + k_{FT}^2)^{1/2}]\}$
13, 24	$\frac{k^2}{2(k^2 + \xi k_F^2)}$	$1/2\xi$ (see footnote j)	$\frac{1}{2}$	$v(r)[1 - \frac{1}{2}\exp(-\sqrt{\xi} k_F r)]$
22, 35	$G_{STLS}(k) = -k \int_0^\infty dr[g(r) - 1] j_1(kr)$ $= -\frac{1}{\rho}\int \frac{d^3q}{(2\pi)^3} \times \frac{\mathbf{k}\cdot\mathbf{q}}{q^2}[S(\mathbf{k} - \mathbf{q}) - 1]$ $= -\frac{3}{4}\int_0^\infty d\eta'\, \eta'^2 [S(\eta') - 1] \times \left[1 + \frac{\eta^2 - \eta'^2}{2\eta\eta'} \ln\left\lvert\frac{\eta + \eta'}{\eta - \eta'}\right\rvert\right]$	Γ	$1 - g(0)$	$\nabla\psi(r) = g(r)\,\nabla v(r)$
35[c]	$G_{STLS}^{(0)}(k) = \frac{9}{32}\eta^2 \left\{\frac{2}{105}\left[\frac{24}{\eta^2} + 44 + \eta^2\right] - \frac{2}{\eta}\left[\frac{8}{35\eta^2} - \frac{4}{15} + \frac{1}{6}\eta^2\right] \times \ln\left\lvert\frac{\eta + 2}{\eta - 2}\right\rvert + \eta^2\left[\frac{\eta^2}{210} - \frac{2}{15}\right] \ln\left\lvert 1 - \frac{4}{\eta^2}\right\rvert\right\}$	$\frac{3}{8}$	$\frac{1}{2}$	$\nabla\psi(r) = g_0(r)\,\nabla v(r)$

14[d]	$1 - \frac{2\nu}{\eta} D\left(\frac{\eta}{2\nu}\right),\ \nu^2 = (9\pi)^{-1/3}$ (see footnote k)	$\frac{1}{6\nu^2} = 0.51$	1	$\nabla\psi(r) = g(r)\,\nabla v(r)$ $g(r) = 1 - \exp(-\nu^2 x^2)$
14[d]	$1 - \exp\left(-\frac{\eta^2}{4\nu_1^2}\right),\ \nu_1^2 = \frac{4}{\pi}\left(\frac{2}{9}\right)^{2/3}$	$\frac{1}{4\nu_1^2} = 0.535$	1	$\nabla\psi(r) = g(r)\,\nabla v(r)$ $g(r) = \mathrm{erf}(\nu_1 x) - 2\nu_1 x \pi^{-1/2} \exp(-\nu_1^2 x^2)$
36	$-\frac{1}{\rho}\int \frac{d^3q}{(2\pi)^3} \times \frac{\mathbf{k}\cdot\mathbf{q}}{q^2\epsilon(q,0)}[S(\mathbf{k}-\mathbf{q}) - 1]$	$-\frac{1}{2k_F}\int_0^\infty dq \times [S(q) - 1]\epsilon^{-1}(q,0) \times \left[1 - \frac{d\ln\epsilon(q,0)}{d\ln q}\right]$	A function of density	—
25,[e] 26[f]	$\left(1 + a\rho\frac{\partial}{\partial\rho}\right)G_{\mathrm{STLS}}(k)$	$\left(1 - \frac{2a}{3} + a\rho\frac{\partial}{\partial\rho}\right)\Gamma$	$1 - g(0) - a\rho\frac{\partial g(0)}{\partial\rho}$	$\nabla\psi(r) = \nabla v(r) \times \left(1 + a\rho\frac{\partial}{\partial\rho}\right)g(r)$
26[g]	$\left(1 + \frac{1}{2}\rho\frac{\partial}{\partial\rho}\right)G^{(0)}_{\mathrm{STLS}}(k) = \left(1 - \frac{1}{6}\eta\frac{\partial}{\partial\eta}\right)G^{(0)}_{\mathrm{STLS}}(k)$	$\frac{1}{4}$	$\frac{1}{2}$	$\nabla\psi(r) = \nabla v(r) \times \left(1 + \frac{1}{2}\rho\frac{\partial}{\partial\rho}\right)g_0(r)$
43[h]	$-\frac{3}{4}\int_0^\infty d\eta'\,\eta'^2[S(\eta') - 1] \times \left[\frac{5}{6} - \frac{\eta'^2}{2\eta^2} + \frac{(\eta'^2 - \eta^2)^2}{4\eta'\eta^3} \times \ln\left\|\frac{\eta + \eta'}{\eta - \eta'}\right\|\right]$	$\frac{2}{3}\Gamma$	$\frac{2}{3}[1 - g(0)]$	—
43[i]	$-\frac{3}{16}\left\{\frac{32}{63\eta^2} - \frac{608}{945} - \frac{142}{315}\eta^2 - \frac{2}{315}\eta^4\right.$	$\frac{3}{20}$	$\frac{1}{3}$	—

Table I. Continued

Ref.	$G(k)$	γ	$\lim_{k\to\infty} G(k)$	$\psi(r)$
	$+\frac{\eta^4}{35}\left(2-\frac{\eta^2}{18}\right)\ln\left\lvert 1-\frac{4}{\eta^2}\right\rvert$			
	$+\frac{1}{\eta}\left(-\frac{32}{63\eta^2}+\frac{24}{35}-\frac{2}{5}\eta^2+\frac{1}{6}\eta^4\right)$			
	$\times \ln\left\lvert\frac{\eta+2}{\eta-2}\right\rvert\Big\}$			

[a] The quantity $\psi(r)$ denotes the effective potential in real space, i.e., the Fourier transform of $\psi(k) = v(k)[1 - G(k)]$. We use the abbreviations $\eta = k/k_F$, $x = k_F r$. Γ is defined by Eqs. (A.11) in the text.

[b] RPA.

[c] STLS,[35] using the free particle (HF) value for $S(k)$, $g(r)$ in $G_{STLS}(k)$.

