The dielectric constant of an interacting electron gas

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A simple method is proposed for finding the local-field correction to the dielectric constant of a system of interacting electrons. In this method, the local distortion of the mean induced density near an individual electron owing to exchange-correlation effects is automatically taken into account by determining the self-consistent potential at the given space-time point under the extra condition that one of the electrons of the system lies at that point. The stated method for accounting for exchange-correlation effects is initially developed within the framework of the single-particle approximation, and then is generalized to the case of analyzing the complete many-electron problem. By using it one can easily reproduce most of the currently known results on the dielectric constant, including those derived by the powerful methods of many-body theory. This study analyzes the contemporary state of the theory of the dielectric constant of an interacting electron gas and briefly presents an application of this theory for describing the physical properties of simple metals.

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CONTENTS

1. INTRODUCTION

One of the central areas in solid-state physics is occupied by studies of the degenerate, strongly interacting electron plasma of metals, which plays a decisive role in engendering the fundamental characteristics of the metal crystal, such as its structure, binding energy, phonon spectrum, and electromagnetic properties. Hence, in order to create a theory of the metallic state, we must know the properties of an electron plasma. The problem of calculating the properties of an interacting electron gas, while complicated *per se*, is even more complicated for a metal by the need of a parallel account for the strong electron-ion interaction. In order to single out the specific effects that stem solely from the Coulomb interaction between the conduction electrons, people often resort to a simplified model of a metal that replaces the ion lattice with a homogeneous passive background that serves only to ensure overall electroneutrality and stability of the system. A model system of N interacting electrons moving in a volume Ω in the background of a uniformly distributed positive charge is commonly called an interacting electron gas (sometimes an electron fluid). The properties of this system can be completely characterized by a single dimensionless rarefaction factor r_s, which is related to the electron number density by the relationship

$$\frac{\Omega}{N} = \frac{4\pi}{3}(a_B r_s)^3 \qquad (1.1)$$

The parameter r_s defines the radius of a sphere of volume equal to the mean volume per electron in the system in units of the Bohr radius $a_B = \hbar^2/me^2$.

This parameter is of the same order of magnitude as the ratio of the potential energy of the particles to their mean kinetic energy.

Owing to the singular behavior of the Fourier component of the Coulomb interaction $v(q) = 4\pi e^2/q^2\Omega$ for small q, which arises from the long-range nature of Coulomb forces, calculations of the properties of an electron gas by perturbation theory yield divergent expressions even in the second order in $v(q)$. As became clear after the studies of Bohm and Pines[1] and the later studies of Hubbard[2] and of Gell-Mann and Brueckner,[3] the long-range component of the interelectron Coulomb interaction is mainly responsible for the collective motions of the particles in the system (plasma oscillations). The latter have a rather high energy of excitation, whereas the individual motions of the electrons are determined by the screened Coulomb interaction with an effective radius of interaction of the order of 1 Å. Such a short-range interaction can be taken into account, even within the framework of elementary perturbation theory, in which no divergence difficulties arise. The corresponding calculations employing the screened interelectronic interaction enable one to obtain both the equilibrium thermodynamic and the kinetic characteristics of the electron gas.

The screening properties of the system of interacting electrons, just as the dispersion law of the plasma oscillations, are governed by the dielectric constant $\varepsilon(q, \omega)$, which depends on the wave vector q and the frequency ω. To calculate $\varepsilon(q, \omega)$ is the central problem in the entire theory of the electron gas. This problem

proves rather simple only in the case of a highly compressed system, i.e., when a small parameter $r_s \ll 1$ exists. As has been shown,[2,3] it suffices to employ the dielectric constant (DC) calculated for a noninteracting electron gas as $\varepsilon(q, \omega)$ in this case. Yet in real metals the conduction electrons have densities for which the corresponding values of the parameter r_s lie in the range $1 < r_s < 6$. During the past three decades, attempts have been repeatedly undertaken to construct a systematic theory of the DC of an electron gas (see, e.g., the reviews[4-6]). Although highly substantial progress has been made toward solving this pressing problem of solid-state physics, a satisfactory solution of it has not yet been found.

This article reviews the current state of the theory of the DC of a system of interacting electrons. Here we shall not adhere strictly to the historical course of development of events, and shall not treat all the numerous studies in this field, since this would require writing an extensive monograph. Instead, we shall show that most of the currently known results for $\varepsilon(q, \omega)$, even those derived by the modern methods of many-body theory, can actually be matched within the framework of a unified single-particle approach based on the method of the self-consistent field. The approach that we have employed automatically allows one to take into account the existence around the electron of an exchange-correlation hole. This is done by determining the self-consistent potential at the given space-time point under the extra condition that one of the electrons of the system lies at that point.

We shall devote the introductory Sec. 2 to presenting the fundamental problems. We shall discuss in detail therein the definition of the DC, its most general properties, and its connection with experimentally observable quantities. The following Sec. 3 briefly describes very simple one-particle approximations for the DC (Hartree-Fock and random-phase approximations). Section 4 of the review is devoted to discussing the problem of accounting for exchange-correlation effects within the framework of the one-particle approximation. The approach developed here will then be extended in Sec. 5 to the case of analyzing the complete many-particle problem. The fundamental idea employed in this section is that the initial Hamiltonian of the system in the presence of an external electromagnetic perturbation does not undergo second quantization on the basis of single-particle states in the form of plane waves, but on the basis of single-electron states that correspond to motion of the electron in the field of the external perturbation and in the self-consistent field of the rest of the electrons of the system. Thus, even in the first stage of calculation, we avail ourselves of an effective Hamiltonian that accounts to a considerable extent for the effect of screening of the probe charge introduced into the system by generation of an induced density. Section 6 of the review will briefly apply the theory of a homogeneous electron gas to describe the properties of simple metals. In particular, this section will generalize the method of the self-consistent field described in Sec. 4 that allows one to account for the effects of exchange and correlation in calculating both pair interionic forces

and many-ion interactions, which have been mainly treated thus far in the random-phase approximation. In conclusion we discuss the potentialities of experimental test of the effects predicted by the theory of the homogeneous electron gas, together with the problems of developing it further.

2. DEFINITION OF THE DIELECTRIC CONSTANT AND ITS FUNDAMENTAL PROPERTIES

Let us probe a system of electrons with an external source that has the Fourier component $\rho_{ext}(q, \omega)$ of charge density. Consequently, the induced charge $\rho_{ind}(\mathbf{r}, t)$, which fluctuates in space and time, arises in the system. In combination with $\rho_{ext}(\mathbf{r}, t)$, it amounts to the total variation of charge $\rho_{tot}(\mathbf{r}, t) = \rho_{ext}(\mathbf{r}, t) + \rho_{ind}(\mathbf{r}, t)$. This perturbation of the system produces in it a macroscopic electric charge whose induction $\mathbf{D}(\mathbf{r}, t)$ and field intensity $\mathbf{E}(\mathbf{r}, t)$ are given by the Maxwell equations

$$\operatorname{div} \mathbf{D} = 4\pi\rho_{ext}, \quad \operatorname{div} \mathbf{E} = 4\pi\rho_{tot}. \tag{2.1}$$

As is usual in the electrodynamics of continuous media,[7,8] the dielectric constant $\varepsilon(q, \omega)$ is defined in terms of the stated quantites by any of the relationships:

$$\begin{aligned} \mathbf{D}(q, \omega) &= \varepsilon(q, \omega) \mathbf{E}(q, \omega), \\ \rho_{ext}(q, \omega) &= \varepsilon(q, \omega) \rho_{tot}(q, \omega). \end{aligned} \tag{2.2}$$

In the general case, the oscillations of the individual harmonic components of the induced charge are phase-shifted with respect to the corresponding oscillations of the external charge. Hence the function $\varepsilon(q, \omega)$ introduced by the formulas of (2.2) proves complex. An extremely important problem here is that of its analytic properties. We shall begin the analysis of the general properties of the function $\varepsilon(q, \omega)$ by discussing it.

In a homogeneous system of interacting electrons, the Fourier components of the induced and external charges in the linear-response case are interrelated by

$$\rho_{ind}(q, \omega) = v(q) \chi(q, \omega) \rho_{ext}(q, \omega). \tag{2.3}$$

Here $v(q) = 4\pi e^2 q^2 \Omega$ is the Fourier component of the Coulomb potential, and $\chi(q, \omega)$ is the response function for the external charge (also called the polarizability of the system), which is defined by the expression

$$\chi(q, \omega) = -\frac{i}{\hbar} \int_0^\infty dt\, e^{i(\omega + i\delta)t} \langle [n(q, t), n^+(q, 0)] \rangle. \tag{2.4}$$

Here $n(q) = \sum_j \exp(-i\mathbf{q} \cdot \mathbf{r})$ is the Fourier component of the electron-density operator, while the quantity $\langle [n(q, t), n^+(q, 0)] \rangle$ is the statistical mean of the commutator of the operators $n(q)$ and $n^+(q)$ in the Heisenberg representation. As a function of the complex variable $\omega, \chi(q, \omega)$ is analytic in the upper half-plane, including the real axis. At infinity it is proportional to $1/\omega^2$. The Cauchy integral for the function $\chi(q, \omega)$ taken along the real axis is equal in this case to

$$\mathscr{P} \int_{-\infty}^\infty d\omega'\, \frac{\chi(q, \omega')}{\omega' - \omega} = i\pi\chi(q, \omega). \tag{2.5}$$

Here $\mathscr{P}$ is the symbol for the principal value. Upon separating the real and imaginary components in (2.5), we arrive at the Kramers-Kronig relationships for the response function $\chi(q, \omega)$:

$$\text{Re}\,\chi(q, \omega) = \frac{1}{\pi}\,\mathscr{P}\int_{-\infty}^{\infty} d\omega'\,\frac{\text{Im}\,\chi(q, \omega')}{\omega' - \omega}, \tag{2.6a}$$

$$\text{Im}\,\chi(q, \omega) = -\frac{1}{\pi}\,\mathscr{P}\int_{-\infty}^{\infty} d\omega'\,\frac{\text{Re}\,\chi(q, \omega')}{\omega' - \omega}. \tag{2.6b}$$

One can also derive these relationships directly by starting with the definition (2.4) for $\chi(q, \omega)$.

The fact that the function $\chi(q, \omega)$ obeys the Kramers-Kronig relationships is a direct consequence of the causal character of the response of the system to an external perturbation. Upon being rewritten by using the corresponding Fourier components with respect to the time, Eq. (2.3) acquires the form

$$\rho_{\text{ind}}(q, t) = \frac{v(q)}{\hbar}\int_{-\infty}^{\infty} dt'\,\chi(q, t - t')\,\rho_{\text{ext}}(q, t'). \tag{2.7}$$

On the other hand, we find from Eq. (2.4) by direct integration that

$$\chi(q, t - t') = \hbar\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\chi(q, \omega)\,e^{-i\omega(t - t')}$$
$$= -i\theta(t - t')\langle[n(q, t), n^+(q, t')]\rangle. \tag{2.8}$$

Here $\theta(t - t')$ is the unit step function

$$\theta(t - t') = \begin{cases} 1, & t > t', \\ 0, & t \leqslant t'. \end{cases}$$

Thus, in full accord with the principle of causality, the result (2.7) implies that the induced charge arising in the system at the instant t of time arises from the cumulative action on it of the external perturbation over all the preceding instants of time $t' < t$.

Now let us discuss the problem of whether the dielectric constant $\varepsilon(q, \omega)$ satisfies the Kramers-Kronig relationships. Upon employing (2.2) and (2.3), and taking account of the fact that $\rho_{\text{tot}}(q, \omega) = \rho_{\text{ext}}(q, \omega) + \rho_{\text{ind}}(q, \omega)$, we arrive at the following general formula for $\varepsilon(q, \omega)$ in the linear-response approximation:

$$\varepsilon^{-1}(q, \omega) = 1 + v(q)\,\chi(q, \omega). \tag{2.9}$$

We see from this formula that the reciprocal of the dielectric constant $1/\varepsilon(q, \omega)$ in any case should satisfy the Kramers-Kronig relationships, which we shall write in the following explicit form:

$$\text{Re}\,\varepsilon^{-1}(q, \omega) = 1 + \frac{2}{\pi}\,\mathscr{P}\int_0^{\infty} d\omega'\,\frac{\omega'}{\omega'^2 - \omega^2}\,\text{Im}\,\varepsilon^{-1}(q, \omega'), \tag{2.10a}$$

$$\text{Im}\,\varepsilon^{-1}(q, \omega) = -\frac{i2\omega}{\pi}\,\mathscr{P}\int_0^{\infty}\frac{d\omega'}{\omega'^2 - \omega^2}\,\text{Re}\,\varepsilon^{-1}(q, \omega'). \tag{2.10b}$$

As concerns the functions $\varepsilon(q, \omega)$ directly, most studies on the electrodynamics of continuous media (see, e.g., Refs. 7, 8) usually assume without the appropriate detailed analysis that it also obeys relationships of the type of (2.10). Starting with this assumption, an entire series of sum rules has been derived that the quantity $\varepsilon(q, \omega)$ must satisfy.[9] Yet $\varepsilon(q, \omega)$ is not generally a causal response function. To prove this, let us introduce into the treatment the screened response function $\pi(q, \omega)$ that establishes the connection between the induced and total charges:

$$\rho_{\text{ind}}(q, \omega) = -v(q)\,\pi(q, \omega)\,\rho_{\text{tot}}(q, \omega). \tag{2.11}$$

We can easily convince ourselves that $\varepsilon(q, \omega)$ can be expressed in terms of the screened response function (often also called the irreducible polarization operator) as follows:

$$\varepsilon(q, \omega) = 1 + v(q)\,\pi(q, \omega). \tag{2.12}$$

This formula shows that the function $\varepsilon(q, \omega)$ actually defines the response of the system to the total charge. It is generally impossible for the induced charge to be governed by the total charge (which in turn itself depends on the induced charge). Hence we cannot treat the quantities $\pi(q, \omega)$ and $\varepsilon(q, \omega)$ as being causal response characteristics and require them to satisfy the Kramers-Kronig relationships.

The idea of the possible breakdown of the Kramers-Kronig relationships for the longitudinal dielectric function $\varepsilon(q, \omega)$ has been advanced in Refs. 10 and 11. This problem has been analyzed in detail in the review of Kirzhnits.[12] He showed that the very fact of breakdown of the Kramers-Kronig relationships for $\varepsilon(q, \omega)$ does not contradict any of the general principles of stability of the system. This same study treats the consequences to which this breakdown leads. In particular, the static DC $\varepsilon(q, 0)$ of the system can prove negative. On the other hand, as was shown in Ref. 12, when $q = 0$, the function $\varepsilon(0, \omega)$ characterizes a causal response, and it obeys the Kramers-Kronig relationships. Reference 13 gives a detailed analysis of the reasons why the Kramers-Kronig relationships for $\varepsilon(q, \omega)$ can break down in different physical systems, including an electron gas. This same study discusses the consequences of the existence of negative values of the static dielectric function $\varepsilon(q, 0)$ for a set of problems of metal theory, in particular, for problems of high-temperature superconductivity. Henceforth in this review, we shall practically not concern ourselves with the stated problems, but shall focus our attention on the quantity $\varepsilon^{-1}(q, \omega)$, which is a causal response function, and which satisfies without reservations the Kramers-Kronig relationships in a dynamically stable system, together with all their consequences.

First let us note that, if the studied model system of interacting electrons actually existed, then one could directly measure the imaginary component of its reciprocal dielectric function $\varepsilon^{-1}(q, \omega)$ by setting up an experiment on inelastic scattering by the system of a beam of probe charges (fast electrons). The double differential cross-section of this scattering in the first Born approximation has the form

$$\frac{d^2\sigma}{d\varepsilon_1\,d\Omega_{k_1}} = \frac{k_1}{k_0}\left(\frac{e^2}{\varepsilon_q}\right)^2 S(q, \omega). \tag{2.13}$$

Here $\hbar k_1$ and $\varepsilon_1 = \hbar^2 k_1^2/2m$ are respectively the momentum and energy of the scattered electron when far from the target; $d\Omega_{k_1}$ is the element of solid angle in which the scattered particles are detected; $\hbar q = \hbar(k_0 - k_1)$ and $\hbar\omega = \hbar^2(k_0^2 - k_1^2)/2m$ are the momentum and energy imparted to the system in the scattering event; $\varepsilon_q = \hbar^2 q^2/2m$; and finally $S(q, \omega)$ denotes the function

$$S(q, \omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\,e^{i\omega t}\langle n(q, t)\,n^+(q, 0)\rangle. \tag{2.14}$$

The latter is called the dynamic structure factor. This function is real and satisfies the relationships

$$S(-q, \omega) = S(q, \omega), \quad S(q, -\omega) = e^{-\hbar\omega/kT}\,S(q, \omega). \tag{2.15}$$

We can easily show by employing Eqs. (2.4), (2.9),

(2.14), and (2.15) that the function $\varepsilon^{-1}(q, \omega)$ is expressed in terms of $S(q, \omega)$ as follows:

$$\varepsilon^{-1}(q, \omega) = 1 + v(q) \int_{-\infty}^{\infty} d\omega' S(q, \omega') \left(\frac{1}{\omega - \omega' + i\delta} - \frac{1}{\omega + \omega' + i\delta} \right). \quad (2.16)$$

Thus the dynamic structure factor plays the role of the spectral density for the function $\varepsilon^{-1}(q, \omega)$. Upon isolating the imaginary component in (2.16), we find the sought formula

$$\text{Im } \varepsilon^{-1}(q, \omega) = -\pi v(q)(1 - e^{-\hbar\omega/kT}) S(q, \omega). \quad (2.17)$$

Equation (2.17) establishes a rigorous connection between the imaginary component of the response function to a longitudinal perturbation and the spectral distribution of density fluctuations in an equilibrium many-electron system. Similar relationships that also hold for the spin susceptibility and for the response functions to transverse fields are called the fluctuation-dissipative theorems.

To see what information we can extract about the system by measuring its dynamic structure factor, let us for simplicity examine the case of $T = 0$, and rewrite Eq. (2.17) in the following form:

$$S(q, \omega) = \frac{\theta(\omega)}{\pi v(q)} \frac{\varepsilon_2(q, \omega)}{\varepsilon_1^2(q, \omega) + \varepsilon_2^2(q, \omega)}. \quad (2.18)$$

Here $\varepsilon_1(q, \omega)$ and $\varepsilon_2(q, \omega)$ are the real and imaginary components of the dielectric function:

$$\varepsilon(q, \omega) = \varepsilon_1(q, \omega) + i\varepsilon_2(q, \omega). \quad (2.19)$$

Let us assume that the imaginary component of the dielectric function vanishes in some region of values of (q, ω). In this case, upon transforming to the limit as $\varepsilon_2 \to 0$ in Eq. (2.18), we get

$$S(q, \omega) = \frac{\theta(\omega)}{v(q)} \delta(\varepsilon_1(q, \omega)). \quad (2.20)$$

Consequently, if we have $\varepsilon_2(q, \omega) = 0$ in some region of values of transferred energies and momenta, then a nonzero contribution to the dynamic structure factor will will arise only from those q and ω in this region for which we also have $\varepsilon_1(q, \omega) = 0$. Upon taking account of (2.19), we can write this condition in the form

$$\varepsilon(q, \omega) = 0. \quad (2.21)$$

The roots of Eq. (2.21) define the dispersion law $\omega = \omega(q)$ of the collective excitation modes in the electron gas whose existence does not stem from the introduction of external charges into the system. Actually, when $\rho_{\text{ext}} = 0$, we can represent Eqs. (2.1) in the form

$$\varepsilon(q, \omega) q E(q, \omega) = 0, \quad q E(q, \omega) = 4\pi\rho_{\text{ind}}(q, \omega).$$

Along with the trivial solution $q \cdot E(q, \omega) = 4\pi\rho_{\text{ind}}(q, \omega) = 0$, when the condition (2.21) is satisfied, these equations allow the existence in the system of a nonzero alternating electric field $E(q, \omega(q))$ caused by free oscillations of the charge density $\rho_{\text{ind}}(q, \omega)(q)$ (i.e., plasma oscillations). In the neighborhood of the frequency $\omega = \omega(q)$, the expression (2.20) for $S(q, \omega)$ acquires the form

$$S(q, \omega) = \frac{\theta(\omega)}{v(q)} \left(\frac{\partial \varepsilon_1}{\partial \omega} \right)^{-1}_{\omega = \omega(q)} \delta(\omega - \omega(q)). \quad (2.22)$$

The formula (2.22) shows that the dynamic structure factor shows a sharp peak of characteristic losses corresponding to production of plasmons (while, owing to (2.13), so does the double differential scattering cross-section for fast electrons).

