2. At a fixed frequency of the wave, the relaxation frequency ν increases with rising temperature and may turn out to be of the order of ω. Then the contribution (3.5) to the oscillating part of the impedance decreases much faster than (3.3). Consequently in the region

$$\omega-\nu\gg\left(\frac{\omega^2+\nu^2}{|\Lambda|}\right)^{1/2}=(2k_0v\Omega)^{1/2},\quad \omega\sim\nu \tag{4.2}$$

the CR manifest itself in the form of the damped harmonic oscillations from (3.3):

$$\Delta Z_\alpha^{\text{osc}}(H)=\frac{\mu_\alpha c^2k_0}{2^7\pi^2\omega}\left(\frac{k_0v\Omega}{\omega^2+v^2}\right)^2|Z(0)|^2(1-\rho)^2 \times\exp\left\{-\frac{2\pi\nu}{\Omega}+2\pi i\left(\frac{\omega}{\Omega}-\frac{2\beta}{\pi}+\frac{1}{6}\right)\right\}. \tag{4.3}$$

3. On going to the low-frequency region, where $\nu>\omega$, the delay effect ceases to play any role, as a result of which the amplitude of the CR oscillations increases sharply. In the limit

$$\nu-\omega\gg(2k_0v\Omega)^{1/2} \tag{4.4}$$

the oscillating part of the impedance does not depend on the parameter Λ and is determined, according to (3.9) by

$$\Delta Z^{\text{osc}}(H)=\frac{2-\cos(\pi z_0/3)}{3\cos^2(\pi z_0/2)}|Z(0)|\exp\left\{-\frac{2\pi\nu}{\Omega}+2\pi i\left(\frac{\omega}{\Omega}+\frac{1}{3}\right)\right\}. \tag{4.5}$$

The foregoing results were obtained for a quadratic and isotropic dispersion law. They can be easily generalized, however, to include the case of an arbitrary Fermi surface, in analogy with what was done earlier in Ref. 2.

In conclusion, we are greatful to V. A. Yampol'skiĭ for interest in the work and for useful discussions.

[1] M. Ya. Azbel' and É. A. Kaner, Zh. Eksp. Teor. Fiz. **30**, 811 (1956); **32**, 896 (1957) [Sov. Phys. JETP **3**, 772 (1956); **5**, 730 (1957)].

[2] É. A. Kaner, O. I. Lyubimov, and N. M. Makarov, Zh. Eksp. Teor. Fiz. **67**, 316 (1974) [Sov. Phys. JETP **40**, 158 (1975)].

[3] É. A. Kaner, N. M. Makarov, V. L. Fal'ko, and V. A. Yampol'skiĭ, Zh. Eksp. Teor. Fiz. **73**, 1400 (1977) [Sov. Phys. JETP **46**, 737 (1977)].

[4] É. A. Kaner and M. Ya. Azbel', Zh. Eksp. Teor. Fiz. **33**, 1461 (1957) [Sov. Phys. JETP **6**, 1126 (1958)].

[5] J. F. Koch and A. F. Kip, Proc. of the Ninth Intern. Conf. on Low Temperature Physics, Columbus, Ohio, USA, Plenum Press, Inc., New York, 1964, p. 126.

[6] D. A. Smith, Proc. Roy. Soc. **A296**, 476 (1967).

[7] A. Kamgar, J. O. Henningsen, and J. F. Koch, Phys. Rev. B **6**, 342 (1972).

[8] H. D. Drew, Phys. Rev. B **5**, 360 (1972).

[9] É. A. Kaner and N. M. Makarov, Zh. Eksp. Teor. Fiz. **57**, 1435 (1969) [Sov. Phys. JETP **30**, 777 (1970)].

[10] D. E. Zherebchevskiĭ and É. A. Kaner, Zh. Eksp. Teor. Fiz. **63**, 1858 (1972) [Sov. Phys. JETP **36**, 983 (1973)].

[11] L. E. Hartmann and J. M. Luttinger, Phys. Rev. **151**, 430 (1966).

Translated by J. G. Adashko

New approach to the theory of the dielectric constant of a system of interacting electrons

V. D. Gorobchenko

I. V. Kurchatov Institute of Atomic Energy

(Submitted 13 April 1979)
Zh. Eksp. Teor. Fiz. 77, 1197–1206 (September 1979)

An exact formula is obtained for the correction, which depends on the wave vector and on the frequency and must be introduced into the dielectric constant of a homogeneous system of interacting electrons to account for the local field $G(\mathbf{q},\omega)$. The simplest approximation for the exact result for $G(\mathbf{q},\omega)$, which takes into account both two-particle and three-particle exchange-correlation effects, is considered. A table is presented of the numerical values of the approximate correction for the local field in the static limit $\omega=0$.