[d] Shaw,[14] using STLS theory.

[e] $a = \frac{1}{2}$.

[f] $1 \gtrsim a \geqslant \frac{1}{2}$.

[g] VS[26] theory with free particle $S(k)$, $g(r)$, and the value $a = \frac{1}{2}$.

[h] Compare Eqs. (43) and (48).

[i] PV[43] theory with free particle $S(k)$, $g(r)$. See Eq. (D.6).

[j] ξ to be determined from compressibility.

[k] The quantity D is Dawson's integral defined as

$$D(x) = \exp(-x^2)\int_0^\infty dt\,\exp(t^2) = \int_0^\infty dt\,\exp(-t^2)\sin(2xt).$$

is the form of the local field correction obtained by STLS.[35] From the above relations one finds that the quantity γ defined for the static MFA as

$$\lim_{k\to 0} G(k) = \gamma k^2/k_F{}^2 \tag{A.8}$$

is given by

$$\gamma = -\tfrac{1}{3}k_F{}^2 \int_0^\infty dr\,\{g(r) - 1 + a\rho[\partial g(r)/\partial\rho]\}r \tag{A.9a}$$

$$= -(1/2k_F)\int_0^\infty dq\,\{(1-a)[S(q) - 1] + a\rho[\partial S(q)/\partial\rho]\} \tag{A.9b}$$

Comparison with (36) shows that for $a = \frac{1}{2}$ we obtain the expression for γ_0 valid in the classical limit where $\langle \mathrm{KE}\rangle = \langle \mathrm{KE}\rangle_0$. By taking a value of $a > \frac{1}{2}$, VS[26] attempted to take into account the fact that for the ground state system $\langle \mathrm{KE}\rangle > \langle \mathrm{KE}\rangle_0$. Note that the above expression for γ can be written as

$$\gamma = \left(1 - \frac{2a}{3} + a\rho\frac{\partial}{\partial\rho}\right)\Gamma \tag{A.10}$$

where $\Gamma = \gamma_{\mathrm{STLS}}$ is a dimensionless measure of the average potential energy per particle, defined by

$$\Gamma = -\frac{\pi}{2e^2k_F}\langle V\rangle = -\frac{k_F{}^2}{3}\int_0^\infty dr\,r[g(r) - 1] \tag{A.11a}$$

$$= -\frac{1}{2k_F}\int_0^\infty dq[S(q) - 1] \tag{A.11b}$$

The quantity Γ enters directly into the calculation of the ground state energy (or free energy, at finite temperature) via the well-known integration over the coupling strength e^2 (cf. Appendix B).

In the limit $k \to \infty$ one obtains from Eqs. (A.6a)–(A.6c)

$$\lim_{k\to\infty} G(k) = 1 - g(0) - a\rho[\partial g(0)/\partial\rho] \tag{A.12}$$

In the literature[6,26] it has usually been found and assumed that $g(0)$ has some finite (positive) value, the reasoning being that even though particles of parallel spin are forbidden by the exclusion principle to be found right next to each other, particles of opposite spin are not thus restricted, leading to a total $g(0) > 0$. Since $g(0)$ is proportional to the probability of finding two electrons at zero separation and since the Coulomb repulsion between the latter would be infinite, it seems not unreasonable to suppose that $g(0)$ should be zero regardless of the spin of the two particles. This is in fact indicated by recent Monte Carlo type computations on the electron gas.[45] Moreover, the results of these computations indicate that $\partial g(r)/\partial r$ also vanishes at $r = 0$. These results are also consistent with a relation obtained recently by Kimball[16]:

$$\left.\frac{\partial g(r)}{\partial r}\right|_{r=0} = \frac{1}{a_0} g(0) \tag{A.13}$$

where a_0 is the Bohr radius. Thus the right side of (A.12) should reduce to the value unity.

As far as the various expressions and values for γ given in Table I are concerned, the basic relation to be kept in mind is the one relating γ to the compressibility ratio. In the MFA this ratio is

$$K_T^{(0)}/K_T = 1 - \gamma(k_{\mathrm{FT}}^2/k_{\mathrm{F}}^2) \tag{A.14}$$

The values of the compressibility ratio obtained from γ via the limiting form for $k \to 0$ of the static local field corrections given in Table I are usually different from those calculated from the second derivative of the ground state energy. Only in the self-consistent calculation of Vashishta and Singwi[26] do the two results almost coincide in the entire metallic density range with the parameter $a = \frac{2}{3}$. It should also be noted that in the MFA theories the quantity γ_0 (which is related to the compressibility) and the quantity γ_∞ [which occurs in the plasma dispersion, Eq. (56b)] have the same value, γ. Thus the MFA's lead to the following dispersion relation in the long-wavelength limit $k \to 0$ and at zero temperature:

$$\begin{aligned}\omega_p(k) &= \omega_p\left[1 + \left(\frac{9}{10} - \frac{1}{2}\gamma\frac{k_{\mathrm{F}T}^2}{k_{\mathrm{F}}^2}\right)\frac{k^2}{k_{\mathrm{F}T}^2} + \cdots\right] \\ &= \omega_p\left[1 + \left(\frac{9}{10} - \frac{2\alpha r_s}{\pi}\gamma(r_s)\right)\frac{k^2}{k_{\mathrm{FT}}^2} + \cdots\right]\end{aligned} \tag{A.15}$$

As seen from Eqs. (112) and (113), $\gamma_0^{(\mathrm{HF})}$ and $\gamma_\infty^{(\mathrm{HF})}$ differ by 10%, which is probably a considerable underestimate of the true difference between γ_0 and γ_∞ in the range of metallic densities $2 \leqslant r_s \leqslant 6$. It is easily verified that for a metal of density corresponding to $r_s \simeq 3$, a 10% difference between γ_0 and γ_∞ leads to a similar difference in the correction to the RPA term, $9k^2/10k_{\mathrm{F}T}^2$. Thus one cannot hope to achieve consistency between values of the compressibility and the plasma dispersion using MFA theories.