Actually the dispersion equation (2.21) has a real solution $\omega = \omega_p \equiv \sqrt{4\pi N e^2/m\Omega}$ only in the long-wavelength limit $q \to 0$, for which the plasmons do not decay. The latter circumstance involves the fact that, when $q = 0$, the Fourier component of the electron-current-density operator

$$j(q) = -\frac{e}{2m} \sum_j (p_j e^{-iqr_j} + e^{-iqr_j} p_j)$$

commutes with the Hamiltonian of the system. Hence the electron-density oscillations of zero wave vector do not decay via interelectron interactions. However, the plasmons decay for finite q. Here, since in a dynamically stable system the function $\varepsilon^{-1}(q, \omega)$ should not have singularities in the upper half-plane of the complex variable ω, the complex plasma frequency $\omega(q)$ defined by Eq. (2.21) can lie only in the lower half-plane. That is, we have

$$\omega(q) = \omega_q - i\gamma_q \quad (\gamma_q > 0).$$

For small q, the laws of conservation of energy and momentum impede the conversion of a plasmon into an electron-hole pair, although they do not forbid its decay with multiple creation of such pairs. Consequently, for small q the decay γ_q proves small, and as before, the dynamic structure factor $S(q, \omega)$ shows a sharp plasmon resonance at the frequency $\omega = \omega_q$. With increasing q, this resonance continues to broaden and becomes ever less distinct, and can even vanish suddenly, provided only that the plasmon branch $\omega = \omega_q$ penetrates into the region of creation of single electron-hole pairs. Far from the plasmon resonance, the dynamic structure factor is mainly governed by the type of behavior of the imaginary component of the dielectric function [see Eq. (2.18)]. Here the dominant contribution to $S(q, \omega)$ comes from processes of excitation of electron-hole pairs.

An important integral characteristic of the overall behavior of the functions $S(q, \omega)$ and $\text{Im}\,\varepsilon^{-1}(q, \omega)$ throughout the spectral range is their moments with respect to the frequency. One can easily show by starting with (2.15) and (2.17) that the following equation holds for the moments of these functions:

$$\int_{-\infty}^{\infty} d\omega \omega^l \text{Im } \varepsilon^{-1}(q, \omega) = -\pi v(q)[1 - (-1)^l] \int_{-\infty}^{\infty} d\omega \omega^l S(q, \omega). \quad (2.23)$$

We see from this that the even moments of the function $\varepsilon^{-1}(q, \omega)$ vanish identically. Upon turning to Eq. (2.14), we obtain

$$\int_{-\infty}^{\infty} d\omega S(q, \omega) e^{i\omega t} = \frac{1}{\hbar} \langle n(q, 0) n^+(q, t) \rangle.$$

If we now differentiate this relationship l times with respect to t, and then set $t = 0$, we arrive at the so-called sum rule for the moments of the dynamic structure factor

$$\int_{-\infty}^{\infty} d\omega \omega^l S(q, \omega) = \frac{1}{\hbar^{l+1}} \langle n(q) \hat{L}^l n^+(q) \rangle. \quad (2.24)$$

Here $\hat{L}$ is the Liouville operator, whose action on the quantum-mechanical operator f is determined by the rule $\hat{L}f = Hf - fH$, where H is the Hamiltonian of the sys-

tem. Finally, by starting with (2.15), (2.23), and (2.24), and also by accounting for the fact that $\langle f \hat{L} f' \rangle = -\langle (\hat{L} f) f' \rangle$, we arrive at the formula for the moments of the function $\text{Im}\,\varepsilon^{-1}(q, \omega)$:

$$\int_0^\infty d\omega \omega^{2l+1}\,\text{Im}\,\varepsilon^{-1}(q,\,\omega) = -\frac{\pi\nu(q)}{2\hbar^{2l+2}}\,\langle[n(q),\,\hat{L}^{2l+1}n^+(q)]\rangle. \qquad (2.25)$$

The sum rule for the first moment has the following form:

$$\int_0^\infty d\omega \omega\,\text{Im}\,\varepsilon^{-1}(q,\,\omega) = -\frac{\pi}{2}\,\omega_p^2. \qquad (2.26)$$

Here ω_p is the plasma frequency of the electron gas in the long-wavelength limit. The corresponding sum rule for the dynamic structure factor is expressed by the formula

$$\int_0^\infty d\omega \omega S(q,\,\omega) = \frac{Nq^2}{2m}. \qquad (2.27)$$

The relationships (2.26) and (2.27) are often called the f sum rule. As we can see well from (2.25), the first moment of the function $\text{Im}\,\varepsilon^{-1}(q,\,\omega)$ does not depend on the interaction between the electrons, and actually the f sum rule reflects only the requirement of conservation of the number of particles.[9] In this sense, the first moment is fully identical for systems of either interacting or free electrons. A difference involving account of the interaction is manifested only in the third moment of the function $\text{Im}\,\varepsilon^{-1}(q,\,\omega)$, an explicit expression which has the form

$$\int_0^\infty d\omega \omega^3\,\text{Im}\,\varepsilon^{-1}(q,\,\omega)$$
$$= -\frac{\pi\omega_p^2}{2\hbar^2}\left\{\varepsilon_q^2 + 4\varepsilon_q\frac{\langle T\rangle}{N} + \frac{\hbar^2\omega_p^2}{N}\sum_{k\neq 0}\frac{(k\cdot q)^2}{k^2q^2}[S(k+q) - S(k)]\right\}. \qquad (2.28)$$

In this formula, we have $\varepsilon_q = \hbar^2 q^2/2m$, $\langle T\rangle$ is the mean kinetic energy of the system, and $S(q)$ is the static structure factor:

$$S(q) = \frac{\hbar}{N}\int_{-\infty}^\infty d\omega S(q,\,\omega) = \frac{T}{N}\langle n(q)\,n^+(q)\rangle. \qquad (2.29)$$

The existence of exact sum rules satisfied by the true function $\varepsilon^{-1}(q,\,\omega)$ enables one to test the accuracy of approximate expressions for the dielectric function. Generally such a test enables one to reveal the physical adequacy of the approximations that some particular concrete theory of the dielectric constant is actually based on.

A serious test for an approximate dielectric function is the so-called compressibility sum rule. One can show rigorously[15] that the polarization operator $\pi(q, \omega)$ for zero q and ω can be expressed in terms of the isothermal compressibility K of the electron gas:

$$\pi(0,\,0) = \frac{N^2 K}{\Omega}. \qquad (2.30)$$

Consequently, in the long-wavelength limit, the formula (2.12) for $\omega = 0$ acquires the following asymptotically exact form:

$$\varepsilon(q,\,0)\xrightarrow[q\to 0]{} 1 + \left(\frac{\varkappa_{TF}}{q}\right)^2\frac{K}{K_f}. \qquad (2.31)$$

Here $\varkappa_{TF} = (6\pi Ne^2/\varepsilon_F\Omega)^{1/2}$ is the Thomas-Fermi wave number, while $K_f = 3\Omega/2N\varepsilon_F$ is the compressibility of

the free-electron gas at $T = 0$. The relationship (2.31) is known as the compressibility sum rule. On the other hand, one can determine the compressibility of the electron gas in another way in addition to (2.30), which now requires a knowledge of the dielectric constant for all q and ω. Namely, one can employ the thermodynamic relationship[9]

$$\frac{K_f}{K} = \frac{1}{6}\alpha^2 r_s^2\left[r_s^2\frac{d^2\varepsilon(r_s)}{dr_s^2} - 2r_s\frac{d\varepsilon(r_s)}{dr_s}\right]. \qquad (2.32)$$

Here $\alpha = (4/9\pi)^{1/3} \approx 0.521$, and $\varepsilon(r_s)$ is the energy of the ground state per electron expressed in Rydbergs, which obeys the formula

$$\varepsilon(r_s) = \frac{3}{5\alpha^2 r_s^2} - \frac{2\hbar^2}{me^4 r_s^2}\int_0^{r_s} dr_s r_s\sum\left[\frac{2\pi e^2}{q^2\Omega} + \frac{\hbar}{N}\int_0^\infty\frac{d\omega}{2\pi}\,\text{Im}\,\varepsilon^{-1}(q,\,\omega)\right]. \qquad (2.33)$$

People generally assume that an approximate dielectric function satisfies the compressibility sum rule if Eqs. (2.31) and (2.32) give the same result for the quantity K. A lack of such agreement indicates lack of self-consistency of the approximate expression for $\varepsilon(q, \omega)$.

In closing this section, we shall discuss briefly the problem of what physical consequences might arise from a possible breakdown of the Kramers-Kronig relationships for the reciprocal dielectric constant $\varepsilon^{-1}(q, \omega)$ in an interacting electron gas. Purely formally, such a situation corresponds to the appearance in this function of at least one pole in the upper half-plane of the complex frequency, e.g., one lying at the point $\omega = \omega_1 + i\omega_2$ ($\omega_2 > 0$). In turn, this means that the dielectric constant of the system vanishes at the stated point:

$$\varepsilon(q,\,\omega_1 + i\omega_2) = 0.$$

Here a singularity arises in the spectrum of density fluctuations at the frequency ω_1 [see Eq. (2.18)], which corresponds physically to an exponentially rapid growth of the contribution from the component $n(q, \omega_1 + i\omega_2)$. Consequently the homogeneous electron gas becomes unstable with respect to formation of the so-called charge-density waves.

The possible transition of a system of interacting electrons to a state characterized by an inhomogeneous distribution of charge density has been discussed for a long time. One example of such a state might be a Wigner crystal. As early as the thirties, Wigner proposed[16] that, when the density of an electron gas is decreased (i.e., the parameter r_s increases), its homogeneous state ceases to be stable, and the electrons must rearrange into a crystal lattice. Concrete calculations of the value of r_s at which a phase transition can occur from a homogeneous electron gas to a Wigner crystal give a very great scatter of critical values of r_s ($6 < r_s < 100$) (see the review[17]). We should note that most of the studies on this problem have treated a transition from a homogeneous gaseous phase directly to a crystal lattice of localized electrons. However, as noted in the review,[13] a situation can occur in which a transition first occurs to an inhomogeneous state having a small amplitude of density modulation, i.e., to a state corresponding to a so-called coherent crystal.[18] Concretely, this possibility has been discussed for the cases of a three-dimensional[19] and a two-dimensional[20,21] electron gas in a magnetic field.

Within the framework of the model of an electron gas with a passive neutralizing background, the possible transition to a Wigner-crystal state arouses some doubt involving the following circumstance. One can show[22] that the instability of the system upon breakdown of the Kramers-Kronig relationships and the onset of an inhomogeneous state having some wave vector q_0 is manifested in the fact that the static polarizability $\chi(q, 0)$ becomes infinite for the given value of the wave vector:

$$\chi(q_0, 0) = \infty. \tag{2.34}$$

In most of the known approximate expressions for the static dielectric constant $\varepsilon(q, 0)$, the polarization operator for a momentum $q = 0$ becomes negative at values of the parameter r_s that are usually smaller than those for which the condition (2.34) is satisfied. In turn, owing to (2.30), the condition $\pi(0, 0) < 0$ implies the appearance of a negative compressibility. In this case, self-compression of the electron gas or a transition resembling an ordinary liquid-gas transition precedes a transition to a state having a charge-density wave. The studies of Wiser and Cohen[23] and of Van Horn[24] have paid attention to this situation. When one accounts for a finite compressibility of the neutralizing background, a transition to the state of a Wigner crystal becomes even more probable.

3. VERY SIMPLE APPROXIMATIONS FOR THE DIELECTRIC CONSTANT (HARTREE-FOCK AND RANDOM-PHASE)

One can actually calculate the dielectric constant of a system of interacting electrons only approximately by employing some particular simplified description of the many-electron system. A very simple approximation for $\varepsilon(q, \omega)$ arises when one completely neglects the Coulomb interactions between the electrons in finding the induced-charge density (but, of course, necessarily accounts for the Pauli principle). In this case $\rho_{ind}(q, \omega)$ is defined by Eq. (2.3). However, in the latter the Lindhard function enters instead of $\chi(q, \omega)$:

$$\chi_0(q, \omega) = 2 \sum_k \frac{n_k - n_{k+q}}{\hbar\omega - \varepsilon_{k+q} + \varepsilon_k + i\delta}. \tag{3.1}$$

This amounts to the polarizability of a system of noninteracting electrons. In this formula, n_k is the Fermi distribution function, while $\varepsilon_k = \hbar^2 k^2 / 2m$ is the energy of a free particle. In this approximation the dielectric constant obeys the formula

$$\varepsilon_0^{-1}(q, \omega) = 1 + v(q) \chi_0(q, \omega). \tag{3.2}$$

The expression (3.2) for the DC is known in the literature as the Hartree-Fock approximation,[25] since substitution of $\varepsilon_0(q, \omega)$ into Eq. (2.33) leads to the Hartree-Fock result for the energy of the ground state of a homogeneous electron gas. The neglect of correlation effects renders the approximation (3.2) physically quite unsound in many respects. In particular, we can easily convince ourselves that $\varepsilon_0(q, \omega)$ incorrectly describes the phenomenon of screening. Actually, if we use the Lindhard function in Eq. (2.3) instead of the true polarizability, then we can write the following expression for the static potential $V_{ind}(q, 0)$ induced in the system under the action of the external source $V_{ext}(q, 0)$:

$$V_{ind}(q, 0) = \frac{4\pi e^2}{q^2 \Omega} \chi_0(q, 0) V_{ext}(q, 0).$$

Let us account for the fact that

$$\lim_{q \to 0} \chi_0(q, 0) = -\frac{3N}{2\varepsilon_F}, \tag{3.3}$$

where ε_F is the Fermi energy of the system of noninteracting electrons. Then we see that the ratio $V_{ind}(q, 0)/V_{ext}(q, 0)$ approaches minus infinity in the limit of small wavenumbers q. Correspondingly, the overall potential proves also to diverge at large distances from the probe charge. Such a gross overscreening is physically evidently meaningless, and it has been a direct consequence of the neglect of the Coulomb repulsion between the electrons in the process of generation of the induced charge.

An approximation is far more reasonable in which the electrons as before are treated formally as independent particles, but now one seeks their response to the overall screened potential, rather than to the external field. In this case the induced-charge density proves to be

$$\rho_{ind}(q, \omega) = v(q) \chi_0(q, \omega) \rho_{tot}(q, \omega). \tag{3.4}$$

Comparison of Eqs. (3.4) and (2.11) shows that, in the studied approximation, the polarization operator is defined by the formula

$$\pi_{RPA}(q, \omega) = -\chi_0(q, \omega). \tag{3.5}$$

In line with (2.12), this leads to the following expression for the DC:

$$\varepsilon_{RPA}(q, \omega) = 1 - v(q) \chi_0(q, \omega). \tag{3.6}$$

The formula (3.6) for the DC was first derived by Lindhard.[26] This result has subsequently been repeatedly reobtained by use of a whole set of theoretical methods, in the approximation on which it is based on has received several names.[25] The most widespread term is apparently the random-phase approximation (RPA), which we shall adopt here.

Upon starting with (2.9) and (3.6), we can easily find the polarizability of a system of interacting electrons in the RPA:

$$\chi_{RPA}(q, \omega) = \frac{\chi_0(q, \omega)}{1 - v(q) \chi_0(q, \omega)}. \tag{3.7}$$

With accounting of (3.3) we have in the limit of small wave numbers

$$\chi_{RPA}(q, 0) \xrightarrow{q \to 0} -\frac{q^2 \Omega}{4\pi e^2}.$$

Hence, in the RPA the static induced potential $V_{ind}(q, 0)$ is related to the external potential $V_{ext}(q, 0)$ by

$$\lim_{q \to 0} \frac{V_{ind}(q, 0)}{V_{ext}(q, 0)} = -1.$$

This is the condition for complete screening of the field from a static probe charge at large distances.

Within the framework of the random-phase approximation, the interacting electrons are treated as free particles moving in the total screened potential

$$V_{tot}(q, \omega) = \frac{V_{ext}(q, \omega)}{\varepsilon(q, \omega)} = V_{ext}(q, \omega) + v(q) n_{ind}(q, \omega). \tag{3.8}$$

This corresponds to the interaction of the electron with the external field and with the mean Hartree field of the induced charge. The Fourier component of the electron

number density $n_{ind}(\mathbf{q}, \omega)$ in the induced charge is then found in self-consistent fashion by the equation

$$n_{ind}(\mathbf{q}, \omega) = \chi_0(\mathbf{q}, \omega) V_{tot}(\mathbf{q}, \omega)$$
$$= \chi_0(\mathbf{q}, \omega) [V_{ext}(\mathbf{q}, \omega) + v(\mathbf{q}) n_{ind}(\mathbf{q}, \omega)]. \quad (3.9)$$

This expression for the induced density can easily be derived by employing the Hartree approximation to describe the motion of the system of interacting electrons in the external field. For this reason, $\varepsilon_{RPA}(\mathbf{q}, \omega)$ is sometimes called the dielectric constant in the self-consistent Hartree approximation.

The general properties of the function $\varepsilon_{RPA}(\mathbf{q}, \omega)$ have been described in a whole series of monographs on solid-state theory and statistical physics (see e.g., Refs. 9, 25, 27–29). Hence we shall not treat this problem globally here, but shall only take up the following aspects: to what extent does the dielectric function $\varepsilon_{RPA}(\mathbf{q}, \omega)$ satisfy the exact sum rules, and how reliable is the random-phase approximation at densities corresponding to the densities of conduction electrons in real metals?