PACS numbers: 05.30.Fk

1. INTRODUCTION

A homogeneous system of N interacting electrons that move in a volume Ω against the background of a uniformly distributed neutralizing postive charge was considered in physics more than 40 years ago[1] as the simplest model of the metallic state of matter. Corresponding to such a state is a Hamiltonian

$$H=\sum_j\frac{\mathbf{p}_j^2}{2m}+\frac{1}{2}\sum_{\mathbf{q}}v(\mathbf{q})\sum_{j\neq j'}\exp[i\mathbf{q}(\mathbf{r}_j-\mathbf{r}_{j'})], \tag{1}$$

where $\mathbf{p}_j$ and $\mathbf{r}_j$ are respectively the momentum operator and the coordinate of the j-th electron, and

$$v(\mathbf{q})=\begin{cases}4\pi e^2/q^2\Omega, & q\neq0,\\ 0, & q=0\end{cases}$$

is the Fourier component of the electron-electron interaction, determined with account taken of the fact that the system as a whole is electrically neutral. Despite the considerable progress reached in the qualitive understanding of the general properties that such a system should possess at various densities N/Ω, no unambiguous answers have been obtained so far to many important questions concerning the details of its behavior precisely in the range of densities typical of conduction electrons in real metals (see, e.g., the review[2]). The key to the answers to most of the unanswered questions might be a reliable practical formula for the dielectric constant $\varepsilon(\mathbf{q}, \omega)$, which depends on the wave vector and on the frequency and charterizes the linear response of the system to an external perturbation in the form

$$V_{ext}(t)=\sum_{q}\int\frac{d\omega}{2\pi}V_{ext}(\mathbf{q},\omega)\sum_{j}\exp(i\mathbf{q}\mathbf{r}_j)\exp(-i(\omega+i\delta)t). \tag{2}$$

It is known that to solve this fundamental physical problem use was made of a great variety of theoretical methods, the usual starting point of the calculations being the exact formula for the dielectric function

$$\varepsilon^{-1}(\mathbf{q},\omega)=1-\frac{i}{\hbar}v(\mathbf{q})\int_0^\infty dt\,e^{i(\omega+i\delta)t}\langle[n(\mathbf{q},t),n^+(\mathbf{q},0)]\rangle, \tag{3}$$

where

$$n(\mathbf{q})=\sum_j\exp(-i\mathbf{q}\mathbf{r}_j)$$

is the Fourier component of the electron-number density operator, and the quantity $\langle[n(\mathbf{q},t),n^+(\mathbf{q},0)]\rangle$ is the statistical mean value of the commutator of the operators $n(\mathbf{q})$ and $n^+(\mathbf{q})$ in the Heisenberg representation. Equation (3) can be easily obtained in first-order perturbation theory and essentially is a formal expression of $\varepsilon(\mathbf{q}, \omega)$ in terms of the exact eigenfunctions and eigenvalues of the multielectron Hamiltonian (1). The latter do not lend themselves to direct calculation at typical metallic densities, when the contribution from the potential energy of the electron interaction in the Hamiltonian (1) turns out to be comparable with the contribution from their kinetic energy. Consequently the approach based on Eq. (3) frequently does not make it possible to estimate the accuracy of the approximations that must be inevitably introduced into the theory at some intermediate stage of the calculation of $\varepsilon(\mathbf{q}, \omega)$.

In present paper is proposed a better method of calculating the dielectric function; it yields for $\varepsilon(\mathbf{q}, \omega)$ an exact formula that does not contain explicitly the eigenvalues of the Hamiltonian (1) and connects $\varepsilon(\mathbf{q}, \omega)$ directly with the mean values of the products of the electron creation and annihilation operators, in the form $\langle c^+c^+c^+ccc\rangle$, taken at one and the same instant of time. These mean values can be approximately estimated by expressing them in terms of the occupation numbers of the single-electron states, as a result of which we obtain for $\varepsilon(\mathbf{q}, \omega)$ a formula that is perfectly suitable for practical calculation. There is also a realistic possibility of systematically improving the indicated simplest approximation for $\varepsilon(\mathbf{q}, \omega)$.

2. EQUATION FOR PERTURBED SINGLE-PARTICLE STATES

We denote by $|\alpha\rangle$ and E_α the eigenfunction and the corresponding eigenvalues of the energy of the Hamiltonian (1). In the general case the eigenfunction of a system of interacting fermions can be formally expressed as a linear superposition of an infinite number of Slater determinants constructed on some orthonormal basis of single-particle states $\psi^{(0)}_{\mathbf{k}\sigma}(\mathbf{r}, \zeta)$. Here ζ is the spin coordinate of the electron, and $\mathbf{k}$ and σ are respectively the orbital and spin quantum numbers.

In the presence of an external perturbation the system of interacting electrons is described by wave functions $\Psi(t)$ determined by the Schrödinger equation

$$i\hbar\frac{\partial\Psi(t)}{\partial t}=[H+V_{ext}(t)]\Psi(t). \tag{4}$$

The external perturbation (2) is adiabatically turned on with a time constant $\delta\to+0$, therefore the solutions of Eq. (4) at $t\to-\infty$ should go over into the stationary states $|\alpha\rangle\exp(-iE_\alpha t/\hbar)$ of the Hamiltonian H. This makes it possible to classify the wave functions $\Psi(t)$ with the aid of the index α.

We seek solutions of (4) in the form

$$\Psi_\alpha(t)=|\alpha(t)\rangle\exp(-iE_\alpha t/\hbar), \tag{5}$$

where the wave function $|\alpha(t)\rangle$ is obtained from the exact eigenstate $|\alpha\rangle$ of the Hamiltonian H by replacing the corresponding basis $\psi^{(0)}_{\mathbf{k}\sigma}(\mathbf{x})$ by some new orthornormal basis $\psi_{\mathbf{k}\sigma}(\mathbf{x}, t)$ of single-particle states (here $\mathbf{x}\equiv\mathbf{r},\zeta$). In other words, assuming that the wave functions $|\alpha(t)\rangle$ and $|\alpha\rangle$ have the same set of occupation numbers of the single-electron states, but are constructed with the aid of different bases. At $t=-\infty$ we should obviously, have $\psi_{\mathbf{k}\sigma}(\mathbf{x},-\infty)=\psi^{(0)}_{\mathbf{k}\sigma}(\mathbf{x})$. This requirement ensures satisfaction of the initial condition $|\alpha(-\infty)\rangle=|\alpha\rangle$.