Finally, it is perhaps of interest to point out that in MFA the plasma oscillations are undamped for k values up to some critical wave number k_c. At k_c it first becomes possible for a plasmon to decay into a particle–hole pair so that a damping of the plasmon sets in (the so-called Landau damping, discussed in detail in Ref. 6). The value of k_c is given by the solution of the equations

$$\omega_p(k_c) = k_c v_{\mathrm{F}} + \omega_0(k_c) \tag{A.16}$$

$$1 + v(k_c)[1 - G(k_c)]\chi_0'[k_c, \omega_p(k_c)] = 0 \tag{A.17}$$

From (110) one finds ($\eta = k/k_F$)

$$\chi_0'[k, kv_F + \omega_0(k)] = \frac{mk_F}{2\pi^2\hbar^2}\left[1 - \left(1 + \frac{\eta}{2}\right)\ln\left(1 + \frac{2}{\eta}\right)\right] \quad (A.18)$$

so that k_c is determined by the equation ($\eta_c = k_c/k_F$)

$$[1 - G(\eta_c)]\left[1 - \left(1 + \frac{\eta_c}{2}\right)\ln\left(1 + \frac{2}{\eta_c}\right)\right] = -2\eta_c^2 \frac{k_F^2}{k_{FT}^2} \quad (A.19)$$

This equation was first considered by Ferrell[46] and Brout *et al.*[5,47] in the RPA where $G(k) \equiv 0$. The effect of $G(k)$ is to decrease the critical wave number from its RPA value; the larger the value of γ, the smaller the value of k_c. The correlations in the particle motions as described by the local field correction $G(k)$ thus act to reduce the number of collective degrees of freedom characteristic of the plasma modes, a result to be expected.

Yasuhara[49] has recently investigated short-range correlations in the electron gas from a diagrammatic analysis of perturbation theory. He has shown that an infinite sum of electron–electron ladder diagrams is indispensable for the short-range correlation at metallic densities. His results are also in the form of the static mean field approximation, with the local field correction $G(k)$ calculated from electron–electron ladder diagrams.

APPENDIX B: RELATIONS BETWEEN GROUND STATE ENERGY, VIRIAL THEOREM, AND COMPRESSIBILITY

First we recall that for the ground state of the noninteracting system

$$\langle \mathrm{KE}\rangle_0 = \tfrac{3}{5}\epsilon_F^{(0)}, \qquad p_0 = \tfrac{2}{5}\epsilon_F^{(0)}\rho, \qquad 1/\rho K^{(0)} = \tfrac{2}{3}\epsilon_F^{(0)} \quad (B.1)$$

where $\epsilon_F^{(0)} = \hbar^2 k_F^2/2m$, $k_F^3 = 3\pi^2\rho$. The ground state energy per particle of the interacting system $E(\rho)$ can be written as[6]

$$E(\rho) = \langle \mathrm{KE}\rangle + \langle V\rangle = \langle \mathrm{KE}\rangle_0 + \int_0^{e^2} \frac{d\lambda}{\lambda}\langle V\rangle_\lambda \quad (B.2)$$

Here $\langle V\rangle_\lambda$ represents the average potential energy per particle for a system with coupling parameter λ. The integration is carried out at constant density ρ. The above ground state energy theorem is a consequence of the relation[6]

$$\partial E(\rho, \lambda)/\partial\lambda = (1/\lambda)\langle V\rangle_\lambda \quad (B.3)$$

We now show that the relations (B.2) and (B.3) imply the equivalence of the virial form for the pressure p and the density derivative of the ground state[39]:

$$\begin{aligned} p/\rho = \rho\, \partial E(\rho)/\partial\rho &= \tfrac{2}{3}\langle \mathrm{KE}\rangle + \tfrac{1}{3}\langle V\rangle \\ &= \tfrac{2}{3}E(\rho) - \tfrac{1}{3}\langle V\rangle \end{aligned} \quad (B.4a)$$

which implies

$$E(\rho) = \langle \mathrm{KE}\rangle_0 - \tfrac{1}{3}\rho^{2/3}\int_\infty^\rho d\rho'\,(\rho')^{-5/3}\langle V\rangle_{\rho'} \quad (B.4b)$$

The differentiation and integration are here carried out at constant coupling strength e^2.

To see this, it is sufficient to express the ground state energy in rydbergs (1 Ry $= e^2/2a_0 = me^4/2\hbar^2 = 13.60$ eV), i.e., to write

$$E(\rho, e^2) = \epsilon(r_s)\,\text{Ry} \tag{B.5}$$

where r_s is the dimensionless parameter defined by $4\pi r_s{}^3 a_0{}^3/3 = 1/\rho$ and $a_0 = \hbar/me^2$ is the Bohr radius. One has

$$e^2 \frac{\partial}{\partial e^2} = -a_0 \frac{\partial}{\partial a_0} = r_s \frac{\partial}{\partial r_s}, \qquad -3\rho \frac{\partial}{\partial \rho} = -k_{\mathrm{F}} \frac{\partial}{\partial k_{\mathrm{F}}} = r_s \frac{\partial}{\partial r_s} \tag{B.6}$$

where the left side refers to differentiations at constant density ρ, and the right side refers to differentiations at constant e^2. With $\langle V\rangle$ also expressed in rydbergs, (B.3), (B.5), and (B.6) imply

$$2\epsilon(r_s) + r_s \frac{\partial \epsilon(r_s)}{\partial r_s} = \langle V\rangle \tag{B.7a}$$

which is the same as (B.4a), with p/ρ expressed in units of Ry:

$$-\frac{3p}{\rho} = r_s \frac{\partial \epsilon(r_s)}{\partial r_s} = -2\epsilon(r_s) + \langle V\rangle \tag{B.7b}$$

Hence if the ground state energy is obtained from an expression for the average potential energy per particle $\langle V\rangle$ via integration over the coupling parameter, or equivalently, via integration over r_s

$$\epsilon(r_s) = (1/r_s{}^2)\left[2.210 + \int_0^{r_s} x\langle V\rangle_x\, dx\right] \tag{B.8}$$

the pressure obtained from the virial theorem is the same as obtained from differentiation of the ground state energy with respect to r_s.