First let us treat the compressibility sum rule. We can easily see from (3.3) and (3.6) that the static dielectric constant $\varepsilon_{RPA}(\mathbf{q}, 0)$ behaves as follows as in the limit of small wave numbers

$$\varepsilon_{RPA}(\mathbf{q}, 0) \xrightarrow[q \to 0]{} 1 + \frac{\varkappa_{TF}^2}{q^2}. \quad (3.10)$$

Comparison of (3.10) with (2.31) shows that the compressibility K of a system of interacting electrons as calculated in the RPA by starting with the behavior of the static DC in the long-wavelength limit is identical with the compressibility K_f of a free electron gas. Yet the thermodynamic definition of the compressibility based on the formulas (2.32) and (2.33) yields a different result. The values of the ratio K/K_f found in the RPA by differentiating the energy of the ground state are given in Table I. Thus we see that the compressibility sum rule is satisfied in the RPA only in the limit $r_s \ll 1$, i.e., outside the range of conduction-electron densities in real metals.

Within the framework of the RPA, we note that the Kramers-Kronig relationships hold for both the function $\varepsilon_{RPA}^{-1}(\mathbf{q}, \omega)$ and the function $\varepsilon_{RPA}(\mathbf{q}, \omega)$. One can directly prove the latter statement by starting with the definitions (3.6) and (3.1). If we employ the identity transformation

$$\mathscr{P} \sum_k \frac{n_k - n_{k+q}}{\hbar\omega - \varepsilon_{k+q} + \varepsilon_k} = \mathscr{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega'} \sum_k (n_k - n_{k+q}) \delta(\hbar\omega' - \varepsilon_{k+q} + \varepsilon_k),$$

then we can easily see that the following relationship holds:

$$Re \, \varepsilon_{RPA}(\mathbf{q}, \omega) = 1 + \frac{1}{\pi} \mathscr{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega' - \omega} Im \, \varepsilon_{RPA}(\mathbf{q}, \omega'). \quad (3.11a)$$

To derive the inverse relationship, we can conveniently

r_s	0	1	2	3	4	5	6
K_f/K	1	0.83	0.64	0.45	0.24	0.03	−0.19

employ the following representation for the δ-function:

$$\mathscr{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega' - \omega} \frac{\omega' - \omega_{nm}}{(\omega' - \omega_{nm})^2 + \delta^2} = \pi \frac{\delta}{(\omega - \omega_{nm})^2 + \delta^2} \xrightarrow[\delta \to 0]{} \pi^2 \delta(\omega - \omega_{nm}).$$

Thereby we can easily convince ourselves that

$$\frac{1}{\pi} \mathscr{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega' - \omega} Re \, \varepsilon_{RPA}(\mathbf{q}, \omega') = -Im \, \varepsilon_{RPA}(\mathbf{q}, \omega). \quad (3.11b)$$

As regards the function $\varepsilon_{RPA}^{-1}(\mathbf{q}, \omega)$, its fulfillment of the Kramers-Kronig relationships is already implied by the fact that the roots of the function $\varepsilon_{RPA}^{-1}(\mathbf{q}, z)$ can only lie on the real axis of the plane of the complex variable z, as can be directly shown from its explicit form.

Now let us examine the situation in the RPA with regard to satisfaction of the sum rules for the moments of the function $Im \, \varepsilon^{-1}(\mathbf{q}, \omega)$. This function has a rather unwieldy explicit form, but we can find its moments without resorting to direct integration. Upon employing the fact that the function $Im \, \varepsilon_{RPA}^{-1}(\mathbf{q}, \omega)$ vanishes at high frequencies, we can represent the Kramers-Kronig relationship of (2.10a) in the form

$$\varepsilon_{RPA}^{-1}(\mathbf{q}, \omega) \xrightarrow[\omega \to \infty]{} 1 - \frac{2}{\pi} \sum_{l=0}^{\infty} \frac{1}{\omega^{2l+2}} \int_0^{\infty} d\omega' \omega'^{2l+1} Im \, \varepsilon_{RPA}^{-1}(\mathbf{q}, \omega). \quad (3.12)$$

On the other hand, the direct expansion of the exact expression for $\varepsilon_{RPA}^{-1}(\mathbf{q}, \omega)$ at large ω has the form

$$\varepsilon_{RPA}^{-1}(\mathbf{q}, \omega) \xrightarrow[\omega \to \infty]{} 1 + \frac{\omega_p^2}{\omega^2} + \frac{\omega_p^2}{\hbar^2 \omega^4} \left(\varepsilon_q^2 + \frac{12}{5} \varepsilon_F \varepsilon_q + \hbar^2 \omega_p^2 \right) + O(\omega^{-6}). \quad (3.13)$$

First, a comparison of the formulas (3.12) and (3.13) indicates that the f sum rule is fulfilled in the RPA. Second, it gives the result for the third moment directly:

$$\int_0^{\infty} d\omega \, \omega^3 \, Im \, \varepsilon_{RPA}^{-1}(\mathbf{q}, \omega) = -\frac{\pi \omega_p^2}{2\hbar^2} \left(\varepsilon_q^2 + 4\varepsilon_q \frac{\langle T \rangle_f}{N} + \hbar^2 \omega_p^2 \right). \quad (3.14)$$

Here $\langle T \rangle_f$ is the mean kinetic energy of a system of free electrons having the same density. One can also derive explicit expressions in quite analogous fashion for the moments of the function $Im \, \varepsilon_{RPA}^{-1}(\mathbf{q}, \omega)$ of higher order.

In order to facilitate the comparison of the third moment in the RPA with the exact result given by Eq. (2.28), it is expedient to integrate over the angular variables in the sum with respect to $\mathbf{k}$ standing on the right-hand side of (2.28). Since, by virtue of its definition (2.29), the static structure factor $S(\mathbf{q})$ has a singularity at $q = 0$ [namely, $S(0) = N$], then we should separate out the contribution having $\mathbf{k} = -\mathbf{q}$ in this sum. Consequently the stated sum is transformed into the form

$$\frac{\hbar^2 \omega_p^2}{N} \sum_{k \neq 0} \left(\frac{\mathbf{k} \cdot \mathbf{q}}{kq} \right)^2 [S(\mathbf{k} + \mathbf{q}) - S(\mathbf{k})] = \hbar^2 \omega_p^2 + J(q). \quad (3.15)$$

Here the quantity $J(q)$ is given by the expression

$$J(q) = \frac{\hbar^2 \omega_p^2}{k_F^2} \int_0^{\infty} dk k^2 [S(k) - 1] \left[1 - \frac{3(q^2 + k^2)}{8q^2} + \frac{3(q^2 - k^2)^2}{16q^3 k} \ln \left| \frac{q+k}{q-k} \right| \right]. \quad (3.16)$$

In the limit of small q, the function $J(q)$ is described by the formula

$$J(q) \xrightarrow[q \to 0]{} \frac{\hbar^2 \omega_p^2 q^2}{5k_F^2} \int_0^{\infty} dk [S(k) - 1] = \frac{8}{15} \varepsilon_q \frac{\langle V \rangle}{N}. \quad (3.17)$$

Here $\langle V \rangle$ is the mean potential energy of the system.

Yet at large q the quantity $J(q)$ asymptotically approaches a constant limit:

$$J(\infty) = \frac{\hbar^2 \omega_p^2}{k_F^2} \int_0^\infty dk\, k^2\, [S(k) - 1] = -\frac{2}{3}\hbar^2\omega_p^2\,[1 - g(0)].\qquad (3.18)$$

Here $g(0)$ is the pair correlation function for $r = 0$ (see below).

As we see from Eqs. (2.28), (3.15), and (3.17), in the long-wavelength limit $q \to 0$, the exact third moment approaches the value $-\pi\omega_p^4/2$. The third moment in (3.14) of the formula $\mathrm{Im}\,\varepsilon_{\mathrm{RPA}}^{-1}(q, \omega)$ takes on this same value as $q \to 0$. Thus the sum rule for the third moment in the RPA is satisfied exactly in the limit $q = 0$. At small but nonzero wavenumbers, this rule is obeyed only approximately. In this region of q, the deviation between the exact third moment and that found in the RPA diminishes with increasing density of the electron gas and with decreasing r_s (when $r_s \to 0$, the kinetic energy of the electrons substantially exceeds the potential energy, and we have $\langle T \rangle \approx \langle T \rangle_f$). As regards the region of large q, the result (3.14) of the RPA can quite considerably differ here from the exact third moment of (2.28), especially at the values of r_s corresponding to the electron density in real metals.

An important physical characteristic of the system is the pair correlation function $g(\mathbf{r})$, which is defined as the ratio of the mean electron number density at the distance $\mathbf{r}$ from a given electron to the quantity $(N-1)/\Omega$ (i.e., to the corresponding density in the absence of any correlations in the spatial distribution of the particles). The function $g(\mathbf{r})$ obeys the formula[25]

$$g(r) = 1 + \frac{1}{N-1}\sum_{q \neq 0} [S(q) - 1]\, e^{i\mathbf{q}\cdot\mathbf{r}} \qquad (3.19)$$

Here $S(q)$ is the static structure factor of the system.

We can easily find the explicit expression that defines the pair correlation function in the Hartree-Fock approximation:

$$g_0(r) = 1 - \frac{9}{2}\left(\frac{\sin x - x\cos x}{x^3}\right)^2.$$

Here we have $x = k_F r$. Figure 1 shows a graph of the function $g_0(r)$, from which we see that the Hartree-Fock approximation accounts for the tendency of electrons to avoid one another at small distances. In this approximation this correlation is connected exclusively with accounts of the Pauli principle, which forbids electrons with parallel spins to exist at the same point. The restriction imposed by the Pauli principle extends over a certain region of space around the electron where the probability of finding another electron with the same spin direction is small. It is said of this effect that an "exchange hole" is formed around the electron. We can judge the radius of the latter from Fig. 1. The fact that
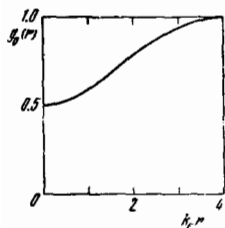

FIG. 1. Pair correlation function $g_0(r)$ in the Hartree-Fock approximation.

$g(0) = 1/2$ in the Hartree-Fock approximation arises from the total neglect of correlation between electrons having antiparallel spins, which actually also avoid one another owing to Coulomb repulsion forces. It is said of the latter effect that the electron is surrounded by a "correlation hole". The existence of this effect causes the true value of the pair correlation function $g(\mathbf{r})$ for $r = 0$ to lie somewhere in the interval from zero to 1/2.

No simple formula exists for $g(\mathbf{r})$ in the RPA, as exists for $g_0(\mathbf{r})$, and finding the pair correlation function involves the need of numerical integration employing Eqs. (3.19), (2.29), (2.17), and (3.6). Such calculations have been performed in Refs. 30 and 31. It turned out that in the RPA the existence of a correlation hole at the electron is manifested to such an extent that the essentially positive physical quantity $g(\mathbf{r})$ becomes negative at small r throughout the range of metallic densities. We can see well from Table II, which gives the values of $g(0)$ as a function of r_s, that the RPA becomes ever less reliable with decreasing density of the electron gas. As regards the region $r_s \ll 1$, here the function $g_{\mathrm{RPA}}(r)$ has no explicit nonphysical singularities.

One can sometimes describe correlation in the motion of particles more conveniently directly in terms of the static structure factor $S(q)$, rather than by using the pair correlation function. At large momenta ($q \gg 2k_F$), the function $S(q)$ approaches unity, while in the long-wavelength limit it is characterized by the behavior[9]

$$S(q) \xrightarrow[q \to 0]{} \frac{\varepsilon_F}{\hbar\omega_p}\left(\frac{q}{k_F}\right)^2 = \frac{1}{2\alpha^3\sqrt{3r_s}}\left(\frac{q}{k_F}\right)^2. \qquad (3.20)$$

In ordinary liquids as well as in liquid metals, the static structure factor shows a sharp peak at $q \approx 2\pi/a$ (a is the mean distance between particles). With further increase in q, it goes over into damped oscillations around a value of unity. This behavior of $S(q)$ indicates local ordering in the mutual arrangement of the particles in the liquid at small distances.

One of the important questions to be answered by the theory of the dielectric constant consists in whether such a close-range order is realized in a system of interacting electrons, and if it is realized, then in what density range. In particular, there is as yet no full clarity in the problem of whether the conduction electrons in real metals behave like a liquid. We shall return again to discussing this problem in the later sections, but now shall merely note here that the static structure factor $S(q)$ in the RPA for small q is exact described by Eq. (3.20) (yet again, this confirms a certain reliability of the RPA in the long-wavelength limit). Then it monotonically increases to unity with increasing q without showing any peaks or oscillations (Fig. 2).

As we have noted in the preceding section, the condition $\varepsilon(\mathbf{q}, \omega) = 0$ determines the dispersion law of the collective excitations in the system. In the RPA this dis-

TABLE II.

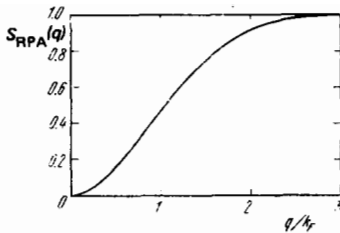| r_s	1	2	3	4	5	6
$g(0)$	−0.06	−0.53	−0.95	−1.33	−1.70	−2.04

FIG. 2. Static structure factor in the random-phase approximation for the case $r_s = 2$.

persion equation has a solution that corresponds to undamped plasma oscillations. This solution exists at values of the momenta q in the range from zero to some critical value q_c at which the plasmon branch enters the region of creation of electron-hole pairs, where $\text{Im}\,\varepsilon_{RPA}(q, \omega) \neq 0$. In the long-wavelength limit, the dispersion law for plasmons in the RPA has the form

$$\omega_{RPA}(q) \xrightarrow[q \to 0]{} \omega_p + \frac{3\varepsilon_F}{5\hbar\omega_p} \frac{\hbar q^2}{m}. \qquad (3.21)$$

Qualitatively, Eq. (3.21) agrees with the results of experiments to measure the inelastic scattering cross-section for electrons and x-rays in metals.[32] However, one usually can get quantitative agreement only after introducing exchange correlation corrections into (3.21) (see the next section). In line with the predictions of the RPA, when $q > q_c$, plasmons practically cease to exist as well-defined excitations ($q_c \sim 0.7 k_F$ in the case of Al with $r_s = 2$). In spite of these predictions, a plasmon-loss peak is observed experimentally even at values of q substantially exceeding q_c (for $q \sim 1.5-2 k_F$ in the case of Al[33,34]).

On the whole, the analysis presented above implies that, from the quantitative standpoint, the RPA satisfactorily describes a system of interacting electrons only in the high-density limit ($r_s \ll 1$). As regards the density region characteristic of real metals, here $\varepsilon_{RPA}(q, \omega)$ gives a rather accurate account of the properties of the system only at small wavenumbers q. Yet the application of the RPA for calculating physical quantities that are sensitive to the behavior of the DC for large q yields answers known to be erroneous, e.g., when estimating the pair correlation function at small distances or the plasmon dispersion law for large momentum transfers.

4. ACCOUNT OF EXCHANGE AND CORRELATION EFFECTS WITHIN THE FRAMEWORK OF THE SELF-CONSISTENT FIELD METHOD

First of all, we should clarify the problem of what are the most important effects from the physical standpoint that are not taken into account in the RPA, so that this approximation proves especially unreliable at large wave vectors. We recall that the effective potential $V_{eff}(q, \omega)$ in the RPA, which perturbs the motion of an individual electron upon introducing the external probe charge into the system, is approximated by the total screening of the potential $V_{ext}(q, \omega)/\varepsilon(q, \omega)$ [see Eq. (3.8)]. In other words, in line with the definition of the DC (2.2) in the RPA, we assume that the mean macroscopic electric field $E(q, \omega)$ that arises in the system

acts on the electron.

As Noziéres and Bines[35] first noted, this assumption, which does not reflect the actual pattern of electron correlations at small distances, precisely constitutes the main defect of the RPA. The point is that the real field at the site r of the electron is not determined by the sum of the contributions from the external field and the mean field induced by the charges. As we noted in the last section, a region of depressed density of other electrons (an exchange-correlation hole) is produced in the vicinity of the point r owing to the restrictions imposed by the Pauli principle, and also because of the strong Coulomb repulsion between electrons at small distances. The actual field whose action the electron must experience must differ from (3.8) by a certain quantity called the local-field correction.

The effect of local fields on the dielectric constant has been studied for a long time within the framework of classical electrodynamics.[36,37] As is well known, the deviation of the local microscopic field E_{mic} acting on the atoms or molecules of the material from the mean macroscopic field E_{mac} means that the DC of such a substance is not determined by the simple sum of the polarizabilities of its constituent particles. In particular, this fact is expressed in the classical Lorentz-Lorenz formula for the dielectric constant:

$$\varepsilon(\omega) = 1 + \frac{4\pi n\alpha(\omega)}{1 - (4\pi/3)\,n\alpha(\omega)}. \qquad (4.1)$$

Here $\alpha(\omega)$ is the polarizability of an individual atom, while n is the density of atoms in the system. Without account for the effects of the local field, the dielectric constant would have the form

$$\varepsilon(\omega) = 1 + 4\pi n\alpha(\omega). \qquad (4.2)$$

Comparison of Eqs. (4.1) and (4.2) shows that an account for the effects of the local field within the framework of classical electrodynamics always increases the DC.

By analogy with classical electrodynamics, one can formally account for the correction to the dielectric constant of a system of interacting electrons due to the effect of the local field by the following generalization of Eqs. (3.8) and (3.9):

$$n_{ind}(q, \omega) = -\pi_{eff}(q, \omega)\,V_{eff}(q, \omega), \qquad (4.3)$$

$$V_{eff}(q, \omega) = V_{ext}(q, \omega) + v(q)[1 - \tilde{G}(q, \omega)]\,n_{ind}(q, \omega). \qquad (4.4)$$

Along with the effective screened response function $\pi_{eff}(q, \omega)$, Eqs. (4.3) and (4.4) also determine the function $\tilde{G}(q, \omega)$, which enters into the local-field correction, and which for this reason bears the same name. We find from Eqs. (4.3) and (4.4) that

$$n_{ind}(q, \omega) = -\frac{\pi_{eff}(q, \omega)}{1 - v(q)\tilde{G}(q, \omega)\pi_{eff}(q, \omega)}\,V_{tot}(q, \omega) \qquad (4.5)$$

[cf. (2.11)]. Finally, by using (4.5) we get the following expression for the dielectric constant:

$$\varepsilon(q, \omega) = 1 - \frac{v(q)\pi_{eff}(q, \omega)}{1 - v(q)\tilde{G}(q, \omega)\pi_{eff}(q, \omega)}. \qquad (4.6)$$

We note that most studies on the theory of the dielectric constant generally write the final result in the form

$$\varepsilon(q, \omega) = 1 - \frac{v(q)\chi_0(q, \omega)}{1 - v(q)G(q, \omega)\chi_0(q, \omega)}. \qquad (4.7)$$

Here $\chi_0(q, \omega)$ is the Lindhard function of (3.1). We can

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easily convince ourselves that Eqs. (4.6) and (4.7) agree identically if we select the renormalized local-field correction $G(\mathbf{q}, \omega)$ as follows:

$$G(\mathbf{q}, \omega) = \bar{G}(\mathbf{q}, \omega) - \frac{1}{v(\mathbf{q})}\left[\frac{1}{\chi_0(\mathbf{q}, \omega)} + \frac{1}{\pi_{\text{eff}}(\mathbf{q}, \omega)}\right]. \qquad (4.8)$$

In the representation of the dielectric constant in the form (4.7), terms appear in the function $G(\mathbf{q}, \omega)$ that have no direct relation from the physical standpoint to the true local-field correction $\bar{G}(\mathbf{q}, \omega)$. However, for practical calculations, the form of writing of the dielectric constant plays no special role.