The problem now consists of finding the equation that must be rigorously satisfied by the perturbed single-particle states $\psi_{\mathbf{k}\sigma}(\mathbf{x}, t)$. To this end we write down the multielectron wave function $\Psi_\alpha(t)$ in the form $\Psi_\alpha(\mathbf{x}, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_N, t)$, multiply the Schrödinger equation from the left by $\Psi^*_\alpha(t)$, and then integrate with respect to the coordinates $\mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_N$ and sum over the spin variables. We write down this operation arbitrarily in the form

$$\left\langle\Psi_\alpha(t)\left|i\hbar\frac{\partial}{\partial t}\right|\Psi_\alpha(t)\right\rangle_{\mathbf{x}}=\langle\alpha(t)|H+V_{ext}(t)|\alpha(t)\rangle_{\mathbf{x}}, \tag{6}$$

which constitutes implicitly the sought equation for $\psi_{\mathbf{k}\sigma}(\mathbf{x}, t)$.

We now consider the left- and right-hand sides of (6) separately. Changing over to the second-quantization operation, we obtain for the left-hand side

$$\begin{aligned}\left\langle \Psi_\alpha(t)\left| i\hbar\frac{\partial}{\partial t}\right| \Psi_\alpha(t)\right\rangle_{\mathbf{x}} &= \frac{E_\alpha}{N}\sum_{\mathbf{k}\mathbf{p}\sigma}\psi_{\mathbf{p}\sigma}^*(\mathbf{x},t)\psi_{\mathbf{k}\sigma}(\mathbf{x},t)\langle\alpha(t)|c_{\mathbf{p}\sigma}^+c_{\mathbf{k}\sigma}|\alpha(t)\rangle\\ &+\frac{i\hbar}{N}\sum_{\mathbf{k}\mathbf{p}\sigma}\psi_{\mathbf{p}\sigma}^*(\mathbf{x},t)\frac{\partial\psi_{\mathbf{k}\sigma}(\mathbf{x},t)}{\partial t}\langle\alpha(t)|c_{\mathbf{p}\sigma}^+c_{\mathbf{k}\sigma}|\alpha(t)\rangle\\ &+\frac{i\hbar}{N}\sum_{\{\mathbf{k}\mathbf{p}\sigma\}}\psi_{\mathbf{p}_1\sigma_1}^*(\mathbf{x},t)\psi_{\mathbf{k}_1\sigma_1}(\mathbf{x},t)\left\langle\psi_{\mathbf{p}_2\sigma_2}\left|\frac{\partial\psi_{\mathbf{k}_2\sigma_2}}{\partial t}\right.\right\rangle\\ &\times\langle\alpha(t)|c_{\mathbf{p}_1\sigma_1}^+c_{\mathbf{p}_2\sigma_2}^+c_{\mathbf{k}_2\sigma_2}c_{\mathbf{k}_1\sigma_1}|\alpha(t)\rangle.\end{aligned} \qquad (7)$$

The first term stems here from the differentiation of the exponential factor in (5) with respect to time, while the two remaining ones are due to direct differentiation of the wave function $|\alpha(t)\rangle$. We note that by virtue of the definitions of the states $|\alpha(t)\rangle$ and $|\alpha\rangle$ we can not distinguish between them when we calculate in (7) the matrix elements of the products of the electron creation and annihilation operators $c_{\mathbf{p}\sigma}^+$ and $c_{\mathbf{k}\sigma}$. Thus, for example,

$$\langle\alpha(t)|c_{\mathbf{p}\sigma}^+c_{\mathbf{k}\sigma}|\alpha(t)\rangle=\langle\alpha|c_{\mathbf{p}\sigma}^+c_{\mathbf{k}\sigma}|\alpha\rangle=n_{\mathbf{k}\sigma}^{(\alpha)}\,\delta_{\mathbf{p},\mathbf{k}},$$

where $n_{\mathbf{k}\sigma}^{(\alpha)}$ are the exact occupation numbers of the single-electron states in the eigenstate $|\alpha\rangle$ of the system of interacting electrons.

As to the right-hand side of (6), it contains in essence the complete Hamiltonian of the system, averaged over the exact perturbed wave function under the additional condition that at the instant of time t there is present in the system and electron with spatial and spin coordinated $\mathbf{x}=\mathbf{r},\xi$. In this averaging it is convenient to break up the Hamiltonian into a sum of the following contributions:

$$\begin{aligned}H+V_{ext}(t)&=\frac{\mathbf{p}^2}{2m}+\sum_{j=2}^{N}\frac{\mathbf{p}_j^2}{2m}+\sum_{\mathbf{q}}v(\mathbf{q})e^{i\mathbf{q}\mathbf{r}}\sum_{j=2}^{N}\exp(-i\mathbf{q}\mathbf{r}_j)\\ &+\frac{1}{2}\sum_{\mathbf{q}}v(\mathbf{q})\sum_{\substack{j\neq j'\\(j,j'=2,\ldots,N)}}\exp[i\mathbf{q}(\mathbf{r}_j-\mathbf{r}_{j'})]\\ &+\sum_{\mathbf{q}}\int\frac{d\omega}{2\pi}V_{ext}(\mathbf{q},\omega)\exp[-i(\omega+i\delta)t]\left[\exp(i\mathbf{q}\mathbf{r})+\sum_{j=2}^{N}\exp(i\mathbf{q}\mathbf{r}_j)\right].\end{aligned} \qquad (8)$$