What has been said about the pressure is equally true about the compressibility. When expressed in rydbergs, the equivalent expressions derived from the virial theorem and ground state energy, respectively, read

$$\frac{1}{\rho K} = \frac{\partial p}{\partial \rho} = \frac{10}{9}\epsilon(r_s) - \frac{5}{9}\langle V\rangle + \frac{1}{9} r_s \frac{\partial \langle V\rangle}{\partial r_s} \tag{B.9a}$$

$$= \frac{1}{9}\left[r_s{}^2 \frac{\partial^2 \epsilon(r_s)}{\partial r_s{}^2} - 2r_s \frac{\partial \epsilon(r_s)}{\partial r_s}\right] \tag{B.9b}$$

as can be easily verified using (B.7b).

It is convenient to restate the above relations in terms of the dimensionless quantities γ_0 and Γ defined by Eqs. (34) and (A.11). First we rewrite the potential energy per particle as

$$\langle V\rangle = -\frac{2e^2 k_{\mathrm{F}}}{\pi}\Gamma = -\frac{4}{\pi\alpha}\frac{\Gamma(r_s)}{r_s}\,\text{Ry} \tag{B.10}$$

where $\alpha = (4/9\pi)^{1/3}$. Equation (B.8) can be rewritten as

$$\epsilon(r_s) = \frac{1}{r_s^2}\left[2.210 - \frac{4}{\pi\alpha}\int_0^{r_s} \Gamma(x)\,dx\right] \tag{B.11}$$

On the other hand, the ratio of the compressibilities of the noninteracting and interacting systems $K^{(0)}/K$ is given in terms of the quantity γ_0. From Eq. (34) we have

$$\frac{K^{(0)}}{K} = 1 - \gamma_0\left(\frac{k_{FT}^2}{k_F^2}\right) = 1 - \frac{4\alpha r_s}{\pi}\gamma_0(r_s) \tag{B.12}$$

Now $\gamma_0^{(V)}$, the contribution from the potential energy, is given by [Eq. (36)]

$$\gamma_0^{(V)}(r_s) = \tfrac{2}{3}\Gamma(r_s) - \tfrac{1}{6}r_s[\partial\Gamma(r_s)/\partial r_s] \tag{B.13}$$

and $\gamma_0^{(KE)}$, the contribution from the kinetic energy, can be written as

$$\gamma_0^{(KE)}(r_s) = \frac{-\pi\alpha r_s}{4}\left(1 - \frac{1}{3}r_s\frac{\partial}{\partial r_s}\right)(\langle KE\rangle - \langle KE\rangle_0) \tag{B.14a}$$

which can be rewritten,[26] using (B.2) and (B.11),

$$\gamma_0^{(KE)}(r_s) = -\frac{5}{3}\left[\Gamma(r_s) - \frac{1}{r_s}\int_0^{r_s}\Gamma(x)\,dx\right] + \frac{1}{3}r_s\frac{\partial\Gamma(r_s)}{\partial r_s} \tag{B.14b}$$

Thus the contribution to the compressibility ratio from the kinetic energy has also been expressed in terms of $\Gamma(r_s)$. Adding (B.13) and (B.14b), we obtain

$$\gamma_0(r_s) = -\Gamma(r_s) + \frac{1}{6}\frac{\partial\Gamma(r_s)}{\partial r_s} + \frac{5}{3r_s}\int_0^{r_s}\Gamma(x)\,dx \tag{B.15}$$

Equations (B.12) and (B.15) give the same value for the compressibility ratio as the one obtained from the ground state energy via (B.9b) (PN)[6]

$$\frac{K^{(0)}}{K} = \frac{1}{6}\alpha^2 r_s^2\left[r_s^2\frac{\partial^2\epsilon(r_s)}{\partial r_s^2} - 2r_s\frac{\partial\epsilon(r_s)}{\partial r_s}\right] \tag{B.16}$$

In connection with the above discussion it is also useful to recall the so-called Ferrell theorem[48] on the ground state energy as a function of r_s

$$((\partial^2/\partial r_s^2)[r_s^2\epsilon(r_s)] \leqslant 0 \tag{B.17a}$$

or equivalently, in terms of $\Gamma(r_s)$, using (B.10) and (B.11),

$$\partial\Gamma(r_s)/\partial r_s \geqslant 0 \tag{B.17b}$$

requiring that $\Gamma(r_s)$ be an increasing function of r_s. In addition, it should be recalled that $\Gamma(r_s)$ is positive and is bounded below by the Hartree–Fock value $\Gamma_{HF} = 3/8$ (see below). The properties of $\Gamma(r_s)$ are further discussed in Ref. 26.

The ground state energy per particle $E(\rho)$ is usually written in terms of the Hartree–Fock value $E_{\mathrm{HF}}(\rho)$ and correlation energy $E_{corr}(\rho)$:

$$E(\rho) = E_{\mathrm{HF}}(\rho) + E_{\mathrm{corr}}(\rho) \tag{B.18}$$

where

$$E_{\mathrm{HF}}(\rho) = \langle \mathrm{KE} \rangle_0 + \langle V \rangle_0 = \frac{2.210}{r_s^2} - \frac{0.916}{r_s}\,\mathrm{Ry} \tag{B.19}$$

The value of $\langle V \rangle_0$ corresponds to $\Gamma = \Gamma_{\mathrm{HF}} = 3/8$ in (B.10).