First of all, we note the evident analogy between the classical Lorentz-Lorenz expression (4.1) and the formulas (4.6) and (4.7) for the dielectric constant. Upon starting with this analogy, we can consider that the local-field correction function $G(\omega)$ in the classical case is reduced to a constant value of $1/3$. We can easily verify that the local-field correction $G_0 = 1$ in the Hartree-Fock approximation discussed above, whereas in the random-phase approximation we have $G_{\text{RPA}} = 0$.

To find the function $G(\mathbf{q}, \omega)$ is the fundamental problem of the theory of an interacting electron gas. In this section we shall restrict the treatment to calculating $G(\mathbf{q}, \omega)$ within the framework of the single-particle approximation based on the self-consistent-field method. As we shall show below, a rather considerable fraction of the currently known approximate formulas for the function $G(\mathbf{q}, \omega)$, which were derived in the original papers by the most varied theoretical approaches, can actually be reproduced withing the framework of a simple, single-particle self-consistent approximation.

In the method of the self-consistent field, one treats the system of interacting electrons as an ensemble of independent quasiparticles, each of which moves in the field of the external charge and in the mean field of all the rest of the electrons. Here the true many-electron wave functions are approximated by simple Slater determinants constructed of the single-particle states $\chi_{q\sigma}(\mathbf{r}, \zeta, t)$ (here ζ is the spin coordinate of the electron, while q and σ are respectively the orbital and spin quantum numbers). In turn, one finds these single-particle states by solving a certain system of equations, e.g., of the type of the well-known Hartree or Hartree-Fock equations.

In the simplest variant of the method of the self-consistent field one assumes that this field is local and is the same for all of the single-electron states. In the absence of a magnetic field and with neglect of spin-orbital interactions, one can naturally choose these states in the form of products of the orbital and spin wave functions:

$$\psi_{q\sigma}(\mathbf{r}, \zeta, t) = \psi_q(\mathbf{r}, t)\chi_\sigma(\zeta).$$

Here the orbital wave functions will be determined by the Schrödinger equation

$$i\hbar\frac{\partial\psi_q(\mathbf{r}, t)}{\partial t} = \left[\frac{\hat{p}^2}{2m} + V_{\text{eff}}(\mathbf{r}, t)\right]\psi_q(\mathbf{r}, t). \qquad (4.9)$$

The following is the effective potential energy of the electron in this case:

$$V_{\text{eff}}(\mathbf{r}, t) = V_{\text{ext}}(\mathbf{r}, t) + V_e(\mathbf{r}, t). \qquad (4.10)$$

This potential energy consists of the potential of interaction of the electron with the external charge $V_{\text{ext}}(\mathbf{r}, t)$ and of its potential energy $V_e(\mathbf{r}, t)$ in the electric field of the rest of the electrons, averaged over the states of the system.

The accuracy with which one can describe the electromagnetic properties of the original system of interacting electrons within the framework of this approach depends considerably on how one concretely defines the potential energy $V_e(\mathbf{r}, t)$, or in other words, on how one averages the operator for the electric field created at the point $\mathbf{r}$ by the remaining $N - 1$ electrons. The latter is given by the expression

$$\mathbf{E}(\mathbf{r}) = i\sum_{\mathbf{q}\neq 0}\frac{4\pi e}{q^2\Omega}\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}}\sum_{j=2}^{N}e^{-i\mathbf{q}\cdot\mathbf{r}_j}. \qquad (4.11)$$

If we average (4.11) over the states of the complete system $\Psi_\alpha(t) = \Psi_\alpha(\mathbf{r}_1, \zeta_1, \mathbf{r}_2\zeta_2, \ldots, \mathbf{r}_N, \zeta_N, t)$ without imposing any restrictions on the relative arrangement of the particles, then we obtain a field corresponding to the mean induced charge, and we arrive at the RPA. We can more correctly account for the existence around the electron of an exchange-correlation hole that dynamically accompanies it during movement if we impose the additional condition in averaging the operator of (4.11) over the wave function $\Psi_\alpha(t)$ that an electron exists at the point $\mathbf{r}$ at the instant of time t with the appropriate probability. In practice this means that we should set $\mathbf{r}_1 = \mathbf{r}$ in the wave function $\Psi_\alpha(t)$, and we should integrate only over the coordinates $\mathbf{r}_2, \ldots, \mathbf{r}_N$ with fixed $\mathbf{r}$ in calculating the matrix element of the operator $\mathbf{E}(\mathbf{r})$. We shall denote the stated procedure symbolically in the form $\langle\ldots\rangle_r$. Then we shall have the following expression for the gradient of the potential energy $V_e(\mathbf{r}, t)$:

$$\nabla V_e(\mathbf{r}, t) = i\sum_{\mathbf{q}\neq 0}\mathbf{q}v(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}\frac{\langle\Psi_\alpha(t)|\sum_{j=2}^{N}e^{-i\mathbf{q}\cdot\mathbf{r}_j}|\Psi_\alpha(t)\rangle_r}{\langle\Psi_\alpha(t)|\Psi_\alpha(t)\rangle_r}. \qquad (4.12)$$

In calculating the matrix elements that enter into Eq. (4.12) in the wave function $\Psi_\alpha(\mathbf{r}\zeta, \mathbf{r}_2\zeta_2, \ldots, \mathbf{r}_N\zeta_N, t)$, we should separate out in explicit form the coordinates $\mathbf{r}\zeta$ of the studied electron and those of one of the remaining $N - 1$ electrons, say $\mathbf{r}_2\zeta_2$. This is performed by employing the formula

$$\Psi_\alpha(\mathbf{r}\zeta, \mathbf{r}_2\zeta_2, \ldots, \mathbf{r}_N\zeta_N, t) \qquad (4.13)$$
$$= \pm\frac{1}{\sqrt{N(N-1)}}\sum_{\mathbf{q}_1\mathbf{q}_2\sigma_1\sigma_2}\psi_{\mathbf{q}_1\sigma_1}(\mathbf{r}, \zeta, t)\psi_{\mathbf{q}_2\sigma_2}(\mathbf{r}_2, \zeta_2, t)c_{\mathbf{q}_1\sigma_1}c_{\mathbf{q}_2\sigma_2}|\alpha).$$

Here $|\alpha\rangle$ is the corresponding state of the sytem in the second-quantization representation, while $c_{q\sigma}$ is the annihilation operator for electrons in the single-particle state $\chi_{q\sigma}$. Consequently we arrive at the following expression for $\nabla V_e(\mathbf{r}, t)$:

$$\nabla V_e(\mathbf{r}, t) = i\sum_{\mathbf{q}\neq 0}\mathbf{q}v(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}\left[\int d^3r'e^{-i\mathbf{q}\cdot\mathbf{r}'}n(\mathbf{r}', t)\right.$$
$$\left. - \frac{1}{n(\mathbf{r}, t)}\sum_{\mathbf{k}p\sigma}n_{\mathbf{k}\sigma}n_{p\sigma}\psi_{\mathbf{k}}^*(\mathbf{r}, t)\psi_p(\mathbf{r}, t)\int d^3r'\psi_p^*(\mathbf{r}', t)e^{-i\mathbf{q}\cdot\mathbf{r}'}\psi_{\mathbf{k}}(\mathbf{r}', t)\right]. \qquad (4.14)$$

Here $n(\mathbf{r}, t)$ is the electron number density at the point $\mathbf{r}$ at the instant of time t, and we have

$$n(\mathbf{r}, t) = \sum_{\mathbf{k}\sigma}n_{\mathbf{k}\sigma}|\psi_{\mathbf{k}}(\mathbf{r}, t)|^2. \qquad (4.15)$$

The first term in (4.14) represents the mean Hartree field taken into account in the RPA, since the second

term is of exchange origin and describes the sought local-field correction.

Together with the self-consistency condition (4.10) and Eq. (4.14), the Schrödinger equation (4.9) forms a closed system of equations with respect to $\psi_q(\mathbf{r}, t)$ and $V_e(\mathbf{r}, t)$, which we must solve to the accuracy of first-order terms in the external perturbation. To this accuracy, the single-electron states are determined by the formula

$$\psi_q(\mathbf{r}, t) = \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{\sqrt{\Omega}}\left[1 - \sum_k \int \frac{d\omega}{2\pi} \frac{V_{eff}(\mathbf{k}, \omega) e^{i\mathbf{k}\cdot\mathbf{r}} e^{-i(\omega+i\delta)t}}{\hbar\omega - \varepsilon_{k+q} + \varepsilon_q + i\delta}\right] e^{-(i/\hbar)\varepsilon_q t}. \quad (4.16)$$

Upon substituting (4.16) into (4.14) and making simple algebraic transformations, we get

$$V_e(\mathbf{q}, \omega) = v(q)[1 - G(\mathbf{q}, \omega)]\chi_0(\mathbf{q}, \omega)V_{eff}(\mathbf{q}, \omega). \quad (4.17)$$

Here $G(\mathbf{q}, \omega)$ denotes the function

$$G(\mathbf{q}, \omega) = \frac{2}{N\chi_0(\mathbf{q}, \omega)}\sum_{kp}\frac{\mathbf{q}\cdot\mathbf{p}}{p^2}(n_{k+p} - n_{k+p+q})\frac{n_k - n_{k+q}}{\hbar\omega - \varepsilon_{k+q} + \varepsilon_k + i\delta}. \quad (4.18)$$

Finally, upon substituting (4.16) into (4.15), we find the Fourier component of the mean induced density

$$n_{ind}(\mathbf{q}, \omega) = \chi_0(\mathbf{q}, \omega)V_{eff}(\mathbf{q}, \omega). \quad (4.19)$$

Comparison of Eqs. (4.3), (4.4), (4.10), (4.17), and (4.19) shows that the function (4.18) is the sought local-field correction [we note that we have $\pi_{eff}(\mathbf{q}, \omega) = -\chi_0(\mathbf{q}, \omega)$ in the self-consistent-field approximation, and owing to (4.8), we have $G(\mathbf{q}, \omega) = \tilde{G}(\mathbf{q}, \omega)$].

The expression (4.18) for the local-field correction was first derived by Toigo and Woodruff[38] (see also Refs. 39–41). These authors started with the exact formula (2.4) for the polarizability $\chi(\mathbf{q}, \omega)$, and uncoupled the equations of motion for the double-time-retarded commutator of $\chi(\mathbf{q}, t - t')$ [see (2.8)]. Here they imposed on the higher-order Green's functions the specific condition that they should be proportional to the Green's function of $\chi(\mathbf{q}, t - t')$, so as to retain in the result the integral of the corresponding spectral densities with respect to the frequency.

The derivation of Eq. (4.18) given above requires far fewer powerful mathematical tools and is distinguished by greater physical perspicuity. In particular, the approach that we have employed allows us to establish directly the form of the effective interaction of the electron with the external charge introduced into the system with account for local-field effects. This is, as we can easily see from (4.10) and (4.17), we have

$$V_{eff}(\mathbf{q}, \omega) = \frac{V_{ext}(\mathbf{q}, \omega)}{\tilde{\varepsilon}(\mathbf{q}, \omega)}. \quad (4.20)$$

Here $\tilde{\varepsilon}(\mathbf{q}, \omega)$ is the so-called effective dielectric constant, for which we have the formula

$$\tilde{\varepsilon}(\mathbf{q}, \omega) = 1 - v(q)[1 - G(\mathbf{q}, \omega)]\chi_0(\mathbf{q}, \omega). \quad (4.21)$$

As we see from (4.20), $V_{eff}(\mathbf{q}, \omega)$ is not determined by the dielectric function $\varepsilon(\mathbf{q}, \omega)$ itself, which characterizes only the mean macroscopic fields in the system, but by the effective dielectric constant of (4.21), which accounts for the local distortion of the mean induced density near an individual electron owing to exchange and correlation effects. In this regard we note that the true spatial induced-charge distribution around the point $\mathbf{r}$ when an electron lies at this point is determined by the

quantity $[1 - G(\mathbf{q}, \omega)]n_{ind}(\mathbf{q}, \omega)$.

Before we proceed to analyze the fundamental properties of the dielectric function of Toigo and Woodruff, we shall show how one can calculate it in practice. We see from (4.7) that we must also know the quantity

$$\Phi(\mathbf{q}, \omega) = G(\mathbf{q}, \omega)\chi_0(\mathbf{q}, \omega),$$

in order to find $\varepsilon(\mathbf{q}, \omega)$, in addition to the well-known function $\chi_0(\mathbf{q}, \omega)$. In line with (4.18), the latter requires one to calculate a sextuple integral. It turns out that the imaginary component of the function $\Phi(\mathbf{q}, \omega)$ can be expressed in terms of elementary functions:

$$\mathrm{Im}\,\Phi(\mathbf{q}, \omega)$$
$$= \begin{cases} -\frac{9\pi N}{64\varepsilon_F}\{x[F(y) - F(1)] - x'[F(y') - F(1)]\}, & 0 \leqslant \omega \leqslant q(2-q), \\ -\frac{9\pi N}{64\varepsilon_F}\{x[F(y) - F(x)] + x'[F(1) - F(x')]\}, & q|2-q| \leqslant \omega \leqslant q(2+q), \\ 0 \end{cases}$$

in the remaining cases; here we have $x = (q^2 + \omega)/2q$, $x' = (q^2 - \omega)/2q$, $y = (1 + \omega)^{1/2}$, $y' = (1 + \omega)^{1/2}$, q is measured in units of k_F, and ω stands for $\hbar\omega/\varepsilon_F$. Finally, $F(t)$ is a function having the following form:

$$F(t) = \frac{1}{3}\left[t^2 + \frac{(3-t)(1+t)^2}{2t}\ln|1+t| - \frac{(3+t)(1-t)^2}{2t}\ln|1-t|\right].$$

If we know the imaginary component of the function $\Phi(\mathbf{q}, \omega)$, we can also find its real component by using the dispersion relationship

$$\mathrm{Re}\,\Phi(\mathbf{q}, \omega) = \frac{2}{\pi}\mathcal{P}\int_0^\infty d\omega' \frac{\omega'}{\omega'^2 - \omega^2}\mathrm{Im}\,\Phi(\mathbf{q}, \omega').$$

In the static case $\omega = 0$, the local-field correction of (4.18) behaves as follows in the limits of small and large q:

$$G(q, 0) \to \begin{cases} \frac{1}{4}\left(\frac{q}{k_F}\right)^2, & q \to 0, \\ \frac{2}{3} + \frac{11}{75}\left(\frac{k_F}{q}\right)^2, & q \to \infty. \end{cases} \quad (4.22)$$

One can judge the character of the function $G(q, 0)$ in the intermediate region of wavenumbers from Fig. 3.

As is implied by the compressibility sum rule (2.31) and Eq. (4.7), the main contribution to the static local-field correction for $q \to 0$ must have the form

$$G(q, 0) \xrightarrow[q \to 0]{} \frac{\gamma q^2}{k_F^2}. \quad (4.23)$$

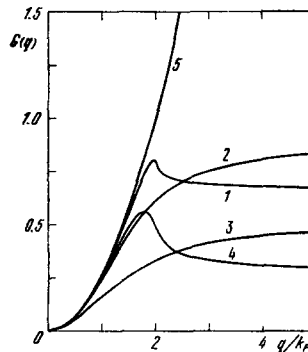Here γ is a dimensionless constant that is related to the

FIG. 3. Static variant of the local-field correction in the theories of Toigo and Woodruff[38] (1), Vashishta and Singwi[54] (r_s =2) (2), and Geldart and Vosko[57] (ξ =2) (3). Curves 4 and 5 calculated according to Eqs. (4.38) and (4.41) while accounting for the factor 2/3 of Gaspar, Kohn, and Sham.[60,61]

isothermal compressibility by

$$\frac{K_f}{K} = 1 - \frac{\gamma \kappa_{TF}^2}{K_F^2} = 1 - \frac{4\gamma \alpha r_s}{\pi}. \qquad (4.24)$$

When $\gamma = 1/4$ [see (4.22)], Eq. (4.24) coincides exactly with the corresponding expression for the compressibility obtained from (2.32) by differentiating the energy of the ground state in the Hartree-Fock approximation:

$$\varepsilon_{HF}^{(0)'}(r_s) = \frac{2}{5\alpha^2 r_s^2} - \frac{3}{2\pi \alpha r_s}. \qquad (4.25)$$

As direct calculations show (see, e.g., Ref. 54), the correction to the compressibility from the correlation energy is much smaller than the contributions from each of the two terms in Eq. (4.25), and it becomes appreciable only when $r_s \sim 6$, when compensation of the main Hartree-Fock contributions occurs. Thus, even though the compressibility sum rule is not obeyed strictly in the approximation of Toigo and Woodruff, yet it is satisfied with good accuracy over a rather broad range of the parameter r_s that covers a substantial part of the range of metallic densities. In this respect, the dielectric function of Toigo and Woodruff has an undoubted advantage over $\varepsilon_{RPA}(q, \omega)$.

In the region of small q and large ω, the local-field correction of (4.18) is approximated by the expression

$$G(q, \omega) \xrightarrow[\substack{q \to 0 \\ \omega \to \infty}]{} \frac{3}{20} \left(\frac{q}{k_F}\right)^2 \left[1 - \frac{24}{35} \left(\frac{\varepsilon_F}{\hbar \omega}\right)^2 \left(\frac{q}{k_F}\right)^2\right].$$

This behavior of $G(q, \omega)$ leads to the ordinary quadratic dispersion law of the long-wavelength plasma oscillations

$$\omega(q) \xrightarrow[q \to 0]{} \omega_p + \frac{a\hbar^2 q^2}{m}. \qquad (4.26)$$

Here the dimensionless parameter a proves equal to

$$a = \frac{3\varepsilon_F}{5\hbar \omega_p} \left(1 - \frac{\alpha r_s}{3\pi}\right). \qquad (4.27)$$

The second term on the right-hand side of (4.27) constitutes the exchange-correlation correction to the result of (3.21) derived in the RPA. Figure 4 shows the experimental values of the ratio a/a_{RPA} for a set of simple metals, together with the corresponding calculated values obtained by Eq. (4.27). As we see from this diagram, Eq. (4.27) satisfactorily describes the experimental data, and this allows us to conclude that the expression (4.18) for $G(\mathbf{q}, \omega)$ is quite reliable for small q. We note that the result of (4.26) and (4.27) was first derived by Nozières and Pines[45] and then has been repeatedly derived by other authors.[46-50]
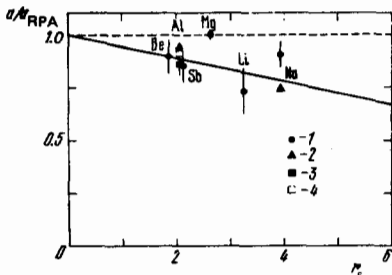
FIG. 4. The ratio a/a_{RPA} as a function of r_s. The solid line corresponds to Eq. (4.27), and the dotted line corresponds to the random-phase approximation. The experimental data are taken from Refs. 42 (1), 43 (2), 33 (3), and 44 (4).

Moreover, the dielectric function of Toigo and Woodruff has the undoubted advantage over ε_{RPA} that it strictly satisfies not only the f sum rule but also the sum rule for the third moment.[14,51] Hence it now satisfactorily describes the development of events in a system of interacting electrons, at least for short times.