As a result, Eq. (6) takes the following explicit form

$$\begin{aligned}&E_\alpha\sum_{\mathbf{k}\sigma}n_{\mathbf{k}\sigma}^{(\alpha)}|\psi_{\mathbf{k}\sigma}(\mathbf{x},t)|^2+i\hbar\sum_{\mathbf{k}\sigma}n_{\mathbf{k}\sigma}^{(\alpha)}\psi_{\mathbf{k}\sigma}^*(\mathbf{x},t)\frac{\partial\psi_{\mathbf{k}\sigma}(\mathbf{x},t)}{\partial t}\\ &+i\hbar\sum_{\{\mathbf{k}\mathbf{p}\sigma\}}\psi_{\mathbf{p}_1\sigma_1}^*(\mathbf{x},t)\psi_{\mathbf{k}_1\sigma_1}(\mathbf{x},t)\left\langle\psi_{\mathbf{p}_2\sigma_2}\left|\frac{\partial\psi_{\mathbf{k}_2\sigma_2}}{\partial t}\right.\right\rangle\\ &\times\langle\alpha|c_{\mathbf{p}_1\sigma_1}^+c_{\mathbf{p}_2\sigma_2}^+c_{\mathbf{k}_2\sigma_2}c_{\mathbf{k}_1\sigma_1}|\alpha\rangle=\sum_{\mathbf{k}\sigma}n_{\mathbf{k}\sigma}^{(\alpha)}\psi_{\mathbf{k}\sigma}^*(\mathbf{x},t)\frac{\mathbf{p}^2}{2m}\psi_{\mathbf{k}\sigma}(\mathbf{x},t)\\ &+\sum_{\{\mathbf{k}\mathbf{p}\sigma\}}\psi_{\mathbf{p}_1\sigma_1}^*(\mathbf{x},t)\psi_{\mathbf{k}_1\sigma_1}(\mathbf{x},t)\left\langle\psi_{\mathbf{p}_2\sigma_2}\left|\frac{\mathbf{p}^2}{2m}\right|\psi_{\mathbf{k}_2\sigma_2}\right\rangle\langle\alpha|c_{\mathbf{p}_1\sigma_1}^+c_{\mathbf{p}_2\sigma_2}^+c_{\mathbf{k}_2\sigma_2}c_{\mathbf{k}_1\sigma_1}|\alpha\rangle\\ &+\sum_{\{\mathbf{k}\mathbf{p}\mathbf{q}\sigma\}}v(\mathbf{q})e^{i\mathbf{q}\mathbf{r}}\psi_{\mathbf{p}_1\sigma_1}^*(\mathbf{x},t)\psi_{\mathbf{k}_1\sigma_1}(\mathbf{x},t)\langle\psi_{\mathbf{p}_2\sigma_2}|e^{-i\mathbf{q}\mathbf{r}}|\psi_{\mathbf{k}_2\sigma_2}\rangle\\ &\times\langle\alpha|c_{\mathbf{p}_1\sigma_1}^+c_{\mathbf{p}_2\sigma_2}^+c_{\mathbf{k}_2\sigma_2}c_{\mathbf{k}_1\sigma_1}|\alpha\rangle+\frac{1}{2}\sum_{\{\mathbf{k}\mathbf{p}\mathbf{q}\sigma\}}v(\mathbf{q})\psi_{\mathbf{p}_1\sigma_1}^*(\mathbf{x},t)\psi_{\mathbf{k}_1\sigma_1}(\mathbf{x},t)\\ &\times\langle\psi_{\mathbf{p}_2\sigma_2}|e^{i\mathbf{q}\mathbf{r}}|\psi_{\mathbf{k}_2\sigma_2}\rangle\langle\psi_{\mathbf{p}_3\sigma_3}|e^{-i\mathbf{q}\mathbf{r}}|\psi_{\mathbf{k}_3\sigma_3}\rangle\langle\alpha|c_{\mathbf{p}_1\sigma_1}^+c_{\mathbf{p}_2\sigma_2}^+c_{\mathbf{p}_3\sigma_3}^+c_{\mathbf{k}_3\sigma_3}c_{\mathbf{k}_2\sigma_2}c_{\mathbf{k}_1\sigma_1}|\alpha\rangle\\ &+\sum_{\mathbf{q}}\int\frac{d\omega}{2\pi}V_{ext}(\mathbf{q},\omega)e^{-i(\omega+i\delta)t}\left[e^{i\mathbf{q}\mathbf{r}}\sum_{\mathbf{k}\sigma}n_{\mathbf{k}\sigma}^{(\alpha)}|\psi_{\mathbf{k}\sigma}(\mathbf{x},t)|^2\right.\\ &\left.+\sum_{\{\mathbf{k}\mathbf{p}\sigma\}}\psi_{\mathbf{p}_1\sigma_1}^*(\mathbf{x},t)\psi_{\mathbf{k}_1\sigma_1}(\mathbf{x},t)\langle\psi_{\mathbf{p}_2\sigma_2}|e^{i\mathbf{q}\mathbf{r}}|\psi_{\mathbf{k}_2\sigma_2}\rangle\langle\alpha|c_{\mathbf{p}_1\sigma_1}^+c_{\mathbf{p}_2\sigma_2}^+c_{\mathbf{k}_2\sigma_2}c_{\mathbf{k}_1\sigma_1}|\alpha\rangle\right].\end{aligned} \qquad (9)$$

The terms in the right-hand side of (9) are the result of successive averaging of each of the separated contributions in the Hamiltonian (8).