The correlation energy per particle is defined by

$$\begin{aligned} E_{\mathrm{corr}}(\rho) &= \int_0^{e^2} d\lambda \left[\frac{\langle V \rangle_\lambda}{\lambda} - \frac{\langle V \rangle_0}{e^2} \right] \\ &= -\frac{4}{\pi \alpha r_s^2} \int_0^{r_s} \left[\Gamma(x) - \frac{3}{8} \right] dx\,\mathrm{Ry} \\ &\equiv \epsilon_{\mathrm{corr}}(r_s)\,\mathrm{Ry} \end{aligned} \tag{B.20}$$

The pressure and compressibility corresponding to the HF ground state energy are

$$\frac{p_{\mathrm{HF}}}{\rho} = \rho \frac{\partial E_{\mathrm{HF}}(\rho)}{\partial \rho} = \frac{2}{5} \epsilon_{\mathrm{F}}^{(0)} - \frac{e^2 k_{\mathrm{F}}}{4\pi} \tag{B.21}$$

$$\frac{1}{\rho K_{\mathrm{HF}}} = \frac{\partial p_{\mathrm{HF}}}{\partial \rho} = \frac{2}{3} \epsilon_{\mathrm{F}}^{(0)} - \frac{e^2 k_{\mathrm{F}}}{3\pi} \tag{B.22a}$$

or

$$\frac{K^{(0)}}{K_{\mathrm{HF}}} = 1 - \frac{\alpha r_s}{\pi} \tag{B.22b}$$

thus giving the value $\gamma_0 = \gamma_0^{(\mathrm{HF})} = 1/4$ for the compressibility factor of the HF ground state.

Finally, the total pressure and compressibility ratio, written in terms of HF and correlation contributions and expressed in rydbergs, are

$$\frac{p}{\rho} = \frac{p_{\mathrm{HF}}}{\rho} + \frac{2}{3} \epsilon_{\mathrm{corr}}(r_s) + \frac{4}{3\pi \alpha r_s} \left[\Gamma(r_s) - \frac{3}{8} \right] \tag{B.23}$$

$$\frac{K^{(0)}}{K} = 1 - \frac{\alpha r_s}{\pi} + \frac{1}{6} \alpha^2 r_s^2 \left[r_s^2 \frac{\partial^2 \epsilon_{\mathrm{corr}}(r_s)}{\partial r_s^2} - 2 r_s \frac{\partial \epsilon_{\mathrm{corr}}(r_s)}{\partial r_s} \right] \tag{B.24}$$

or, in terms of the compressibility factor $\gamma_0(r_s)$ [cf. (B.12) and (B.15)]

$$\gamma_0(r_s) = \frac{1}{4} - \left[\Gamma(r_s) - \frac{3}{8} \right] + \frac{1}{6} r_s \frac{\partial \Gamma(r_s)}{\partial r_s} + \frac{5}{3 r_s} \int_0^{r_s} \left[\Gamma(x) - \frac{3}{8} \right] dx \tag{B.25}$$

APPENDIX C: CALCULATION OF THE QUANTITY $P''(k,\omega)$

At $T = 0$ the expression (96) for $P''(k, \omega)$ becomes

$$P''(k, \omega) = -\frac{g\pi}{\hbar}\int \frac{d^3q}{(2\pi)^3}\left\{\theta\left[k_F^2 - \left(\mathbf{q} + \frac{\mathbf{k}}{2}\right)^2\right] - \theta\left[k_F^2 - \left(\mathbf{q} - \frac{\mathbf{k}}{2}\right)^2\right]\right\}$$
$$\times f(\mathbf{q}, \mathbf{k})\,\delta\left[\omega - \frac{\hbar\mathbf{q}\cdot\mathbf{k}}{m}\right] \tag{C.1}$$

where $g = 2$ is the spin degeneracy and the expression (103) for $f(\mathbf{q}, \mathbf{k})$ is to be substituted. The angular integration involving the δ function can be carried out, using

$$\int_{-1}^{1} dx\,\delta\left[\omega - \frac{\hbar qk}{m}x\right]h(x) = \frac{m}{\hbar qk}h\left(\frac{m\omega}{\hbar qk}\right)\theta\left[q - \left|\frac{m\omega}{\hbar k}\right|\right] \tag{C.2}$$

for an arbitrary function $h(x)$. We shall take $\omega > 0$. Thus $\mathbf{q}\cdot\mathbf{k}$ in the above integral is replaced by $m\omega/\hbar$ and we have under the integral sign

$$\left(\mathbf{q} + \frac{\mathbf{k}}{2}\right)^2 = q^2 + \frac{k^2}{4} + \frac{m\omega}{\hbar} \equiv q^2 + \alpha_+, \qquad \left|\mathbf{q} + \frac{\mathbf{k}}{2}\right| = (q^2 + \alpha_+)^{1/2}$$
$$\left(\mathbf{q} - \frac{\mathbf{k}}{2}\right)^2 = q^2 + \frac{k^2}{4} - \frac{m\omega}{\hbar} \equiv q^2 + \alpha_-, \qquad \left|\mathbf{q} - \frac{\mathbf{k}}{2}\right| = (q^2 + \alpha_-)^{1/2} \tag{C.3}$$

Using the abbreviations

$$q_+^2 = k_F^2 - \alpha_- = k_F^2 - \frac{k^2}{4} + \frac{m\omega}{\hbar}$$
$$q_-^2 = k_F^2 - \alpha_+ = k_F^2 - \frac{k^2}{4} - \frac{m\omega}{\hbar}, \qquad q_0 = \frac{m\omega}{\hbar k} \tag{C.4}$$

we then have

$$P''(k, \omega) = -\frac{gm}{4\pi\hbar^2 k}\int_0^\infty q\,dq\,\theta(q - q_0)[\theta(q_-^2 - q^2) - \theta(q_+^2 - q^2)]$$
$$\times\left\{\frac{3(\alpha_+ + \frac{1}{4}k^2)}{16k_F^2}\left[1 + \frac{k_F^2}{q^2 + \alpha_+} - \frac{(q^2 + \alpha_+)^{1/2}}{2k_F}\left(1 - \frac{k_F^2}{q^2 + \alpha_+}\right)^2\right.\right.$$
$$\left.\times\ln\left|\frac{(q^2 + \alpha_+)^{1/2} + k_F}{(q^2 + \alpha_+)^{1/2} - k_F}\right|\right]$$
$$+\frac{3(\alpha_- + \frac{1}{4}k^2)}{16k_F^2}\left[1 + \frac{k_F^2}{q^2 + \alpha_-} - \frac{(q^2 + \alpha_-)^{1/2}}{2k_F}\left(1 - \frac{k_F^2}{q^2 + \alpha_-}\right)^2\right.$$
$$\left.\left.\times\ln\left[\frac{(q^2 + \alpha_-)^{1/2} + k_F}{(q^2 + \alpha_-)^{1/2} - k_F}\right|\right]\right\} \tag{C.5}$$

Now the integrand of (C.5) is nonvanishing only for $q_0 < q$ and $q_- < q < q_+$. There are two cases to consider:

(i) $k < 2k_F$. Here we can have contributions to the integral if $q_0 < q_- < q < q_+$ corresponding to $0 < \omega < kv_F - \omega_0(k)$, or if $q_- < q_0 < q < q_+$ corresponding to $kv_F - \omega_0(k) < \omega < kv_F + \omega_0(k)$.