The study of Toigo and Woodruff[38] was historically the first study that found a method for accounting for the dynamic character of the exchange-correlation hole, and thus obtained a frequency-dependent local-field correction. Prior to that, all attempts to improve the result (3.6) of the RPA, beginning with the first publication of Hubbard,[2] led to a formula for the DC of the form of (4.7). However, in these formulas the static local-field correction $G(q)$ figured instead of $G(q, \omega)$. One of these attempts was undertaken in the well-known series of studies of Singwi et al.[52-55] These authors proposed a method based on a classical analogy that was quite attractive from the physical standpoint for accounting for exchange-correlation effects via pair correlation functions (see also the study of Hubbard[56]). We shall show below how the fundamental postulate of the theory of Singwi et al. can be substantiated within the scope of the method that led us to the theory of Toigo and Woodruff.

Let us assume that an electron exists at the point $\mathbf{r}$, while we are interested in the mean number density of the rest of the electrons at the point $\mathbf{r}'$ under conditions in which an external perturbation acts on the system. Upon employing the same notation as in Eq. (4.12), we have the following expression for the sought density:

$$n_{eff}(\mathbf{r}, \mathbf{r}'; t) = \langle \Psi_\alpha(t) | \sum_{j=2}^{N} \delta(\mathbf{r}' - \mathbf{r}_j) | \Psi_\alpha(t) \rangle / \langle \Psi_\alpha(t) | \Psi_\alpha(t) \rangle_\mathbf{r}. \qquad (4.28)$$

If we were to remove the restriction on the right-hand side of (4.28) that the designated (first) electron is rigidly fixed at the point $\mathbf{r}$, then we would obtain simply the mean density $n(\mathbf{r}', t)$ instead of $n_{eff}(\mathbf{r}, \mathbf{r}'; t)$. The relation is established between these two quantities that

$$n_{eff}(\mathbf{r}, \mathbf{r}'; t) = g(\mathbf{r}, \mathbf{r}'; t) n(\mathbf{r}', t). \qquad (4.29)$$

This defines the pair correlation function $g(\mathbf{r}, \mathbf{r}'; t)$ in the perturbed system. Upon employing (4.28) and (4.29), we can rewrite Eq. (4.12) in the following equivalent form:

$$\nabla V_e(\mathbf{r}, t) = \int d^3 r' g(\mathbf{r}, \mathbf{r}'; t) n(\mathbf{r}', t) \nabla v(\mathbf{r} - \mathbf{r}'). \qquad (4.30)$$

Here $v(\mathbf{r} - \mathbf{r}') = e^2 / |\mathbf{r} - \mathbf{r}'|$ is the Coulomb potential. This notation has a quite evident structure in terms of classical electrodynamics.

Equation (4.30) is the fundamental equation in the theory of Singwi et al. These authors actually postulated it by generalizing the corresponding classical expression to the quantum-mechanical case. This approach per se gives no hint how one can calculate in practice the perturbed pair correlation function that enters into (4.30). The further course of construction of the theory fully depended only on the physical intuition and inventiveness of the authors.

In the first variant of their theory,[52] instead of $g(\mathbf{r}, \mathbf{r}'; t)$, Singwi et al. employed in (4.30) the equilibrium pair correlation function $g(\mathbf{r} - \mathbf{r}')$, which is associated with the static structure factor $S(q)$ by the relationship (3.19). Here Eq. (4.30), upon being rewritten in

terms of the corresponding Fourier components, acquires the form

$$V_e (q, \omega) = v (q) \{1 - G (q)\} n_{\text{ind}} (q, \omega). \qquad (4.31)$$

Here the static correction for the local field $G(q)$ is given by the expression

$$G(q) = \frac{1}{N-1} \sum_k \frac{k \cdot q}{k^2} \{1 - S(k-q)\}. \qquad (4.32)$$

In turn, the static structure factor $S(q)$ is associated with the dielectric function by the relationship

$$S(q) = -\frac{\hbar}{\pi v(q) N} \int_0^\infty d\omega \operatorname{Im} \varepsilon^{-1} (q, \omega). \qquad (4.33)$$

Equations (4.33), (4.32), and (4.7) [with the function $G(q)$ instead of $G(q, \omega)$] form a closed system of equations with respect to $S(q)$, $G(q)$, and $\varepsilon(q, \omega)$, which can be solved by the iteration scheme

$$\varepsilon^{(0)} (q, \omega) \to S^{(0)} (q) \to G^{(0)} (q) \to \varepsilon^{(1)} (q, \omega) \to \dots .$$

An essential achievement of the theory of Singwi et al. was that it led to a physically reasonable pair correlation function. As we see from Table III, in this theory $g(0)$ remains positive up to $r_s \approx 4$, while for $r_s \gtrsim 4$, it takes on very small negative values that we can consider zero for all practical purposes. However, the compressibility calculated by Eq. (4.24) becomes negative even at $r_s \gtrsim 3$. Moreover, the theory[52] gives an extremely unsatisfactory description of the plasmon dispersion law (which, moreover, is characteristic of all the known dielectric functions having a static local-field correction).

The theory of Singwi et al. culminated in the study of Vashishta and Singwi,[54] which to some extent accounted for the effect of reorganization of the pair correlation function upon imposing the external field. In analyzing the classical case, these authors employed the following approximation for the function $g(\mathbf{r}, \mathbf{r}'; t)$:

$$g(\mathbf{r}, \mathbf{r}'; t) = g(\mathbf{r}' - \mathbf{r}) + \frac{1}{2} \frac{\partial g(\mathbf{r}' - \mathbf{r})}{\partial n} [n_{\text{ind}} (\mathbf{r}, t) + n_{\text{ind}} (\mathbf{r}', t)].$$

This was chosen by calculation to satisfy the compressibility sum rule exactly. The local-field correction in this approximation remains static as before, and is determined by the formula

$$G_{\text{VS}}^{(\text{cl})} (q) = \left(1 + \frac{n}{2} \frac{\partial}{\partial n}\right) G(q). \qquad (4.34)$$

Here the function $G(q)$ has the form of (4.32). In generalizing the result of (4.34) to the quantum-mechanical case, Vashishta and Singwi simply replaced the factor $1/2$ in the second term by the empirical parameter a. Numerical calculations showed that a choice of $a = 2/3$ causes the compressibility sum rule in the quantum-mechanical case to be almost exactly satisfied throughout the range of metallic densities. Simultaneously it describes the pair correlation function almost as satisfactorily in the original variant of the theory. Figure 3 shows the behavior of the local-field correction of

TABLE III.

r_s	1	2	3	4	5	6
$g(0)$	0.24	0.11	0.04	0.006	−0.02	−0.003

Vashishta and Singwi for the case $r_s = 2$. As the authors themselves note, the assumptions underlying the theory are difficult to substantiate in any rigorous way, and their only justification is that this theory gives a physically acceptable description of the static properties of a system of interacting electrons.

Rajagopal et al.[49] have undertaken a special attempt to elucidate the reason for the success of the theory of Singwi et al. However, they could not correlate the approach used therein with the well-known schemes of calculating the dielectric function in many-body theory. At the same time, even the first study of Singwi et al.[52] noted that one can start with Eq. (4.32) to derive in explicit form the first known local-field correction, which was found by Hubbard by partial summation of the perturbation-theory series for the irreducible polarization operator.[2] Namely, if one substitutes the static structure factor of a system of noninteracting electrons

$$S_0 (q) = 1 - \frac{2}{N} \sum_k n_k n_{k+q},$$

into Eq. (4.32) then it acquires the form

$$G(q) = \frac{2}{N^2} \sum_{kp} \frac{q \cdot (k+p+q)}{(k+p+q)^2} n_k n_p.$$

If now we replace the quantity $(k+p+q)^2$ in the denominator by $q^2 + k_F^2$ (an approximation to which Hubbard also resorted), then this formula transforms into Hubbard's result

$$G(q) = \frac{1}{2} \frac{q^2}{q^2 + k_F^2}. \qquad (4.35)$$

Comparison of (4.35) with (4.23) shows that the parameter γ is $1/2$ in Hubbard's approximation. This implies that the compressibility calculated by Eq. (4.24) begins to take on negative values at $r_s \approx 3$.

Geldart and Vosko[57] have proposed a modified variant of Hubbard's formula (4.35), which preserves its fundamental merit, namely, its extreme simplicity:

$$G(q) = \frac{1}{2} \frac{q^2}{q^2 + \xi(r_s) k_F^2}. \qquad (4.36)$$

Here $\xi(r_s)$ is a parameter that is chosen by calculation so that the compressibility sum rule is strictly obeyed. The static dielectric function with the local-field correction of (4.36) gives quite satisfactory results in calculating the phonon spectra of simple metals.[6]

However, one should approach with some caution the problem of employing dielectric functions with a static local-field correction in estimating any concrete property of a system of interacting electrons. A common serious defect is inherent in these dielectric functions—once cannot in principle construct them so as to satisfy all the exact sum rules simultaneously without leading to physical contradictions.[58] Consequently, theories involving dielectric functions with a static local-field correction unavoidably have only a limited field of applicability.

In closing this section, we shall again touch upon the problem of choosing the self-consistent potential $V_e(\mathbf{r}, t)$ in Eq. (4.10). First we shall show how the dielectric function arises when one employs the above-proposed method for accounting for local-field effects for constructing $V_e(\mathbf{r}, t)$, but directly averages the ener-

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gy of interelectronic interaction, rather than the electric-field operator of (4.11). In this case, as we can easily see, we have

$$V_e(\mathbf{r},\ t) = \int d^3r' v(\mathbf{r}-\mathbf{r}')\, n(\mathbf{r}',\ t)$$
$$- \sum_{\mathbf{k}p\sigma} n_{\mathbf{k}\sigma} n_{p\sigma} \frac{\psi_{\mathbf{k}}^*(\mathbf{r},\ t)\psi_p(\mathbf{r},\ t)}{n(\mathbf{r},\ t)} \int d^3r' \psi_p^*(\mathbf{r}',\ t)\, v(\mathbf{r}-\mathbf{r}')\, \psi_{\mathbf{k}}(\mathbf{r}',\ t). \tag{4.37}$$

Consequently we obtain the following expression for the local-field correction:

$$G(q,\ \omega)$$
$$= \frac{2q^2}{N\chi_0(q,\ \omega)} \sum_{\mathbf{k}p} \frac{1}{p^2}\, (n_{\mathbf{k}+\mathbf{p}} + n_{\mathbf{k}+\mathbf{p}+\mathbf{q}})\, \frac{n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{\hbar\omega - \varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_{\mathbf{k}} + i\delta} - \frac{9}{8}\left(\frac{q}{k_F}\right)^2. \tag{4.38}$$

In the static limit, the function of (4.38) has the following asymptotic behavior at small and large q:

$$G(q,\ 0) \to \begin{cases} \frac{3}{8}\left(\dfrac{q}{k_F}\right)^2, & q \to 0, \\[2mm] \frac{13}{30}, & q \to \infty. \end{cases} \tag{4.39}$$

Upon comparing (4.39) with (4.23), we see that $\gamma = 3/8$ in the considered approximation. Hence the compressibility calculated by Eq. (4.24) already becomes negative for $r_s \gtrsim 4$, whereas this happens only for $r_s \gtrsim 6$ in Toigo and Woodruff's approximation. Thus the replacement of Eq. (4.14) by (4.37) expands the range of values of r_s in which the compressibility sum rule fails.

Interestingly, the potential energy of (4.37) amounts to nothing but a generalization to the nonstationary case of the expression proposed by Slater as early as 1950 for the effective energy of interelectronic interaction, which he derived by specific averaging of the nonlocal exchange potential in the Hartree-Fock equation.[59] Since the one-electron Schrödinger equation with the potential energy $V_e(\mathbf{r})$ proved not much simpler to calculate than the original Hartree-Fock equation, Slater further approximated $V_e(\mathbf{r})$ by its value in a free electron gas having the same local density. That is, he assumed that

$$V_e(\mathbf{r}) = -\frac{3e^2 k_F(\mathbf{r})}{2\pi} = -\frac{3}{2}e^2\left[\frac{3}{\pi}n(\mathbf{r})\right]^{1/3}. \tag{4.40}$$

If we replace $n(\mathbf{r})$ in (4.40) by $n(\mathbf{r},\ t)$ and employ the resulting potential $V_e(\mathbf{r},\ t)$ to find the dielectric constant within the framework of the self-consistent-field method, then, as we can easily convince ourselves, we arrive at the static local-field correction in the form

$$G(q) = \frac{3}{8}\left(\frac{q}{k_F}\right)^2. \tag{4.41}$$

Comparison of (4.41) with (4.39) indicates that the approximation (4.40) for the initial Slater potential of (4.37) does not distort the description of the correlations between the electrons at large distances, although it is unsatisfactory for small r.

Gaspar[60] and Kohn and Sham[61] have shown that is is far better warranted in accounting for exchange-correlation effects in a system of interacting electrons not to employ directly the Slater potential of (4.40), but only 2/3 of its value. This is precisely the factor that reconciles the behavior of the local-field corrections of (4.39) and (4.41) in the limit of small q with the analogous behavior of the function $G(q, 0)$ in the theory of Toigo and Woodruff [see (4.22)]. Figure 3 shows the static variant $G(q, 0)$ of the function of (4.38) and also the function of

(4.41) with account for the factor 2/3.

The self-consistent-field method with the Slater exchange-correlation potential of (4.40) multiplied by some empirical coefficient $\alpha(2/3 \leqslant \alpha \leqslant 1)$ has been termed the $X\alpha$ method, and it is widely applied for calculating the electronic structure of solids, atoms, and molecules.[62] Yet the original potential of (4.37) has found no practical application. Nevertheless, one could have used it to construct a dielectric function with the dynamic local-field correction of (4.38), even before the development of the random-phase approximation.

Upon turning to Eq. (4.41), we note that the static local-field correction, which behaves like q^2 in the region of both small and large q, has also been derived by Kleinman[63] and by Langreth.[64] Singwi et al.[52,53,65] have advanced a serious argument against results of this type. They pointed out that the quadratic behavior of $G(q, 0)$ for large q gives rise to a nonphysical singularity of the $1/r$ type in the pair correlation function as $r \to 0$.

The erroneous results for the asymptotic behavior of $G(q, 0)$ for large q in the work of Kleinman[63] and Langreth[64] did not stem from physical inadequacy of the general scheme of calculation that they employed, but from incorrect approximations that they introduced into their calculations in the final stage. These authors started with a self-consistent-field method resembling that presented in this section. However, they based their calculations on a time-dependent one-electron equation with a nonlocal exchange potential of Hartree-Fock type

$$i\hbar\frac{\partial\psi_{\mathbf{k}}(\mathbf{r},\ t)}{\partial t} = \left[\frac{\hat{\mathbf{p}}^2}{2m} + V_{\text{ext}}(\mathbf{r},\ t) + \int d^3r' v(\mathbf{r}-\mathbf{r}')\, n(\mathbf{r}',\ t)\right]\psi_{\mathbf{k}}(\mathbf{r},\ t)$$
$$- \sum_p n_p \psi_p(\mathbf{r},\ t) \int d^3r' \psi_p^*(\mathbf{r}',\ t)\, v(\mathbf{r}-\mathbf{r}')\, \psi_{\mathbf{k}}(\mathbf{r}',\ t). \tag{4.42}$$

(They treat the case of a paramagnetic many-electron system.) In the absence of an external perturbation, Eq. (4.42) admits solutions in the form of the usual plane waves

$$\psi_{\mathbf{k}}(\mathbf{r},\ t) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\Omega}}\, e^{-(i/\hbar)E_{\mathbf{k}}t}.$$

Here we have

$$E_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \sum_{\mathbf{q}} v(\mathbf{k}-\mathbf{q})\, n_{\mathbf{q}} \tag{4.43}$$

as the dispersion law of the one-electron excitations in the Hartree-Fock approximation. To an accuracy of first-order terms in the external perturbation, the single-particle states satisfying Eq. (4.42) have the form

$$\psi_{\mathbf{k}}(\mathbf{r},\ t) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\Omega}}\left[1 + \sum_{\mathbf{q}} \int \frac{d\omega}{2\pi}\, \frac{V_{\mathbf{k}}^{\text{eff}}(\mathbf{q},\ \omega)\, e^{i\mathbf{q}\cdot\mathbf{r}} e^{-i(\omega+i\delta)t}}{\hbar\omega - E_{\mathbf{k}+\mathbf{q}} + E_{\mathbf{k}} + i\delta}\right] e^{-(i/\hbar)E_{\mathbf{k}}t}. \tag{4.44}$$

Here $V_{\mathbf{k}}^{\text{eff}}(\mathbf{q},\ \omega)$ is the Fourier component of the effective one-electron potential:

$$V_{\mathbf{k}}^{\text{eff}}(\mathbf{q},\ \omega) = V_{\text{ext}}(\mathbf{q},\ \omega) + v(\mathbf{q})\, n_{\text{ind}}(\mathbf{q},\ \omega) + V_{\mathbf{k}}^{\text{xc}}(\mathbf{q},\ \omega). \tag{4.45}$$

In turn, $V_{\mathbf{k}}^{\text{xc}}(\mathbf{q},\ \omega)$ is the component of the Hartree-Fock nonlocal exchange-correlation potential in Eq. (4.42), which is defined as follows:

$$V_{\mathbf{k}}^{\text{xc}}(\mathbf{k}'-\mathbf{k},\ \omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, \langle \mathbf{k}'|\hat{V}^{\text{xc}}(t)|\mathbf{k}\rangle \tag{4.46}$$
$$= -\sum_p n_p \int_{-\infty}^{\infty} dt\, e^{i\omega t} \int d^3r \int d^3r'\, \frac{e^{-i\mathbf{k}'\cdot\mathbf{r}}}{\sqrt{\Omega}}\psi_p(\mathbf{r},\ t)\, v(\mathbf{r}-\mathbf{r}')\psi_p^*(\mathbf{r}',\ t)\, \frac{e^{i\mathbf{k}\cdot\mathbf{r}'}}{\sqrt{\Omega}}.$$

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We can clearly see the Hermitian character of the operator V^{xc} from this relationship, whereby the Fourier components $V_k^{xc}(q, \omega)$ and $V_k^{eff}(q, \omega)$ possess the following transformational property with respect to the operation of finding the complex conjugate:

$$V_k^*(q, \omega) = V_{k+q}(-q, -\omega). \tag{4.47}$$

Upon substituting the trial solutions of (4.44) into Eq. (4.15) and employing (4.47), we find the Fourier component of the induced density:

$$n_{ind}(q, \omega) = 2 \sum_p \frac{n_p - n_{p+q}}{\hbar\omega - E_{p+q} + E_p + i\delta} V_p^{eff}(q, \omega). \tag{4.48}$$

Finally, upon substituting (4.44) into (4.46) and assuming that $k' = k + q$, we find the following relationship that we needed:

$$V_k^{xc}(q, \omega) = -\sum_p v(k-p) \frac{n_p - n_{p+q}}{\hbar\omega - E_{p+q} + E_p + i\delta} V_p^{eff}(q, \omega). \tag{4.49}$$

In contrast to the case of a local potential, in which the self-consistency equation reduces to a simple algebraic equation for $V_{eff}(q, \omega)$, substitution of (4.48) and (4.49) into (4.45) yields an integral equation with respect to $V_k^{eff}(q, \omega)$. In order to simplify the writing of this equation, let us introduce the so-called vertex function $\Lambda_k(q, \omega)$, which is defined by the relationship

$$V_k^{eff}(q, \omega) = \Lambda_k(q, \omega) V_{tot}(q, \omega) \tag{4.50}$$
$$= \Lambda_k(q, \omega) [V_{ext}(q, \omega) + v(q) n_{ind}(q, \omega)].$$

Upon substituting (4.49) into (4.45) and taking account of (4.50), we arrive at the following equation for the vertex function in the self-consistent Hartree-Fock approximation:

$$\Lambda_k(q, \omega) = 1 - \sum_p v(k-p) \frac{n_p - n_{p+q}}{\hbar\omega - E_{p+q} + E_p + i\delta} \Lambda_p(q, \omega). \tag{4.51}$$

If now we recall the definition (2.11) of the irreducible polarization operator $\pi(q, \omega)$, then we can easily see from (4.48) and (4.50) that the following expression holds in the considered approximation:

$$\pi(q, \omega) = -2 \sum_p \frac{n_p - n_{p+q}}{\hbar\omega - E_{p+q} + E_p + i\delta} \Lambda_p(q, \omega). \tag{4.52}$$

Equation (4.52) exactly matches the well-known expression for the screened response function, which is usually derived by diagram technique within the framework of the self-consistent Hartree-Fock approximation.[66,57]

As we have already noted, the dielectric constant is commonly written in the form (4.7). Hence we shall give here another formula that relates the local-field correction $G(q, \omega)$ to the function $\pi(q, \omega)$:

$$G(q, \omega) = -\frac{1}{v(q)} \left[\frac{1}{\chi_0(q, \omega)} + \frac{1}{\pi(q, \omega)} \right]. \tag{4.53}$$

In finding the approximate solutions of the integral equation (4.51) for the vertex function, Kleinman[63] and Langreth[64] employed different methods. However, subsequently both of these authors actually replaced the Hartree-Fock energy E_k of (4.43) by the corresponding value ε_k for free electrons in the formulas that they had derived. Consequently they arrived at the false asymptotic behavior $G(q, 0) \to \alpha q^2$. Geldart and Taylor[67,68] have performed a painstaking analysis of the formula (4.52) for the screened response function in the static case $\omega = 0$ within the framework of diagram technique. As these authors stressed, a correct account for the re-

normalization of the one-electron eigenvalues of the energy is extremely important in the self-consistent Hartree-Fock approximation. In particular, Geldart and Taylor calculated the asymptotic form of the vertex function in explicit form in the limit of large wavenumbers. They showed that all orders of the perturbation-theory series yield strict compensation for large wave vectors between the contributions from the vertex components and from the renormalization of the one-electron energies, which are proportional to q^2.