We are interested in the linear response of the system to an external perturbation, so that it suffices to obtain solutions of the integro-differential equation (9) accurate to terms of first order in V_{ext}. Since this equation is cumbersome, the task seems at first glance very complicated, but it will be shown in the next section that the problem has a very simple solution.

3. EXACT FORMULA FOR THE DIELECTRIC-FUNCTION CORRECTION FOR THE LOCAL FIELD

Since the total Hamiltonian does not depend on the spins of the individual particles, it is natural to choose the sought single-electron states in the form of products of orbital and spin wave functions

$$\psi_{\mathbf{k}\sigma}(\mathbf{x},t)=\psi_{\mathbf{k}}(\mathbf{r},t)\chi_\sigma(\xi).$$

The presence of the spin functions $\chi_\sigma(\xi)$ as factors has no effect whatever on the values of the single-particle matrix elements in Eq. (9), so that we shall take the wave functions $\psi_{\mathbf{k}\sigma}(\mathbf{x},t)$ in this equation to mean simply their orbital parts $\psi_{\mathbf{k}}(\mathbf{r},t)$. As to the unperturbed single-electron states $\psi_{\mathbf{k}}^{(0)}(\mathbf{r})$, we identify them for simplicity with ordinary plane waves:

$$\psi_{\mathbf{k}}^{(0)}(\mathbf{r})=e^{i\mathbf{k}\mathbf{r}}/\sqrt{\Omega}.$$

We seek the solutions of (9) in the form

$$\psi_{\mathbf{k}}(\mathbf{r},t)=\psi_{\mathbf{k}}^{(0)}(\mathbf{r})\left[1+\sum_{\mathbf{q}}\int\frac{d\omega}{2\pi}\frac{V_{eff}(\mathbf{q},\omega)e^{i\mathbf{q}\mathbf{r}}e^{-i(\omega+i\delta)t}}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta}\right]. \qquad (10)$$

Here $\eta_{\mathbf{k}}=\hbar^2\mathbf{k}^2/2m$, and $V_{eff}(\mathbf{q},\omega)$ is the Fourier component of the effective interaction of the electron with the external charge. This component is to be determined, and is of the same order of smallness as $V_{ext}(\mathbf{q},\omega)$ and, just as the latter, it possesses the property $V^*(\mathbf{q},\omega)=V(-\mathbf{q},-\omega)$.

Substituting (10) in (9) we arrive after fundamentally straightforward but technically quite cumbersome algebraic transformation at the following equation for

$$\begin{aligned}S_\alpha(\mathbf{q})V_{eff}(\mathbf{q},\omega)&=S_\alpha(\mathbf{q})[V_{ext}(\mathbf{q},\omega)+v(\mathbf{q})\chi_0^{(\alpha)}(\mathbf{q},\omega)V_{eff}(\mathbf{q},\omega)]\\ &+\frac{1}{N}V_{eff}(\mathbf{q},\omega)\left[\sum_{\mathbf{k}\sigma}\sum_{\mathbf{p}\neq\mathbf{q}}v(\mathbf{p})\left(\frac{1}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta}\right.\right.\\ &\left.-\frac{1}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}-\mathbf{p}}+\eta_{\mathbf{k}-\mathbf{p}}+i\delta}\right)\langle\alpha|c_{\mathbf{k}+\mathbf{q}-\mathbf{p}\sigma}^+\hat{n}(\mathbf{q})\hat{n}(-\mathbf{p})c_{\mathbf{k}\sigma}|\alpha\rangle\\ &\left.+v(\mathbf{q})\sum_{\mathbf{k}\sigma}\left(\frac{1}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta}-\frac{1}{\hbar\omega-\eta_{\mathbf{k}}+\eta_{\mathbf{k}-\mathbf{q}}+i\delta}\right)\langle\alpha|c_{\mathbf{k}\sigma}^+\hat{\Delta}(\mathbf{q})c_{\mathbf{k}\sigma}|\alpha\rangle\right].\end{aligned} \qquad (11)$$