(ii) $k > 2k_F$. In this case $\theta(q_-{}^2 - q^2) = \theta(k_F{}^2 - \frac{1}{4}k^2 - (m\omega/\hbar) - q^2) = 0$ and we must have $q_0 < q < q_+$ corresponding to $\omega_0(k) - kv_F < \omega < \omega_0(k) + kv_F$.

Thus for $k < 2k_F$ and $0 < \omega < kv_F - \omega_0(k)$

$$P''(k, \omega) = \frac{gm}{4\pi\hbar^2 k}\int_{q_-}^{q_+} q\,dq\left\{\ \right\} \tag{C.6}$$

while for $|kv_F - \omega_0(k)| \leqslant \omega \leqslant kv_F + \omega_0(k)$ and all k,

$$P''(k, \omega) = \frac{gm}{4\pi\hbar^2 k}\int_{q_0}^{q_+} q\,dq\left\{\ \right\} \tag{C.7}$$

where { } is the quantity in the curly brackets of (C.5).

Letting $Q_1 = (q^2 + \alpha_+)^{1/2}$ and $Q_2 = (q^2 + \alpha_-)^{1/2}$, one has

$$\begin{aligned}\int q\,dq\{\,\} = {}& \frac{3(\alpha_+ + \frac{1}{4}k^2)}{16k_F{}^2}\int Q_1\,dQ_1\left[1 + \frac{k_F{}^2}{Q_1{}^2} - \frac{Q_1}{2k_F}\left(1 - \frac{k_F{}^2}{Q_1{}^2}\right)^2 \right. \\ & \left. \times \ln\left|\frac{Q_1 + k_F}{Q_1 - k_F}\right|\right] \\ & + \frac{3(\alpha_- + \frac{1}{4}k^2)}{16k_F{}^2}\int Q_2\,dQ_2\left[1 + \frac{k_F{}^2}{Q_2{}^2} - \frac{Q_2}{2k_F}\left(1 - \frac{k_F{}^2}{Q_2{}^2}\right)^2 \right. \\ & \left. \times \ln\left|\frac{Q_2 + k_F}{Q_2 - k_F}\right|\right]\end{aligned} \tag{C.8}$$

which are identical integrals, except that the upper and lower limits are different. The limits on the Q_1 integral are

$$\begin{aligned} Q_{1+} &= k_F\left(1 + \frac{\omega}{\omega_F}\right)^{1/2} && \text{corresponding to } q = q_+ \\ Q_{1-} &= k_F && q = q_- \\ Q_{10} &= \frac{m}{\hbar k}[\omega + \omega_0(k)] && q = q_0 \end{aligned} \tag{C.9}$$

while those on the Q_2 integral are

$$
\begin{aligned}
Q_{2+} &= k_F && \text{corresponding to } q = q_+ \\
Q_{2-} &= k_F\left(1 - \frac{\omega}{\omega_F}\right)^{1/2} && q = q_- \\
Q_{20} &= \frac{m}{\hbar k}\,|\omega - \omega_0(k)| && q = q_0
\end{aligned}
\tag{C.10}
$$

The integrals in (C.8) are tedious but elementary and lead to the results (104a)–(104c).

APPENDIX D: THE QUANTITIES $G(k,\infty)$ AND $G(k,0)$

Here we give the expressions for the above quantities corresponding to the theory of Section 5 [as embodied by the expressions (104a)–(104c) for $P''(k, \omega)$]. First we give the values of the moments $P_{-1}(k)$, $P_1(k)$, and $P_3(k)$ for small k. In this case, using (106), one finds for $k \to 0$

$$
P_{-1}(k) = \frac{mk^2}{4\pi^2\hbar^2 k_F}, \qquad P_1(k) = \frac{3\rho k^4}{20 m k_F^2}, \qquad P_3(k) = P_1(k)\frac{3(kv_F)^2}{7} \tag{D.1}
$$

Thus, using (100), (106), and (40), one obtains for large ω and $k \to 0$

$$
G(k, \omega) \sim \frac{3k^2}{20k_F^2}\left[1 - \frac{6}{35}\left(\frac{kv_F}{\omega}\right)^2 + \cdots\right] \tag{D.2}
$$

The expression for $G(k, \infty)$ is

$$
G(k, \infty) = P_1(k)m/\rho k^2 \tag{D.3}
$$

This can be evaluated for arbitrary k by computing the first frequency moment of the function $P''(k, \omega)$ given by (104). Alternatively, we can obtain $G(k, \infty)$ by substituting the ground state static form factor of the free Fermi gas,

$$
\begin{aligned}
S_0(k) &= \frac{3k}{4k_F} - \frac{k^3}{16k_F^3}, && 0 < k \leqslant 2k_F \\
&= 1, && 2k_F \leqslant k
\end{aligned}
\tag{D.4}
$$

into the integral $I(k)$ defined by Eq. (42), realizing that $G(k, \infty)$ is also given by

$$
G(k, \infty) = -(1/\omega_p^2)I(k) \tag{D.5}
$$

within the approximation considered. For, the basic ingredients of the calculation presented in Section 5 have been a decoupling which conserves the first and third frequency moments $M_1(k)$ and $M_3(k)$, followed by the HF factorization (87). Hence the result (D.3) must be the same as (D.5) in which the HF factorization appears via the above expression for $S_0(k)$. The result, then, obtained either way is

$$G(k,\infty) = -\frac{3}{16}\left\{\frac{32}{63\eta^2} - \frac{608}{945} - \frac{142\eta^2}{315} - \frac{2\eta^4}{315} + \frac{\eta^4}{35}\left(2 - \frac{\eta^2}{18}\right)\ln\left|1 - \frac{4}{\eta^2}\right|\right.$$
$$\left. + \left(-\frac{32}{63\eta^2} + \frac{24}{35} - \frac{2\eta^2}{5} + \frac{\eta^4}{6}\right)\frac{1}{\eta}\ln\left|\frac{\eta+2}{\eta-2}\right|\right\} \tag{D.6}$$