In spite of the fact that the self-consistent Hartree-Fock approximation for the dielectric function was developed in general outline long ago, nevertheless it has not been possible up to now to establish, even by numerical methods, the nature of the behavior of the corresponding local-field correction $G_{SHF}(q, \omega)$ throughout the region of values of q and ω. In the static case with $\omega = 0$, Geldart and Vosko showed[57] that we have the following expression in the limit of small wavenumbers:

$$G_{SHF}(q, 0) \xrightarrow[q \to 0]{} \frac{1}{4} \left(\frac{q}{k_F} \right)^2. \tag{4.54}$$

(We note that the static local-field correction of Toigo and Woodruff has the same asymptotic behavior.) Moreover, it was found that[41]

$$G_{SHF}(q, 0) \xrightarrow[q \to \infty]{} \frac{1}{3}. \tag{4.55}$$

In the intermediate region of q values, the behavior of the function $G_{SHF}(q, 0)$ has unfortunately not yet been established. Moreover, in essence, the very question remains unclear of the degree of accuracy on which one can generally rely in describing the dielectric properties of a system of interacting electrons within the framework of the self-consistent Hartree-Fock approximation.

5. THE MANY-PARTICLE APPROACH BASED ON THE METHOD OF THE GENERALIZED SELF-CONSISTENT FIELD

The previous sections have treated a set of the known formulas for the dielectric constant, for whose derivation it sufficed to employ a simple one-particle approximation combined with the standard method of the self-consistent field. We cannot view the potentialities of this approach as being full exhausted, since apparently one can find more suitable equations for the exchange-correlation contribution to the effective interelectronic interaction potential. However, on this pathway one still must rely mainly on physical intuition. We shall present below a more systematic method for finding the dielectric function of an interacting electron gas based on the many-electron approach, but in which the sequence of ideas employed in the method of the self-consistent field is explicitly followed. Within the framework of this new approach, we shall see that even the crudest approximation, in a certain sense analogous to the very simple Hartree-Fock approximation treated in Sec. 3, directly yields a result for $\varepsilon(q, \omega)$ that constitutes the latest advance in the theory of the dielectric constant in its current stage of development.

In the coordinate-momentum representation, the complete Hamiltonian of a system of interacting electrons

in the presence of an external perturbation has the form

$$H = \sum_j \frac{\mathbf{p}_j^2}{2m} + \frac{1}{2} \sum_q v(q) \sum_{j \neq j'} e^{i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_{j'})}$$
$$+ \sum_q \int \frac{d\omega}{2\pi} V_{ext}(q, \omega) \sum_j e^{i\mathbf{q}\cdot\mathbf{r}_j} e^{-i(\omega + i\delta)t}. \tag{5.1}$$

In order to account for the positive neutralizing background, we shall preassign the Fourier component $v(q)$ of the Coulomb potential by the condition $v(0) \equiv 0$, and we shall also assume that $V_{ext}(0, \omega) = 0$.

In contrast to the usual practice, we shall not perform the second quantization of the Hamiltonian (5.1) on the basis of plane waves, but on that of single-particle states that account, even in the first approximation, for the presence in the system of both the external perturbation and of the Coulomb repulsion between the electrons. Namely, we shall employ a basis of one-electron states of the form

$$\psi_k(\mathbf{r}, t) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\Omega}}\left[1 + \sum_q \int \frac{d\omega}{2\pi} \frac{V_{ext}(q,\omega)}{\tilde{\varepsilon}(q, \omega)} \frac{e^{i\mathbf{q}\cdot\mathbf{r}} e^{-i(\omega+i\delta)t}}{\hbar\omega - \varepsilon_{k+q} + \varepsilon_k + i\delta} \right]. \tag{5.2}$$

Comparison of (5.2) with (4.16) and (4.20) shows that one can treat these states as approximate solutions of the single-particle Schrödinger equation describing the motion of an electron in the field of the external source and in the self-consistent field of the other electrons of the system. The concrete form of this self-consistent field will be determined from the self-consistency equation. We assume the effective dielectric constant $\tilde{\varepsilon}(q, \omega)$ entering into Eq. (5.2) to possess the general property $\tilde{\varepsilon}^*(q, \omega) = \tilde{\varepsilon}(-q, -\omega)$. Without loss of generality we shall assume that the function $\varepsilon(q, \omega)$ has the structure of (4.21), where $G(q, \omega)$ is the sought local-field correction.

To an accuracy of terms linear in the external perturbation, the Hamiltonian of (5.1) acquires the following form in the second-quantization representation on the basis of (5.2):

$$H = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma}$$
$$+ \sum_{kq\sigma} \int \frac{d\omega}{2\pi} e^{-i(\omega+i\delta)t} V_{eff}(q,\omega)\left[\tilde{\varepsilon}(q,\omega) + \frac{\varepsilon_{k+q} - \varepsilon_k}{\hbar\omega - \varepsilon_{k+q} + \varepsilon_k + i\delta}\right] c_{k+q\sigma}^\dagger c_{k\sigma} + H_C. \tag{5.3}$$

Here the contribution H_C corresponds to the Coulomb interelectronic interaction in the original Hamiltonian of (5.2). It is given by the expression

$$H_C = \frac{1}{2} \sum_{\substack{kk'q \\ \sigma\sigma'}} v(q) c_{k+q\sigma}^\dagger c_{k'-q\sigma'}^\dagger c_{k'\sigma'} c_{k\sigma}$$
$$+ \sum_{\substack{kqpp' \\ \sigma\sigma'}} \int \frac{d\omega}{2\pi} e^{-i(\omega+i\delta)t} v(q+p-p') V_{eff}(q, \omega) \tag{5.4}$$
$$\times \left(\frac{1}{\hbar\omega - \varepsilon_{p+q} + \varepsilon_p + i\delta} - \frac{1}{\hbar\omega - \varepsilon_{p'} + \varepsilon_{p'-q} + i\delta} \right) c_{k+q+p-p'\sigma}^\dagger c_{p'\sigma'}^\dagger c_{p\sigma'} c_{k\sigma}.$$

The states of the perturbed system are described by the wave functions $\Psi_\alpha(t)$, which are the solutions of the Schrödinger equation

$$i\hbar \frac{\partial \Psi_\alpha(t)}{\partial t} = H(t) \Psi_\alpha(t). \tag{5.5}$$

Here the subscript α numbers the eigenstates of the unperturbed system that correspond to the eigenvalues of the energy E_α. The Fourier component of the mean in-

duced density will now be determined by the relationship

$$n(q, t) = Z^{-1} \sum_\alpha e^{-E_\alpha/kT} \langle \Psi_\alpha(t) | \sum_j e^{-i\mathbf{q}\cdot\mathbf{r}_j} | \Psi_\alpha(t) \rangle. \tag{5.6}$$

The operator $\sum_j \exp(-i\mathbf{q}\cdot\mathbf{r}_j)$ entering into Eq. (5.6) in the second-quantization representation on the basis of (5.2) acquires the form

$$\hat{n}(q, t) = \sum_{k\sigma} c_{k\sigma}^\dagger c_{k+q\sigma}$$
$$+ \sum_{kk'\sigma} \int \frac{d\omega}{2\pi} e^{-i(\omega+i\delta)t} V_{eff}(q+k-k', \omega) \frac{c_{k\sigma}^\dagger c_{k'\sigma} - c_{k+q\sigma}^\dagger c_{k'+q\sigma}}{\hbar\omega - \varepsilon_{k+q} + \varepsilon_{k'} + i\delta}. \tag{5.7}$$

Since we are interested in the linear response, it suffices in averaging the second term in (5.7) after it has been substituted into (5.6) to assume therein that

$$\langle c_{k\sigma}^\dagger c_{k'\sigma} \rangle \approx n_{k\sigma} \delta_{k, k'}.$$

Here the $n_{k\sigma}$ are the mean occupation numbers of the single-electron states in the system of interacting electrons. Here, as we can easily see, the summation in the second term in (5.7) reduces to an expression having the same structure as the Lindhard function of (3.1), with the sole difference that the exact occupation numbers of the single-particle states in the interacting system enter into this expression. Recalling this, we keep the previous symbol $\chi_0(q, \omega)$ for this expression. Thus, upon substituting (5.7) into (5.6), we get

$$n(q, t) = \overline{\left\langle \sum_{k\sigma} c_{k\sigma}^\dagger c_{k+q\sigma} \right\rangle^t} + \int \frac{d\omega}{2\pi} e^{-i(\omega+i\delta)t} \chi_0(q, \omega) V_{eff}(q, \omega). \tag{5.8}$$

Comparison of (5.8) with (4.3) shows that Eq. (5.8) defines implicitly the effective screened response function $\pi_{eff}(q, \omega)$.

In calculating the first term in (5.8), we must already know the concrete form of the perturbed wave functions $\Psi_\alpha(t)$. That is, we must find the solution of the Schrödinger equation (5.5) in some approximation. Upon performing these calculations, we arrive at a formula for the dielectric constant of the form of (4.6), where $\pi_{eff}(q, \omega)$ and $G(q, \omega)$ will in turn amount to certain functionals of the sought local-field correction $G(q, \omega)$ that enters into the definition (4.21) of the effective dielectric constant $\tilde{\varepsilon}(q, \omega)$. In principle we can then find the unknown function $G(q, \omega)$ from the self-consistency condition (4.8).

We can simplify this unwieldy scheme of calculation substantially by requiring the dielectric constant directly to have the standard form (4.7), where $\chi_0(q, \omega)$ is the Lindhard function with the exact occupation numbers of the single-electron states. As we can easily see from from (5.8), it suffices for this to require that

$$\overline{\left\langle \sum_{k\sigma} c_{k\sigma}^\dagger c_{k+q\sigma} \right\rangle^t_{q\neq 0}} = 0. \tag{5.9}$$

This simple condition will serve us as the equation for finding the local-field correction $G(q, \omega)$.

In solving the Schrödinger equation (5.5), the fundamental difficulties arise from the first term in the operator of (5.4), which do not contain any small parameter. We shall get the crudest approximation, which makes the problem elementarily simple, by simply neglecting this term. Here the complete Hamiltonian of the system is reduced to the form

$$H(t) = H_0 + H_1(t). \tag{5.10}$$

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The "unperturbed" Hamiltonian is given by the expression

$$H_0 = \sum_{\mathbf{k}\sigma} \varepsilon_\mathbf{k} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma}, \qquad (5.11)$$

while the "perturbation" $H_1(t)$ amounts to the sum of the second terms in Eqs. (5.3) and (5.4). Although the Hamiltonian of (5.11) does not depend explicitly on the time, yet we note that its eigenfunctions must depend on the time, since we are employing the perturbed basis of (5.2). In their structure the eigenfunctions $\Psi_\alpha^{(0)}(t)$ of the Hamiltonian H_0 amount to Slater determinants constructed from the single-electron states of (5.2). The eigenvalues corresponding to them are equal to

$$E_\alpha^{(0)} = \sum_{\mathbf{k}\sigma} \varepsilon_\mathbf{k} n_{\mathbf{k}\sigma}^{(\alpha)}.$$

Here the $n_{\mathbf{k}\sigma}^{(\alpha)}$ are the occupation numbers of the state $\Psi_\alpha^{(0)}(t)$.

The solutions of the Schrödinger equation (5.5) with the Hamiltonian of (5.10) in the approximation linear in the external perturbation have the form

$$\Psi_\alpha(t) = \Psi_\alpha^{(0)}(t) e^{-(i/\hbar)E_\alpha^{(0)}t}$$
$$- \frac{i}{\hbar} \sum_\beta \Psi_\beta^{(0)}(t) e^{-(i/\hbar)E_\beta^{(0)}t} \int_{-\infty}^t dt' e^{(i/\hbar)(E_\beta^{(0)}-E_\alpha^{(0)})t'}$$
$$\times \left\langle \Psi_\beta^{(0)}(t') \left| H_1(t') - i\hbar \frac{\partial}{\partial t'} \right| \Psi_\alpha^{(0)}(t') \right\rangle. \qquad (5.12)$$

If now we average the first term in (5.7) over the states of (5.12), and by virtue of the condition (5.8), equate the result to zero, then the following equation arises for the local-field correction:

$$0 = \sum_{\mathbf{k}\sigma} \frac{n_\mathbf{k} - n_{\mathbf{k}+\mathbf{q}}}{\hbar\omega - \varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_\mathbf{k} + i\delta} \Big[v(q) G(\mathbf{q},\,\omega) \chi_0(\mathbf{q},\,\omega)$$
$$+ \sum_\mathbf{p} v(\mathbf{p}-\mathbf{k})(n_\mathbf{p} - n_{\mathbf{p}+\mathbf{k}}) \left(\frac{1}{\hbar\omega - \varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_\mathbf{k} + i\delta} - \frac{1}{\hbar\omega - \varepsilon_{\mathbf{p}+\mathbf{q}} + \varepsilon_\mathbf{p} + i\delta} \right) \Big]. \qquad (5.13)$$

Here the $n_\mathbf{k}$ are the mean occupation numbers of the single-electron states in a free electron gas. In order to facilitate the comparison of this result with those of other authors, and also for computational considerations, we shall assume that the function $\chi_0(\mathbf{q},\omega)$ in (5.13) is the ordinary Lindhard function of (3.1). In this approximation, we find from Eq. (5.13) directly that

$$G(\mathbf{q},\,\omega) = \frac{4e_q}{\gamma_0^2(\mathbf{q},\,\omega)} \sum_{\mathbf{k}\mathbf{p}} \frac{q(\mathbf{p}-\mathbf{k})}{(\mathbf{p}-\mathbf{k})^2} \frac{n_\mathbf{p} - n_{\mathbf{p}+\mathbf{q}}}{\hbar\omega - \varepsilon_{\mathbf{p}+\mathbf{q}} + \varepsilon_\mathbf{p} + i\delta} \frac{n_\mathbf{k} - n_{\mathbf{k}+\mathbf{q}}}{(\hbar\omega - \varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_\mathbf{k} + i\delta)^2}. \qquad (5.14)$$

In the static case $\omega = 0$, we can transform Eq. (5.14) into the form

$$G(\mathbf{q},\,0) = \frac{8e_q}{\gamma_0^2(\mathbf{q})} \sum_{\mathbf{k}\mathbf{p}} \left[\frac{q(\mathbf{k}-\mathbf{p})}{(\mathbf{k}-\mathbf{p})^2} + \frac{q(\mathbf{k}+\mathbf{p}+\mathbf{q})}{(\mathbf{k}+\mathbf{p}+\mathbf{q})^2} \right] \frac{n_\mathbf{p} n_\mathbf{k}}{(\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_\mathbf{p})(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_\mathbf{k})^2}. \qquad (5.15)$$

In the limits of small and large q, this function has the following asymptotic behavior:

$$G(\mathbf{q},\,0) \rightarrow \begin{cases} \frac{1}{4} \left(\frac{q}{k_\mathrm{F}} \right)^2, & q \rightarrow 0, \\ \frac{1}{3}, & q \rightarrow \infty. \end{cases} \qquad (5.16)$$

Upon comparing (5.16) with (4.54) and (4.55), we see that the function of (5.15) reaches the same asymptotic limits as the static local-field correction in the self-consistent Hartree-Fock approximation. Figure 5 shows the behavior of the function of (5.15) in the intermediate wavenumber region.

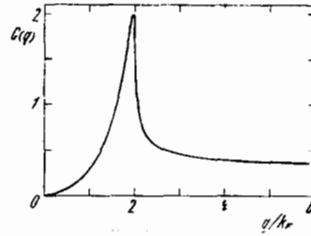The approximation (5.14) for the local-field correction

FIG. 5. Static local-field correction calculated by Eq. (5.15).

possesses a rather long history, though as yet it has received no generally accepted name. As we can show from the results of Geldart and Taylor,[67] who treated only the static case $\omega = 0$, the local-field correction of (5.15) corresponds to an approximation in which one introduces first-order exchange corrections for the Coulomb interaction into the zero-order polarization operator

$$\pi_0(q) = \chi_0(q) = \bigcirc .$$

That is, one employs the approximation

$$\pi(q) \approx \bigcirc + \langle\!\Box\!\rangle + \langle\!\bigcirc\!\rangle + \langle\!\bigcirc\!\rangle .$$

Although Geldart and Taylor did not find the function of (5.15) in explicit form, yet in Ref. 67 they tabulated the numerical values of the integral entering into (5.15) in the interval of wave vectors $0 \leqslant q \leqslant 2k_\mathrm{F}$.