Here $S_\alpha(\mathbf{q})$ is the static structure factor of the system in the state $|\alpha\rangle$:

$$S_\alpha(\mathbf{q})=1+\frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'}\langle\alpha|c_{\mathbf{k}-\mathbf{q}\sigma}^+c_{\mathbf{k}'+\mathbf{q}\sigma'}^+c_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}|\alpha\rangle; \qquad (12)$$

by $\chi_0^{(\alpha)}(\mathbf{q},\omega)$ we denote the function

$$\chi_0^{(\alpha)}(\mathbf{q},\omega)=2\sum_{\mathbf{k}}\frac{n_{\mathbf{k}}^{(\alpha)}-n_{\mathbf{k}+\mathbf{q}}^{(\alpha)}}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta}, \qquad (13)$$

which goes over into the known Lindhard function[4] if the exact occupation numbers $n_{\mathbf{k}}$ are replaced by the usual Fermi steps $f_{\mathbf{k}}$; next

$$\hat{n}(\mathbf{q})=\sum_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}{}^{+}c_{\mathbf{k}+\mathbf{q}\sigma} \tag{14}$$

is the operator of the Fourier components of the electron-number density in the unperturbed system, finally, $\hat{\Delta}(\mathbf{q})$ is an operator in the form

$$\hat{\Delta}(\mathbf{q})=\sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'}[\overset{+}{c}_{\mathbf{k}+\mathbf{q}\sigma}\overset{+}{c}_{\mathbf{k}'-\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}-\langle\alpha|\overset{+}{c}_{\mathbf{k}+\mathbf{q}\sigma}\overset{+}{c}_{\mathbf{k}'-\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}|\alpha\rangle].$$

We note that Eq. (11) does not contain the eigenvalue E_α; the corresponding term are strictly cancelled out in the course of the transformation from (9) to (11). We shall henceforth take $|\alpha\rangle$ to mean the ground state of the system of interacting electrons and will not write out the index α explicitly.

Solving Eq. (11) for $V_{eff}(\mathbf{q},\omega)$, we get

$$V_{eff}(\mathbf{q},\omega)=V_{ext}(\mathbf{q},\omega)/\tilde{\varepsilon}(\mathbf{q},\omega), \tag{15}$$

where the effective dielectric constant $\tilde{\varepsilon}(\mathbf{q},\omega)$ is defined by

$$\tilde{\varepsilon}(\mathbf{q},\omega)=1-v(\mathbf{q})[1-G(\mathbf{q},\omega)]\chi_0(\mathbf{q},\omega). \tag{16}$$

Here $G(\mathbf{q},\omega)$ is the so called correction for the local field and is given by the following exact formula:

$$\begin{aligned}S(\mathbf{q})v(\mathbf{q})G(\mathbf{q},\omega)\chi_0(\mathbf{q},\omega)&=\frac{1}{N}\sum_{\mathbf{k}\sigma}\sum_{\mathbf{p}\neq\mathbf{q}}v(\mathbf{p})\left(\frac{1}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}-\mathbf{p}}+\eta_{\mathbf{k}-\mathbf{p}}+i\delta}\right.\\&\left.-\frac{1}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta}\right)\langle\overset{+}{c}_{\mathbf{k}+\mathbf{q}-\mathbf{p}\sigma}\hat{n}(\mathbf{q})\hat{n}(-\mathbf{p})c_{\mathbf{k}\sigma}\rangle\\&+\frac{v(\mathbf{q})}{N}\sum_{\mathbf{k}\sigma}\left(\frac{1}{\hbar\omega-\eta_{\mathbf{k}}+\eta_{\mathbf{k}-\mathbf{q}}+i\delta}\right.\\&\left.-\frac{1}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta}\right)\langle c_{\mathbf{k}\sigma}{}^{+}\hat{\Delta}(\mathbf{q})c_{\mathbf{k}\sigma}\rangle.\end{aligned} \tag{17}$$

The angle brackets in this expression mean averaging over the ground state of the system of interacting electrons. We note that in accordance with our result (17), the correction for the local field is inversely proportional to the static structure factor—a circumstance not discerned in other known theories of the dielectric constant.

Using the explicit form (10) of the single-particle states and taking (15) into account, we obtain the Fourier component of the averaged induced density.

$$n_{ind}(\mathbf{q},\omega)=\chi_0(\mathbf{q},\omega)V_{ext}(\mathbf{q},\omega)/\tilde{\varepsilon}(\mathbf{q},\omega). \tag{18}$$

In turn, the longitudinal dielectric function $\varepsilon(\mathbf{q},\omega)$ of the system is connected with $\eta_{ind}(\mathbf{q},\omega)$ by the relation

$$\varepsilon^{-1}(\mathbf{q},\omega)=[V_{ext}(\mathbf{q},\omega)+v(\mathbf{q})n_{ind}(\mathbf{q},\omega)]/V_{ext}(\mathbf{q},\omega).$$

When account is taken of (15), (16), and (18), this relation leads to an equation for $\varepsilon(\mathbf{q},\omega)$ in the usual form:

$$\varepsilon(\mathbf{q},\omega)=1-\frac{v(\mathbf{q})\chi_0(\mathbf{q},\omega)}{1+v(\mathbf{q})G(\mathbf{q},\omega)\chi_0(\mathbf{q},\omega)}. \tag{19}$$

As seen from (17), to calculate the corrections for the local field it is necessary to known, besides the function $\chi_0(\mathbf{q},\omega)$ also the static structure factor $S(\mathbf{q})$, whose behavior at all values of q has not yet been reliably established so far. This, however, is no fundamental obstacle, since $S(\mathbf{q})$ is connected with the dielector constant by the relation

$$S(\mathbf{q})=-\frac{\hbar q^2}{\pi m\omega_p{}^2}\int_0^{\infty} d\omega\,\mathrm{Im}\,\varepsilon^{-1}(\mathbf{q},\omega), \tag{20}$$

where $\omega_p=(4\pi Ne^2/m\Omega)^{1/2}$ is the plasma frequency.