In the limit $k \to 0$ one obtains

$$\lim_{k\to 0} G(k,\infty) = \frac{3}{20}\eta^2\left\{1 - \frac{\eta^2}{14}\left(\frac{247}{105} - 2\ln\frac{\eta}{2}\right) + \cdots\right\} \tag{D.7}$$

while for $k \to \infty$, (D.6) takes the form

$$\lim_{k\to\infty} G(k,\infty) = \frac{1}{3}\left\{1 - \frac{6}{5\eta^2} + O\left(\frac{1}{\eta^4}\right)\right\} \tag{D.8}$$

These results are consistent with the limits stated in Eqs. (44) and (45) when it is recalled that $\langle V\rangle_0 = -3e^2k_F/4\pi$ and $g_0(0) = 1/2$.

We now consider the static limit given by

$$G(k,0) = \mathrm{P}(k,0)/\chi_0(k,0) = P_{-1}(k)/\chi_0(k) \tag{D.9}$$

where

$$P_{-1}(k) = \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{P''(k,\omega)}{\omega} \tag{D.10}$$

The calculation of the inverse first frequency moment of the function $P''(k,\omega)$ defined in (104) is very lengthy and tedious but straightforward and leads to the following results ($\eta = k/k_F$):

For $k < 2k_F$

$$P_{-1}(k) = \frac{mk_F}{16\pi^2\hbar^2}\left\{-\frac{24}{5} + \frac{23}{30}\eta^2 + 8\left(1 - \frac{\eta}{2}\right)\ln\left|1 - \frac{2}{\eta}\right|\right.$$
$$+ \left(-8 + 2\eta - 2\eta^2 + \frac{1}{3}\eta^4\right)\ln\left|1 - \frac{4}{\eta^2}\right|$$
$$+ \left(4\ln 2 + 4\ln\eta + \ln\left|1 - \frac{4}{\eta^2}\right|\right)\eta\ln\left|\frac{\eta+2}{\eta-2}\right|$$
$$+ \left(\frac{12}{5\eta} + 4 - 6\eta + \frac{3}{4}\eta^3\right)\ln\left|\frac{\eta+2}{\eta-2}\right|$$
$$+ \left(\frac{12}{5\eta} + \frac{8}{5} + \frac{41}{15}\eta - \frac{11}{15}\eta^2 - \frac{4}{15}\eta^3\right)(1+\eta)\ln\left|1 + \frac{2}{\eta}\right|$$

$$- \left(\frac{12}{5\eta} - \frac{8}{5} + \frac{41}{15}\eta + \frac{11}{15}\eta^2 - \frac{4}{15}\eta^3\right)|1 - \eta| \ln\left|\frac{1 + |1 - \eta|}{1 - |1 - \eta|}\right|$$

$$+ \eta\left(\ln^2\left|\frac{1 + |1 - \eta|}{1 - |1 - \eta|}\right| - \ln^2\left|1 + \frac{2}{\eta}\right|\right)$$

$$- 2\eta\left[\int_{1-\eta}^{1} dx \frac{1}{x + \frac{1}{2}\eta} \ln|x^2 - 1| + \int_{1}^{1+\eta} dx \frac{1}{x - \frac{1}{2}\eta} \ln|x^2 - 1|\right]$$

$$+ \frac{3}{2}\left(1 + \frac{\eta^2}{2} - \frac{\eta^4}{48}\right)\left[\int_{1-\eta}^{1} dx \frac{1}{x + \frac{1}{2}\eta} \ln\left|\frac{x + 1}{x - 1}\right|\right.$$

$$\left.\left. - \int_{1}^{1+\eta} dx \frac{1}{x - \frac{1}{2}\eta} \ln\left|\frac{x + 1}{x - 1}\right|\right]\right\} \tag{D.11a}$$

For $k > 2k_F$

$$P_{-1}(k) = \frac{mk_F}{16\pi^2\hbar^2}\left\{-\frac{24}{5} + \frac{23}{30}\eta^2 + \frac{\eta^4}{15}\ln\left|1 - \frac{4}{\eta^2}\right|\right.$$

$$+ \left(-\frac{1}{4}\eta^2 + \frac{1}{3} + \frac{24}{5\eta^2}\right)\eta \ln\left|\frac{\eta + 2}{\eta - 2}\right|$$

$$+ 4\eta(\ln 2 + \ln\eta)\ln\left|\frac{\eta + 2}{\eta - 2}\right|$$

$$- 2\eta\int_{-1}^{1} dx \frac{1}{x + \frac{1}{2}\eta}[\ln|x^2 - 1| + \ln|(x + \eta)^2 - 1|]$$

$$\left. + \frac{3}{2}\left(1 + \frac{\eta^2}{2} - \frac{\eta^4}{48}\right)\int_{-1}^{1} dx \frac{1}{x + \frac{1}{2}\eta}\left[\ln\left|\frac{x + 1}{x - 1}\right| - \ln\left|\frac{\eta + x + 1}{\eta + x - 1}\right|\right]\right\} \tag{D.11b}$$