The local-field correction to the static dielectric constant of (5.15) has alos been derived by Dagens[69] and by Sham,[70] who used the method developed by Kohn and Sham[61] of accounting for exchange-correlation effects on the basis of functionals of the density. Moreover, Dagens showed[71] that the values of the function of (5.15) for all q are an upper bound for the possible values of the local-field correction $G_{\mathrm{SHF}}(q, 0)$ in the self-consistent Hartree-Fock approximation.

Rajagopal and Jain[72] first derived the local-field correction of (5.14) dependent on the frequency and the wave vector. Like Langreth,[64] these authors started with the integral equation for the nonlocal vertex function $\Lambda_\mathbf{p}(\mathbf{q}, \omega)$ in the self-consistent Hartree-Fock approximation. They found approximate solutions of this equation by the variational method. The idea of this method is very simple and consists in the following. Initially one seeks some functional $S[\Lambda]$, that acquires an extremal value whenever the vertex function satisfies Eq. (4.51). Let us choose the functional $S[\Lambda]$ in the form

$$S[\Lambda] = \sum_\mathbf{p} \chi_\mathbf{p} \Lambda_\mathbf{p}^2 + \sum_{\mathbf{p}\mathbf{p}'} \Lambda_\mathbf{p} \chi_\mathbf{p} v(\mathbf{p}-\mathbf{p}') \chi_{\mathbf{p}'} \Lambda_{\mathbf{p}'} - 2\sum_\mathbf{p} \chi_\mathbf{p} \Lambda_\mathbf{p}. \qquad (5.17)$$

To shorten the notation here we have introduced the symbol

$$\chi_\mathbf{p}(\mathbf{q},\,\omega) = \frac{n_\mathbf{p} - n_{\mathbf{p}+\mathbf{q}}}{\hbar\omega - E_{\mathbf{p}+\mathbf{q}} + E_\mathbf{p} + i\delta}. \qquad (5.18)$$

Also we have omitted the common arguments $(\mathbf{q}, \omega)$ in the functions $\chi_\mathbf{p}(\mathbf{q}, \omega)$ and $\Lambda_\mathbf{p}(\mathbf{q}, \omega)$. Upon varying (5.17) with respect to $\Lambda_\mathbf{p}$, we get

$$\frac{\delta S[\Lambda]}{\delta \Lambda_\mathbf{p}} = 2\chi_\mathbf{p} \Big[\Lambda_\mathbf{p} - 1 + \sum_{\mathbf{p}'} v(\mathbf{p}-\mathbf{p}') \chi_{\mathbf{p}'} \Lambda_{\mathbf{p}'} \Big]. \qquad (5.19)$$

By comparing (5.19) with (4.51), we see that, if $\Lambda_\mathbf{p}$ is a

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solution of the integral equation (4.51), then the functional of (5.17) actually reaches an extremum. Then one employs the variational principle, namely, one seeks the best "solution" of Eq. (4.51) of the local type of $\Lambda(q, \omega)$ that doesn't depend on the wave vector p. In the class of such local vertex functions, the functional of (5.17) has the form

$$S[\Lambda] = \Lambda^2 \left[\sum_p \chi_p + \sum_{pp'} v(p-p')\chi_p\chi_{p'} \right] - 2\Lambda \sum_p \chi_p.$$

It reaches an extremum when

$$\Lambda = \sum_p \chi_p \left[\sum_p \chi_p + \sum_{pp'} v(p-p')\chi_p\chi_{p'} \right]^{-1}. \tag{5.20}$$

Upon employing (5.20), (4.52), and (4.53), we finally find the following expression for the local-field correction:

$$G(q, \omega) = \frac{1}{v(q)} \left[\frac{1}{\tilde{\chi}(q, \omega)} - \frac{1}{\chi_0(q, \omega)} \right. \tag{5.21}$$
$$\left. + \frac{2}{\tilde{\chi}^2(q, \omega)} \sum_{pp'} v(p-p')\chi_p(q, \omega)\chi_{p'}(q, \omega) \right].$$

Here we have introduced the notation

$$\tilde{\chi}(q, \omega) = 2 \sum_p \chi_p(q, \omega).$$

The approximation (5.20) for the vertex function was first derived by Langreth[64] (in fact, he proposed in this study to use the shielded potential $4\pi e^2/[(p-p')^2 + K_s^2]$ instead of $v(p-p')$). As regards the study by Rajagopal and Jain,[72] they took account of the Coulomb interaction to an accuracy of terms of the first order in $v(p-p')$. Upon considering (4.43) and (5.18), we have the following expression in this approximation for the first term in brackets in (5.21):

$$\frac{1}{\tilde{\chi}(q, \omega)} \approx \frac{1}{\chi_0(q, \omega)} - \frac{2}{\chi_0^2(q, \omega)} \sum_{pp'} v(p-p') \frac{(n_p - n_{p+q})(n_{p'} - n_{p'+q})}{(\hbar\omega - \varepsilon_{p+q} + \varepsilon_p + i\delta)^2}, \tag{5.22}$$

whereas it suffices to set the third term in brackets equal to

$$\frac{2}{\chi_0^2(q, \omega)} \sum_{pp'} v(p-p') \frac{(n_p - n_{p+q})(n_{p'} - n_{p'+q})}{(\hbar\omega - \varepsilon_{p+q} + \varepsilon_p + i\delta)(\hbar\omega - \varepsilon_{p'+q} + \varepsilon_{p'} + i\delta)}. \tag{5.23}$$

Upon substituting (5.22) and (5.23) into (5.21), we arrive at Eq. (5.14) directly.

We note that Rajagopal and Jain[72] found formulas for the spin and orbital magnetic susceptibility of a system of interacting electrons in the same approximation.

The dynamic local-field correction of (5.14) also figures in the study of Dharma-Wardana[73] [see Eq. (4.6c) of the cited study]. For finding the linear response function, he uses the formalism developed by Zubarev[74] of double-time Green's functions, while to estimate the mass operators, he applies the approach of Tyablikov and Bonch-Bruevich[75] based on perturbation theory. An analysis is also performed in Ref. 73 of the contributions to the function $G(q, \omega)$ of the second order in the Coulomb interaction that are not accounted for in Eq. (5.14). These contributions now arise from three-particle correlations, and were shown not be small. Geldart and Taylor[68] had previously reached the same conclusion.

In addition, the expression (5.14) for the function $G(q, \omega)$ has been derived by Brosens et al.[50] following the Hartree-Fock scheme, they uncoupled the equations of motion for the Wigner distribution function $f(p, r, t)$,

which is the quantum-mechanical analog of the classical Boltzmann distribution function. Here they obtained an integral equation for $f(p, r, t)$, which they solved by the above-described Langreth-Rajagopal-Jain variational procedure.

Finally, the local-field correction of (5.14) has appeared in a study by Tripathy and Mandal,[76] who followed the general scheme of Toigo and Woodruff,[38] while introducing a certain new feature into it. As mentioned in the previous section, Toigo and Woodruff started with a chain of equations of motion for the Green's functions that stemmed from the equation for the response function $\chi(q, \omega)$. Here the Green's functions of the next order were equated to $\chi(q, \omega)$ with a certain proportionality constant $A(q)$. They required the corresponding integrals with respect to the frequency to coincide. Tripathy and Mandal applied the same method, but employed here the coefficient $A(q, \omega)$ that also depends on the frequency. We should note that, although this calculational scheme has a certain mathematical elegance, the underlying physics requires special elucidation.

Thus we see that the approximation (5.14) for the local-field correction proves very "popular", and is yielded by an entire set of theoretical methods that are often difficult to correlate with one another. Within the framework of the approach developed in this section, however, we see well that this approximation is still rather crude. It corresponds to the simplest treatment of the problem in which one drops the first term, which is not at all small, in the Coulomb interaction operator of (5.4). Yet the behavior of the dielectric constant with the local-field correction of (5.14) is characterized by qualitatively new features that merit thorough study. Thus, Brosens et al.[77] calculated the real component of $\varepsilon(q, \omega)$ as well as the dynamic structure factor. As these calculations showed, an important qualitative feature of the dielectric constant with the local-field correction of (5.14) is that it yields a plasmon branch that doesn't penetrate into the region of creation of single electron-hole pairs with increasing wave vector. Instead, the plasmon branch asymptotically approaches the boundary $\hbar\omega/\varepsilon_F \approx 2(q/k_F) + (q/k_F)^2$ of the continuum of single-pair excitations. Thus here, for example, at $q = 1.5k_F$ the plasmons are still conserved as well-defined collective excitations even at $r_s = 3$. Tripathy et al.[78] showed that, within the framework of the studied approximation, the static structure factor $S(q)$ shows a maximum at $q \approx 2k_F$ for all values of the parameter r_s in the range of metallic densities. This indicates that close-range order is established in a system of interacting electrons at these densities. Thus this system more resembles a liquid than a gas. With further growth in r_s, the maximum at $q \approx 2k_F$ on the $S(q)$ curve becomes even sharper. Moreover, extra maximum appear at $q > 2k_F$, which indicate establishment of correlation between ever more remote neighbors. However, it remains unknown how much one can trust the stated behavior of the static structure factor for large q and large r_s, since the calculations of the pair correlation function $g(r)$ performed by Mandal et al.[79] show that $g(0)$ becomes negative for $r_s \gtrsim 4$ in the studied approximation.

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6. THE INTERACTING ELECTRON GAS AND THE THEORY OF SIMPLE METALS

The homogeneous system of interacting electrons moving in a background of neutralizing positive charge that we have treated in the previous sections is, of course, purely a model and is not realized in nature. Yet real objects exist for which one can easily adapt the theory of the homogeneous electron gas to describe their properties. The most important example of such systems is the simple metals.

Many elements that have incomplete s and p electron shells in the atomic state collectivize all their valence electrons in forming a metal, and convert into a distinctive two-component electron-ion plasma. As a rule, the dimensions of the ionic cores in such metals are small in comparison with the lattice parameter, so that the direct interionic interaction amounts mainly to a pure Coulomb repulsion of the point charges $+Ze$, where Z is the number of valence electrons released by the metal atom into the conduction band. The stability of both the ionic and the electronic subsystems is ensured by their mutual interaction.

In order to create a quantitative theory of the metallic state, one must first make specific such an important characteristic as the electron-ion interaction. We shall condense to an extreme the discussion of this far-from-simple problem, whose solution is involved in the development of an entire field in metal theory. We note that the concept of the pseudopotential (or model potential)[80,81] proves very useful in describing the effective electron-ion interaction in simple metals, whose fundamental properties primarily owe to the character of the behavior of the conduction electrons in the region of space outside the ionic cores. In the intervals between the ions, the total potential acting on an electron is highly smoothed, and the wave function of the electron has a form close to a plane wave. Hence it proves possible in describing the behavior of the electrons in this region of space to replace the true Coulomb potential of the ions, which generally is not at all small, with some relatively weak pseudopotential that has the same scattering properties. In this case, the calculation of the electronic properties of a metal can start with treatment of a homogeneous electron gas, and then account for the effect of the weak electron-ion interaction by perturbation theory. In the simplest variant of the pseudopotential method, to which we shall restrict our analysis, one assumes that the pseudopotential is a local operator, and that the effective electron-ion interaction can be written in the following form:

$$V_{ei} = \sum_{jn} V\left(\mathbf{r}_j - \mathbf{R}_n\right) = \sum_{q} V(q) \sum_{jn} e^{i \cdot q(r_j - R_n)}. \tag{6.1}$$

Here $\mathbf{r}_j$ and $\mathbf{R}_n$ are the coordinates of the jth electron and the nth ion respecitvely, while $V(q)$ is the form factor of the electron-ion pseudopotential, which is a characteristic of the individual ion and is assumed to be fixed.

As we know, the concept of the pseudopotential initially arose within the framework of the problem of calculating the electronic band structure.[80] However, the fruitfulness of this idea has also been demonstrated subsequently in the calculation of other characteristics of simple metals, such as the binding energy and phonon spectra.[6,81] The formation of the phonon spectrum of a metal is a very complicated process, in which the interactions between all the particles existing in the metal play a substantial role. Here an especially important role belongs to screening effects arising from interelectron interaction. We shall discuss the influence of these effects on the phonon spectrum of a simple metal in the next section.

Upon accounting for the picture formulated above of a simple metal, we can write the model Hamiltonian for it in the following form:

$$H = \sum \frac{P_n^2}{2M} + \frac{1}{2} \sum_{n \ne n'} \frac{Z^2 e^2}{|R_n - R_{n'}|} + \sum_j \frac{p_j^2}{2m} + \frac{1}{2} \sum_{j \ne j'} \frac{e^2}{|r_j - r_{j'}|} + \sum_{jn} V\left(r_j - R_n\right). \tag{6.2}$$

One usually calculates the phonon spectrum of a metal on the basis of the Hamiltonian of (6.2) within the framework of the adiabatic approximation first proposed by Born and Oppenheimer.[82] This approximation is based on the following physical arguments. Owing to the large difference between the masses of the electrons and the ions, the characteristic velocities of the conduction electrons in metals greatly exceed the velocities of the ions. Hence, in studying the motion of the electrons, one can consider the ions in first approximation to be at rest with some given configuration $\{\mathbf{R}_n\}$. On the other hand, in treating the motion of the ions, we get a good approximation if we replace all the quantities that depend on the electronic variables and which affect the dynamics of the ionic subsystem with their mean values calculated for the corresponding concrete configurations of the ions. Thus, within the framework of the adiabatic approximation, the effective potential energy of the ionic subsystem $U_{eff}(\{\mathbf{R}_n\})$ can be represented as the sum of the direct Coulomb interionic interaction $U_{ii}(\{\mathbf{R}_n\})$ and the mean energy of the electrons $E_0(\{\mathbf{R}_n\})$ for the given configuration $\{\mathbf{R}_n\}$ of the ions:

$$U_{eff}(\{R_n\}) = U_{ii}(\{R_n\}) + E_0(\{R_n\}).$$

In finding in practice the lattice-vibration spectrum from $U_{eff}(\{\mathbf{R}_n\})$, one separates out the harmonic component (which is quadratic in the small deviations u_n of the ions from their equilibrium lattice positions), and then solves the system of classical equations of motion of Newton for the ions:

$$M\ddot{u}_n = -\frac{\partial}{\partial u_n} U_{eff}(\{R_n\}). \tag{6.3}$$

In this equation, the right-hand side contains the effective force exerted on the nth ion by the other ions and electrons.

The most difficult point in this scheme of calculation consists in finding a reasonable approximate estimate of the mean energy of the electrons $E_0(\{\mathbf{R}_n\})$ for a given ionic configuration. The theory of simple metals takes as the zero-order approximation for this quantity the energy of the ground state of a homogeneous interacting electron gas, while the contribution from the electron-ion interaction is taken into account in the form of a perturbation-theory series in powers of the pseudopotential $V(q)$. This procedure has been carried out most

consistently within the framework of a many-particle approach to the electronic subsystem in a series of studies by E. G. Brovman and Yu. M. Kagan (see the review[6]). They showed that the contribution to $E_0(\{R_n\})$ quadratic in $V(q)$ is responsible in the lattice dynamics for the pairwise interionic interactions, whereas the contributions of higher order in $V(q)$ are equivalent to many-particle ion-ion forces, which indicate the existence in metals of a sort of covalent bonding. The painstaking analysis of these many-ion interactions by Brovman and Kagan showed that one can use them to solve the problem of the compressibility and that of the breakdown of the Cauchy relationships for the elastic constants of a metal. They also found that these interactions must lead to a certain type of anomalies in the phonon spectra of metals.

Evidently, in calculating the mean electron energy $E_0(\{R_n\})$, and hence also in calculating the effective interionic potential, accounting for the exchange-correlation effects in the electronic subsystem is an extremely difficult problem. Owing to the electron-ion interaction, this problem proves substantially more complicated than, say, the calculation of the dielectric constant of a homogeneous electron gas. As regards the pairwise interionic interactions, which correspond to accounting for the pseudopotential $V(q)$ in second-order perturbation theory, they are completely described by using the DC of a homogeneous electron gas. In calculating them, this allows one to use the already existing approximate expressions for the DC that account for exchange and correlation effects. Yet a calculation of the non-pairwise many-ion interactions requires a knowledge of the nonlinear polarizabilities of an interacting electron gas. No procedure that is to any extent systematic has yet been developed for accounting for exchange-correlation effects in finding the nonlinear polarizabilities of an electron gas. Hence, in calculating the many-ion non-pairwise forces, most studies have actually been restricted to the framework of the random-phase approximation.[6,83-85] Recently attempts[86-88] have been undertaken on the basis of the formalism of functionals of the density[61] to take account to an equal extent of exchange-correlation effects in calculations of both the linear and the nonlinear polarizability. We shall return later to discussing this problem, but first we shall present a method of calculating the electronic contribution to the effective ion-ion interaction based on ideas close to those employed in Sec. 4.

In full accord with the spirit of the adiabatic approximation and with account for the explicit form (6.1) of the electron-ion interaction potential, we can write the following obvious formula directly for the effective force exerted by the electrons on the nth ion:

$$\mathbf{F}_{el}(\mathbf{R}_n) = -i \sum_q \mathbf{q} V^*(q)\, e^{i\mathbf{q}\mathbf{R}_n} \left\langle \sum_j e^{-i\mathbf{q}\mathbf{r}_j} \right\rangle_{\{R_n\}}. \qquad (6.4)$$

Here the subscript applied to the brackets denotes averaging over the states of the electronic subsystem that are realized in the given ionic configuration $\{R_n\}$. The characteristic of the electronic subsystem to be averaged is

$$n_e(\mathbf{q}) = \sum_j e^{-i\mathbf{q}\mathbf{r}_j}. \qquad (6.5)$$

This amounts to the Fourier component of the operator for the electron number density. Thus, in finding the effective force of (6.4), we must actually know only the mean induced-density distribution in the system of interacting electrons into which the ions in the configuration $\{R_n\}$ have been introduced.

To solve this problem, we shall apply the self-consistent-field method that we employed in Sec. 4 in deriving the expression for the dielectric function of Toigo and Woodruff. In this case, owing to the static nature of the perturbation of the electronic subsystem by the motionless ions, we must know the stationary solutions of the one-particle Schrödinger equation, in which the total potential energy of an electron is defined by the expression

$$V_{eff}(\mathbf{r}) = \sum_k V(k)\, e^{i\mathbf{k}\cdot\mathbf{r}} \sum_n e^{-i\mathbf{k}\cdot\mathbf{R}_n} + V_a(\mathbf{r}). \qquad (6.6)$$

Here $V_e(\mathbf{r})$ is the potential energy of the electron in the self-consistent field of the rest of the electrons, which we shall find by Eq. (4.4). In order to allow in explicit form for the overall electroneutrality of the system, we shall stipulate that the Fourier components of the potentials that figure in (6.6) have no components of zero wave vector. That is, we have $V(q=0) = V_e(q=0) = 0$.