Formulas (17), (19), and (20) make it possible to carry out a self-consistent calculation of both the correction for the local field and of the static structure factor.

4. SIMPLEST APPROXIMATION FOR THE FUNCTION $G(\mathbf{q},\omega)$

To gain an idea about the character of the correction for the local field (17), we estimate all the quantities that enter in this formula in the very simplest approximation, namely, as if we were dealing with a system of non-interacting electrons. In this approximation we take the function $\chi_0(\mathbf{q},\omega)$ to mean the usual Lindhard function, while for the static structure factor $S(\mathbf{q})$ we assume its Hartree-Fock value

$$S_0(\mathbf{q})=1-\frac{2}{N}\sum_{\mathbf{k}}f_{\mathbf{k}}f_{\mathbf{k}+\mathbf{q}}=\begin{cases}\dfrac{3q}{4k_F}\left(1-\dfrac{q^2}{12k_F{}^2}\right), & q\leqslant 2k_F\\ 1, & q\geqslant 2k_F\end{cases} \tag{21}$$

where k_F is the Fermi wave number for a system of non-interacting electrons of the same density. As a result we obtain for the correction for the local field

$$\begin{aligned}G(\mathbf{q},\omega)&=\frac{2q^2}{S_0(\mathbf{q})\chi_0(\mathbf{q},\omega)N}\sum_{\mathbf{k}\mathbf{p}}\frac{1}{p^2(\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta)}\\&\times[f_{\mathbf{k}}f_{\mathbf{k}+\mathbf{p}+\mathbf{q}}-f_{\mathbf{k}+\mathbf{p}}f_{\mathbf{k}+\mathbf{q}}+f_{\mathbf{k}}f_{\mathbf{k}+\mathbf{q}}(f_{\mathbf{k}+\mathbf{p}}-f_{\mathbf{k}+\mathbf{p}+\mathbf{q}})-f_{\mathbf{k}+\mathbf{p}}f_{\mathbf{k}+\mathbf{p}+\mathbf{q}}(f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}})].\end{aligned} \tag{22}$$

It is easy to establish the limit to which the correction (22) for the local field tends as $q\to\infty$. To this end it is convenient to break up $G(\mathbf{q},\omega)$ into a sum of two contributions

$$G(\mathbf{q},\omega)=G^{(1)}(\mathbf{q},\omega)+G^{(2)}(\mathbf{q},\omega).$$

The first of these contributions corresponds to those terms of (22) which contain products of only two Fermi distribution functions, and this contribution can be represented in the form

$$\begin{aligned}G^{(1)}(\mathbf{q},\omega)&=\frac{2q^2}{S_0(\mathbf{q})\chi_0(\mathbf{q},\omega)N}\sum_{\mathbf{k}\mathbf{p}}\frac{f_{\mathbf{k}}f_{\mathbf{p}}}{|\mathbf{k}+\mathbf{p}+\mathbf{q}|^2}\\&\times\left(\frac{1}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta}-\frac{1}{\hbar\omega-\eta_{\mathbf{k}}+\eta_{\mathbf{k}+\mathbf{q}}+i\delta}\right).\end{aligned} \tag{23}$$

The remaining terms of (22) make up the contribution $G^{(2)}(\mathbf{q},\omega)$, which is somewhat more complicated in structure:

$$\begin{aligned}G^{(2)}(\mathbf{q},\omega)&=\frac{2q^2}{S_0(\mathbf{q})\chi_0(\mathbf{q},\omega)N}\sum_{\mathbf{k}\mathbf{p}}\frac{f_{\mathbf{k}}f_{\mathbf{k}+\mathbf{q}}}{|\mathbf{k}+\mathbf{p}+\mathbf{q}|^2}(f_{\mathbf{p}}-f_{\mathbf{p}+\mathbf{q}})\\&\times\left(\frac{1}{\hbar\omega-\eta_{\mathbf{p}}+\eta_{\mathbf{p}+\mathbf{q}}+i\delta}-\frac{1}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta}\right).\end{aligned} \tag{24}$$

As seen from (24), the function $G^{(2)}(\mathbf{q},\omega)$ vanishes at q $2k_F$ and consequently in this region of wave-number values the correction for the local field is determined completely by Eq. (23). In particular, in the limit of large q we have

$$G(\mathbf{q},\omega)\xrightarrow[q\to\infty]{}\frac{q^2}{\chi_0(\mathbf{q},\omega)}\frac{1}{q^2}\left(\frac{2}{N}\sum_{\mathbf{p}}f_{\mathbf{p}}\right)\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}}{\hbar\omega-\eta_{\mathbf{k}+\mathbf{q}}+\eta_{\mathbf{k}}+i\delta}=\frac{1}{2}.$$

In the important static case $\omega=0$ the expression (22) for the correction for the local field takes the form

TABLE I. Values of the functions $G(q, 0)$ as functions of the ratio q/k_F.