The functions $G(k, 0)$ and $G(k, \infty)$ are shown in Fig. 7. For k near $2k_F$ one finds from (D.11a) and (D.11b) (see below) $(0 < \Delta \ll 1)$

$$P_{-1}\left[2k_F\left(1 \pm \frac{\Delta}{2}\right)\right] = \frac{mk_F}{16\pi^2\hbar^2}\left\{-\frac{26}{15} + \frac{32}{15}\ln 2 + \frac{2\pi^2}{3}\right.$$

$$\left. \pm 6\Delta\ln\Delta + O(\Delta, \Delta^2\ln\Delta)\right\} \tag{D.12}$$

Thus $P_{-1}(k)$ is continuous at $k = 2k_F$ but its slope has a logarithmic singularity there. A similar behavior is known for the function $\chi_0(k)$ given by Eq. (111). Near $2k_F$ the latter behaves as

$$\chi_0\left[2k_F\left(1 \pm \frac{\Delta}{2}\right)\right] = \frac{mk_F}{2\pi^2\hbar^2}\left[1 \pm \frac{\Delta}{2}\ln\Delta + O(\Delta, \Delta^2\ln\Delta)\right] \tag{D.13}$$

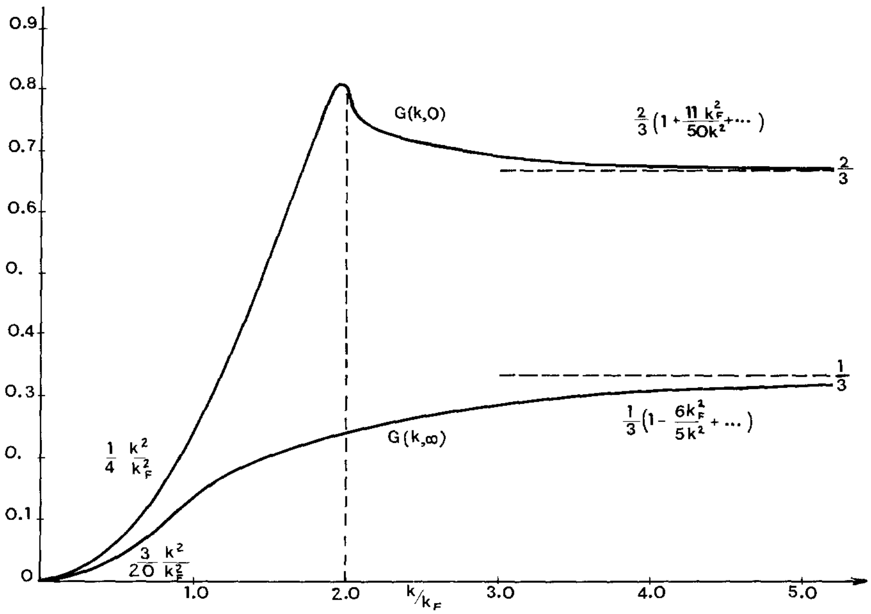

Fig. 7. The static limit $G(k, 0)$ and high-frequency limit $G(k, \infty)$ of the local field correction plotted vs. k/k_F. The indicated behavior for small and large k follows from the expressions given in Appendix D.

Hence one obtains for the static local field correction for k near $2k_F$ the result

$$G\left[2k_F\left(1 \pm \frac{\Delta}{2}\right), 0\right] = \frac{1}{8}\left\{-\frac{26}{15} + \frac{32}{15}\ln 2 + \frac{2\pi^2}{3}\right.$$
$$\left. \pm \left[6 + \frac{13}{15} - \frac{16}{15}\ln 2 - \frac{\pi^2}{3}\right]\Delta \ln \Delta\right\}$$
$$\simeq 0.791 \pm 0.354\, \Delta \ln \Delta \tag{D.14}$$

To see how the result (D.12) is obtained, we first use integration by parts on some of the integrals occurring in (D.11a):

$$\int_1^{1+\eta} dx \frac{1}{x - \frac{1}{2}\eta} \ln|x + 1| = \ln^2(\eta + 2) + \ln^2 2 - \ln 2 \ln|\eta^2 - 4|$$
$$- \int_{-1}^{\eta - 1} dx \frac{1}{x + 3} \ln\left|x + 2 - \frac{\eta}{2}\right| \tag{D.15}$$

Now for $\eta = 2 - \Delta$, $0 < \Delta \ll 1$, one has

$$\int_{-1}^{\eta-1} dx \frac{1}{x+3} \ln\left|x + 2 - \frac{\eta}{2}\right| = \int_{-1}^{1-\Delta} dx \frac{1}{x+3} \ln\left|x + 1 + \frac{\Delta}{2}\right|$$

$$= \int_{\Delta/2}^{\infty} dy \frac{\ln 2 - y + \frac{1}{4}\Delta e^y}{e^y + 1}$$

$$= \ln^2 2 - \frac{\pi^2}{12} - \frac{1}{4}\Delta \ln \Delta + O(\Delta, \Delta^2, \Delta^2 \ln \Delta) \tag{D.16}$$

Similarly, one has

$$\int_{1-\eta}^{1} dx \frac{1}{x + \frac{1}{2}\eta} \ln|x - 1| = \int_{-1+\Delta}^{1} dx \frac{1}{x + 1 - \frac{1}{2}\Delta} \ln|x - 1|$$

$$= \int_{\Delta/2}^{\infty} \frac{\ln 2 - y}{(1 - \frac{1}{4}\Delta)e^y - 1}$$

$$= -\ln 2 \ln\left(\frac{\Delta}{4}\right) - \frac{\pi^2}{6} + \frac{1}{4}\Delta \ln \Delta$$

$$+ O(\Delta, \Delta^2, \Delta^2 \ln \Delta) \tag{D.17}$$

where we have used the fact that $\ln \Delta$ can be written as

$$\ln \Delta = -\int_0^{\infty} dy \frac{1}{e^{\Delta + y} - 1}$$

Similar manipulations can be used for the integrals occurring in (D.11b) to show that for $\eta = 2 + \Delta$, $0 < \Delta \ll 1$, one obtains the result (D.12) where the sign of the $\Delta \ln \Delta$ term is reversed.

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