To an accuracy of second-order terms in the perturbation of (6.6), the solutions of the one-electron Schrödinger equation have the form

$$\psi_q(\mathbf{r}) \approx c_q \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{\sqrt{\Omega}}\left[1 + \sum_k \frac{V_{eff}(k)\, e^{i\mathbf{k}\cdot\mathbf{r}}}{\varepsilon_q - \varepsilon_{q+k}} + \sum_{k,p} \frac{V_{eff}(k-p)\, V_{eff}(p)\, e^{i\mathbf{k}\cdot\mathbf{r}}}{(\varepsilon_q - \varepsilon_{q+k})(\varepsilon_q - \varepsilon_{q+p})}\right]. \qquad (6.7)$$

Here c_q is a normalizing factor. Equation (6.7) directly allows us to write down an expression for the sought mean value of the operator for the Fourier component of the electron density of (6.5):

$$\langle n_e(q) \rangle_{\{R_n\}} \approx \chi_0(q) V_{eff}(q) + \sum_k J^{(3)}(k, q) V_{eff}^*(k) V_{eff}(k+q). \qquad (6.8)$$

Here $\chi_0(q)$ is the static Lindhard function, while $J^{(3)}(k, q)$ denotes the function

$$J^{(3)}(k, q) = 2 \sum_p n_p \left[\frac{1}{(\varepsilon_p - \varepsilon_{p+k})(\varepsilon_p - \varepsilon_{p-q})} \right.$$
$$\left. + \frac{1}{(\varepsilon_p - \varepsilon_{p+q})(\varepsilon_p - \varepsilon_{p+k+q})} + \frac{1}{(\varepsilon_p - \varepsilon_{p-k-q})(\varepsilon_p - \varepsilon_{p-k})} \right]. \qquad (6.9)$$

The latter was first introduced by Kagan and Brovman[89] and is called the tripole. The review[6] gives an explicit expression for the tripole. As we see from Eq. (6.4), the approximation (6.8) for the induced electron density allows one to establish the form of the effective interionic interaction to an accuracy of third-order terms in the form factor of the electron-ion pseudopotential, and thus to gain a picture of the three-particle interionic interactions.

We must still find the Fourier components $V_{eff}(q)$ that enter into (6.8), which we can do by using Eqs. (4,4), (6.6), and (6.7). To facilitate tracing the scheme of this calculation, we shall first account only for the first term in Eq. (4.4), which corresponds to the self-consistent Hartree field. This simplification corresponds to employing the random-phase approximation.

In the RPA, we have actually already performed the main part of the calculation, since the Hartree contribu-

tion to the potential $V_e(\mathbf{q})$ is determined by the expression

$$V_e^{11}(\mathbf{q}) = v(\mathbf{q}) \langle n_e(\mathbf{q}) \rangle_{\{\mathbf{R}n\}}. \qquad (6.10)$$

Upon employing the approximation (6.10) for $V_e(\mathbf{q})$ and accounting for (6.8), we arrive from the self-consistency condition (6.6) at the following integral equation for the sought Fourier components:

$$
\begin{aligned}
V_{\text{eff}}(\mathbf{q}) \\
\approx \frac{V(\mathbf{q})}{\varepsilon_{\text{RPA}}(\mathbf{q})} \sum_n{}' e^{-i\mathbf{q}\cdot\mathbf{R}n} + \frac{v(\mathbf{q})}{\varepsilon_{\text{RPA}}(\mathbf{q})} \sum_k{}' J^{(3)}(\mathbf{k},\mathbf{q}) V_{\text{eff}}^*(\mathbf{k}) V_{\text{eff}}(\mathbf{k}+\mathbf{q}).
\end{aligned}
$$
$$(6.11)$$

Here $\varepsilon_{\text{RPA}}(\mathbf{q})$ is the dielectric constant in the RPA. We must find a solution of Eq. (6.11) to an accuracy of terms quadratic in the form factor of the electron-ion pseudopotential $V(\mathbf{q})$. This problem can be easily solved by the iteration method, and as a result we get

$$
\begin{aligned}
V_{\text{eff}}(\mathbf{q}) \approx \frac{V(\mathbf{q})}{\varepsilon_{\text{RPA}}(\mathbf{q})} \sum_n{}' e^{-i\mathbf{q}\cdot\mathbf{R}n} \\
+ \frac{v(\mathbf{q})}{\varepsilon_{\text{RPA}}(\mathbf{q})} \sum_k{}' J^{(3)}(\mathbf{k},\mathbf{q}) \frac{V^*(\mathbf{k})}{\varepsilon_{\text{RPA}}(\mathbf{k})} \frac{V(\mathbf{k}+\mathbf{q})}{\varepsilon_{\text{RPA}}(\mathbf{k}+\mathbf{q})} \sum_n{}' e^{i\mathbf{k}\cdot\mathbf{R}n} \sum_m{}' e^{-i(\mathbf{k}+\mathbf{q})\cdot\mathbf{R}m}.
\end{aligned}
$$
$$(6.12)$$

Finally, upon substituting (6.12) into (6.8) and taking (6.4) into account, we arrive at the following expression for the effective force exerted by the ions and electrons on the nth ion:

$$
\begin{aligned}
\mathbf{F}_{\text{eff}}(\mathbf{R}_n) \approx -i \sum_q{}' \mathbf{q} \left[Z^2 v(\mathbf{q}) + \chi_0(\mathbf{q}) \frac{|V(\mathbf{q})|^2}{\varepsilon_{\text{RPA}}(\mathbf{q})} \right] e^{i\mathbf{q}\cdot\mathbf{R}n} \sum{}' e^{-i\mathbf{q}\cdot\mathbf{R}n} \\
- i \sum_{\mathbf{k},\mathbf{q}}{}' \mathbf{q} J^{(3)}(\mathbf{k},\mathbf{q}) \frac{V^*(\mathbf{q})}{\varepsilon_{\text{RPA}}(\mathbf{q})} \frac{V^*(\mathbf{k})}{\varepsilon_{\text{RPA}}(\mathbf{k})} \frac{V(\mathbf{k}+\mathbf{q})}{\varepsilon_{\text{RPA}}(\mathbf{k}+\mathbf{q})} e^{i\mathbf{q}\cdot\mathbf{R}n} \sum_m{}' e^{i\mathbf{k}\cdot\mathbf{R}m} \sum_{m'}{}' e^{-i(\mathbf{k}+\mathbf{q})\cdot\mathbf{R}m'}.
\end{aligned}
$$
$$(6.13)$$

The first term on the right-hand side of Eq. (6.13) describes the pairwise effective interionic interaction forces, which consist of direct Coulomb repulsion between the ions and their indirect attraction via the conduction electrons [the function $\chi_0(\mathbf{q})$ is negative for all q]. This term determines the dominant contribution to the total interionic interaction and plays the major role in forming the phonon spectrum of a simple metal. The term of the third order in $V(\mathbf{q})$ in Eq. (6.13) describes the effective forces of covalent type that correspond to indirect interaction of one ion with two others. In structure, this term corresponds exactly to the analogous term in Brovman and Kagan's theory. Its fundamental role in the lattice dynamics of a simple metal is discussed in the review.[6] We recall that Eq. (6.13) was derived in an approximation that neglected the second term in Eq. (4.4) for the potential $V_e(\mathbf{r})$. We shall see below how the expression for $E_{\text{eff}}(\mathbf{R}_n)$ is altered when we account for exchange and correlation effects in the electronic subsystem.

Upon substituting the single-electron states of (6.7) into the second term in Eq. (4.4), after rather unwieldy, but fundamentally uncomplicated algebraic transformations, we arrive at the following expression for the Fourier component of the exchange-correlation correction to the potential $V_e(\mathbf{q})$:

$$
\begin{aligned}
V_e^{\text{xc}}(\mathbf{q}) = -v(\mathbf{q}) G(\mathbf{q}) \chi_0(\mathbf{q}) V_{\text{eff}}(\mathbf{q}) \\
+ \frac{v(\mathbf{q})}{N} \sum_k [G(\mathbf{k}) + g(\mathbf{k},\mathbf{q})] \chi_0(\mathbf{k}) \chi_0(\mathbf{k}+\mathbf{q}) V_{\text{eff}}^*(\mathbf{k}) V_{\text{eff}}(\mathbf{k}+\mathbf{q}).
\end{aligned}
$$
$$(6.14)$$

Here $G(\mathbf{q})$ is the static local-field correction of Toigo and Woodruff, while $g(\mathbf{k},\mathbf{q})$ denotes a function defined by the expression

$$
\begin{aligned}
\chi_0(\mathbf{k}) \chi_0(\mathbf{k}-\mathbf{q}) g(\mathbf{k},\mathbf{q}) \qquad (6.15) \\
-2 \sum_{\mathbf{p},\mathbf{p'}}{}' \frac{\mathbf{q}(\mathbf{p'}-\mathbf{p})}{|\mathbf{p'}-\mathbf{p}|^2} \frac{n_{\mathbf{p}}-n_{\mathbf{p}+\mathbf{k}}}{\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}+\mathbf{k}}} \left(\frac{n_{\mathbf{p'}}-n_{\mathbf{p'}+\mathbf{k}+\mathbf{q}}}{\varepsilon_{\mathbf{p'}}-\varepsilon_{\mathbf{p'}+\mathbf{k}+\mathbf{q}}} + 2 \frac{n_{\mathbf{p'}}-n_{\mathbf{p'}+\mathbf{q}}}{\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}+\mathbf{q}}} \right).
\end{aligned}
$$

The subsequent calculation is performed in full analogy with the scheme that we used above in deriving the result in the RPA, with the sole difference that now $V_e(\mathbf{q})$ is determined by the sum of the expressions (6.10) and (6.14). Consequently we get the following expression for the effective force acting on the nth ion:

$$
\begin{aligned}
\mathbf{F}_{\text{eff}}(\mathbf{R}_n) \approx -i \sum_q{}' \mathbf{q} \left[Z^2 v(\mathbf{q}) + \chi_0(\mathbf{q}) \frac{|V(\mathbf{q})|^2}{\tilde\varepsilon(\mathbf{q})} \right] e^{i\mathbf{q}\cdot\mathbf{R}n} \sum_m{}' e^{-i\mathbf{q}\cdot\mathbf{R}n} \\
- i \sum_{\mathbf{k},\mathbf{q}}{}' \mathbf{q} \tilde J(\mathbf{k},\mathbf{q}) \frac{V^*(\mathbf{q})}{\tilde\varepsilon(\mathbf{q})} \frac{V^*(\mathbf{k})}{\tilde\varepsilon(\mathbf{k})} \frac{V(\mathbf{k}+\mathbf{q})}{\tilde\varepsilon(\mathbf{k}+\mathbf{q})} e^{i\mathbf{q}\cdot\mathbf{R}n} \sum_m{}' e^{i\mathbf{k}\cdot\mathbf{R}m} \sum_{m'}{}' e^{-i(\mathbf{k}+\mathbf{q})\cdot\mathbf{R}m'}.
\end{aligned}
$$
$$(6.16)$$

Here $\tilde\varepsilon(\mathbf{q})$ is the effective dielectric constant of (4.10) in the static case $\omega = 0$, while $\tilde J(\mathbf{k},\mathbf{q})$ is the renormalized tripole, which is given by the formula

$$
\begin{aligned}
\tilde J(\mathbf{k},\mathbf{q}) = [1 + v(\mathbf{q}) G(\mathbf{q}) \chi_0(\mathbf{q})] J^{(3)}(\mathbf{k},\mathbf{q}) \qquad (6.17) \\
+ \frac{1}{N} v(\mathbf{q}) \chi_0(\mathbf{q}) \chi_0(\mathbf{k}) \chi_0(\mathbf{k}+\mathbf{q}) [G(\mathbf{k}) + g(\mathbf{k},\mathbf{q})].
\end{aligned}
$$

We note that Eq. (6.16) has been derived for an arbitrary configuration of ions $\{\mathbf{R}_n\}$, so that it can be employed in the rather general case. In the problem of the dynamics of a stable regular lattice, in which the ions perform small oscillations around their equilibrium positions, the exponentials entering into (6.16) can be expanded in a series in the displacements of the ions. In the harmonic approximation, it suffices to restrict the treatment to terms that are linear in the displacements. This immediately yields the force matrix, with which can find the dynamic matrix by standard procedures. Diagonalization of the latter enables one to obtain the phonon spectrum. For concrete calculations we must also know the explicit form of the function $g(\mathbf{k},\mathbf{q})$, in addition to $V(\mathbf{q})$ as well as the known functions $\chi_0(\mathbf{q})$, $G(\mathbf{q})$, and $J^{(3)}(\mathbf{k},\mathbf{q})$. One can easily convert the sixfold integral in (6.15) into a double integral, which can be found by numerical integration. The corresponding formulas are rather unwieldy, and we shall not present them here.

The merit of the method given above for calculating the effective interionic interaction is simple metals lies in the fact that it enables one simultaneously and self-consistently to find both the effective dielectric constant, which determines the linear response of the electronic subsystem to the electron-ion interaction and the renormalized tripole, which characterizes the nonlinear polarizability of the electron gas with account for exchange and correlation effects. Within the framework of this method, apparently one can actually take the next step and find an explicit expression for $\mathbf{F}_{\text{eff}}(\mathbf{R}_n)$ to an accuracy of fourth-order terms in the form factor of the electron-ion pseudopotential. However, with further increase in accuracy, we shall evidently obtain formulas that are ever more unwieldy and less suitable for direct calculations.

Attempts have been undertaken[87,88,90] to construct a theory of the lattice dynamics of simple metals with account for the contributions from higher-order terms in the electron-ion interaction. The fundamental idea of these studies is the following. In line with the theorem of Hohenberg and Kohn,[91] the energy of the ground state

of the electron gas $E_0(\{\mathbf{R}_n\})$ is a functional of the electron density $n(\mathbf{r}, \{\mathbf{R}_n\})$. Hence we should assign the central role in the whole problem to calculating this specific physical quantity as accurately as possible. This calculation is performed in the stated studies by the following, highly nontrivial scheme. First one solves the auxiliary problem of finding the true induced electron density in a system of interacting electrons into which a single ion of the given type has been introduced [in practice one employs the Slater-Gaspar-Kohn-Sham approach[59-62] for this purpose with an approximate exchange-correlation potential of the form $n^{1/3}(\mathbf{r})$]. In the region of space outside the ion core ($r \geqslant R_c$), the exact induced density $n(\mathbf{r})$ is a smoothly varying function of $\mathbf{r}$, whereas inside the ion it undergoes frequent, short-wave oscillations. From the data of this auxiliary calculation, one constructs the "smoothed" electron density $\bar{n}(\mathbf{r})$, which coincides with $n(\mathbf{r})$ for $r > R_c$, and has the same mean value over the volume as $n(\mathbf{r})$, but now behaves smoothly (without oscillations) inside the ionic core. Further, one introduces a certain effective electron-ion potential, which even in the lowest order of perturbation theory leads to an induced density that coincides with the smoothed electron density $\bar{n}(\mathbf{r})$. Thus, two variants of the local effective potential were tested in Ref. 88, namely the first-order potential $W^{(1)}(\mathbf{q})$ defined by the formula

$$\bar{n}(\mathbf{q}) = \chi_0(\mathbf{q}) \frac{W^{(1)}(\mathbf{q})}{\bar{\varepsilon}(\mathbf{q})},$$

together with the effective second-order potential $W^{(2)}(\mathbf{q})$, which is introduced by the relationship

$$\bar{n}(\mathbf{q}) = \chi_0(\mathbf{q}) \frac{W^{(2)}(\mathbf{q})}{\bar{\varepsilon}(\mathbf{q})} + \sum_{\mathbf{k}} \frac{J^{(3)}(\mathbf{k}, \mathbf{q})}{\bar{\varepsilon}(\mathbf{q})} \frac{W^{(2)*}(\mathbf{k})}{\bar{\varepsilon}(\mathbf{k})} \frac{W^{(2)}(\mathbf{k}+\mathbf{q})}{\bar{\varepsilon}(\mathbf{k}+\mathbf{q})}.$$

Here $\bar{\varepsilon}(\mathbf{q})$ is the static effective dielectric constant of (4.10) (to be specific function $\bar{\varepsilon}(\mathbf{q})$ was used in Ref. 88 with the local-field correction $G(\mathbf{q})$ of Geldart and Taylor[68]). The effective electron-ion potential thus defined differs from the ordinary pseudopotential, and actually proves even weaker. The latter fact facilitates its use for calculating phonon spectra, as is done by the same scheme as in the approach based on the pseudopotential method. It is clear, however, that by definition $W(\mathbf{q})$ also partially incorporates the effects of higher-order terms in the electron-ion interaction (e.g., those that correspond to multiple scattering of electrons by the same ion). On the whole, this approach seems highly promising, though systematic pursuit of it in practice faces the same difficulties of accurate accounting for exchange and correlation effects.

7. CONCLUSIONS

It is practically impossible in such a short review to examine all the aspects of the theory of a system of interacting electrons, which continues to develop actively. Hence we have focused attention on deriving the fundamental, currently known formulas for the dielectric constant of this system. Here we have actually not touched upon such an important question as the relative merits of the various methods of solving this problem. At present it seems very difficult to advance any cogent arguments on the advantage of any given approach to calculating the DC of an electron gas at intermediate

and low densities. This involves the following two circumstances. First, the absence of a small parameter in the problem rules out a pure theoretical analysis of the degree of accuracy of the different methods of calculating $\varepsilon(\mathbf{q}, \omega)$. Second, a system of a homogeneous electron gas in a neutralizing background is not realized in pure form in nature. Hence one cannot test experimentally all the consequences of the various theoretical calculations.

The sole system at our disposal that most closely corresponds to a homogeneous electron gas in the ensemble of conduction electrons in simple metals. The few known experiments to measure the contribution of the conduction electrons to the dynamic structure factor of a set of simple metals have been performed by the method of inealstic scattering of both x-rays[92,93] and an electron beam.[34,44] Apparently they indicate that not one of the existing approximate expressions for the DC can be deemed fully satisfactory. The results of these experiments also show that the collective response of the conduction electrons to the probe beam recalls the response of a strongly interacting liquid, rather than of an ideal gas. Study of the static structure factor in liquid sodium and aluminum[94] also reveals strong close-range order in the electronic subsystem that propagates to distances of 30–40 Å. However, we should note, first that the experimental data of Refs. 93, 44 are not in full agreement and second, that we do not possess complete theoretical clarity on the problem of the role of electron-ion interaction in these phenomena.

The problem of the behavior of a homogeneous electron gas in the background of a neutralizing positive charge can also be studied in the classical limit. The problem of studying the properties of a classical, strongly nonideal plasma is currently also the topic of intensive theoretical studies.[95] However, the situation in this field is far more definite, since detailed calculations exist on the properties of a classical, one-component plasma by the method of molecular dynamics,[96,97] with which we can compare the approximate theoretical results. Very recently molecular-dynamic calculations have also been performed by the Monte Carlo method on a quantum one-component plasma.[98] This study calculated the energy of the ground state of an interacting electron gas over a broad range of values of the parameter r_s. Three phases were shown to exist in the electron system: a homogeneous unpolarized liquid ($1 < r_s < 13$), a ferromagnetic homogeneous liquid with fully polarized spins ($13 < r_s < 33$), and a Wigner crystal for $r_s > 33$. The compressibility of a homogeneous electron gas was also found[98] to become negative even at $r_s \geqslant 5.4$. This means, first, that the stability of this system at the corresponding densities can be ensured only by the compressibility of the neutralizing background, and second, that the onset of negative compressibilities at $r_s > 5.4$ in calculations that start with a concrete expression for the dielectric constant cannot be treated as evidence of the inconsistency of the given approximation for the DC. Undoubtedly, it is of great interest to continue the study of the properties of the quantum interacting electron gas by the Monte Carlo method, and in particular, to calculate the various cor-

relation functions by this method.

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