q/k_F	$G(q, 0)$	q/k_F	$G(q, 0)$	q/k_F	$G(q, 0)$
0.10	0.00250	2.01	0.91167	4.50	0.53286
0.20	0.01003	2.02	0.89007	5.00	0.52606
0.30	0.02263	2.03	0.87272	5.50	0.52122
0.40	0.04040	2.04	0.85794	6.00	0.51763
0.50	0.06348	2.05	0.84496	6.50	0.51489
0.60	0.09204	2.06	0.83334	7.00	0.51276
0.70	0.12629	2.10	0.79592	7.50	0.51105
0.80	0.16648	2.15	0.76148	8.00	0.50967
0.90	0.21290	2.20	0.73500	8.50	0.50854
1.00	0.26585	2.25	0.71365	9.00	0.50759
1.10	0.32569	2.30	0.69591	9.50	0.50680
1.20	0.39271	2.40	0.66786	10.00	0.50612
1.30	0.46720	2.50	0.64648	11.00	0.50504
1.40	0.54924	2.60	0.62956	12.00	0.50422
1.50	0.63859	2.70	0.61581	13.00	0.50359
1.60	0.73423	2.80	0.60439	14.00	0.50309
1.70	0.83342	2.90	0.59476	15.00	0.50269
1.80	0.92939	3.00	0.58654	16.00	0.50236
1.85	0.97116	3.10	0.57943	17.00	0.50209
1.90	1.00258	3.20	0.57324	18.00	0.50186
1.93	1.01220	3.30	0.56779	19.00	0.50167
1.94	1.01292	3.40	0.56298	20.00	0.50151
1.95	1.01194	3.50	0.55869	21.00	0.05137
1.96	1.00884	3.60	0.55485	22.0	0.50124
1.97	1.00293	3.70	0.55140	23.00	0.50114
1.98	0.99318	3.80	0.54828	30.00	0.50067
1.99	0.97732	3.90	0.54545	50.00	0.50024
2.00	0.94593	4.00	0.54287	100.00	0.50006

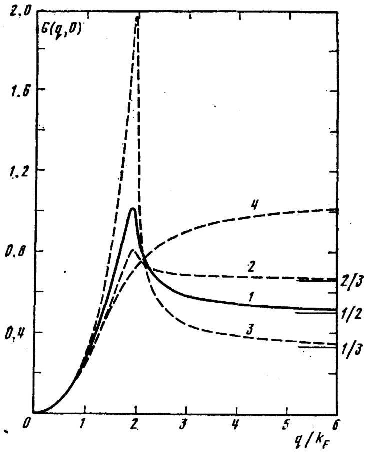

FIG. 1. Behavior of the static correction (25) for the local field as a function of the wave number (curve 1). The dashed curves show the analogous functions obtained by Toigo and Woodruff,[5] (curve 2), Tripathy and Mandal,[6] (curve 3), and of Vashishta and Singwi[7] (curve 4, case $r=4$).

$$G(\mathbf{q},0)=\frac{4q^2}{S_0(\mathbf{q})\chi_0(\mathbf{q})N}\times\sum_{\mathbf{kp}}\frac{f_{\mathbf{k}}f_{\mathbf{p}}(1-f_{\mathbf{k+q}}-f_{\mathbf{p+q}})}{|\mathbf{k}+\mathbf{p}+\mathbf{q}|^2(\eta_{\mathbf{k}}-\eta_{\mathbf{k+q}})}\to\begin{cases}(q/2k_F)^2, & q\to0,\\ {}^1/_2+{}^3/_5(k_F/q)^2, & q\to\infty.\end{cases}\qquad(25)$$

The sextuple integral over momentum space in (25) is analytically converted into a double integral, the calculation of which calls already for the use of numerical methods. A plot of the function $G(\mathbf{q}, 0)$ is shown in the figure, which shows also for comparison the corresponding results obtained in Refs. 5–7. We note that in the long-wave $q\to0$ the function (25) behaves in exactly the same manner as the correction for the local field in the known self-consistent Hartree-Fock approximation for the dielectric constant.[8] The limit $\frac{1}{2}$ to which the function (25) tends asymptotically at large q is typical also of static corrections for the local field, obtained by Hubbard[9] and by Geldard and Vosko,[8] and it is located exactly half-way between the corresponding limits in the theories of Toigo and Woodruff[9] and Tripathy and Mandal.[6] In the wave-number region near $2k_F$ the function (25) has a maximum, whose existence is confirmed also by other dielectric-constant theories that are regarded as the most reliable. We see thus that even the simplest approximation (22) of the exact expression (17) for the function $G(\mathbf{q}, \omega)$ is quite satisfactory in light of the information available at the present time concerning the true behavior of the correction for the local field.

It is known that to calculate the phonon spectra of metals in the adiabatic approximation, in which it is assumed that the conduction electrons align themselves synchronously to each new configuration of the relatively slowly moving ions, calls for knowledge of the static dielectric constant $\varepsilon(\mathbf{q}, 0)$ of the system of interacting electrons, and the results of such calculations are extremely sensitive to the dependence of $G(\mathbf{q}, 0)$ on the wave number.[10] Bearing in mind the possible practical applications of the approximate dielectric function, obtained in the present section, in calculations of similar kind, we have tabulated the numerical values of the correction (25) for the local field.

In conclusion, the author is grateful to N. A. Chernoplekov for constant interest in the work, and V. G. Kon and V. V. Pokrovskiĭ for help with the numerical calculations.

[1] E. P. Wigner, Phys. Rev. **46**, 1002 (1934); Trans. Faraday Soc. **34**, 678 (1938).
[2] C. M. Care and N. H. March, Adv. Phys. **24**, 101 (1975).
[3] D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [Sov. Phys. Usp. **3**, 320 (1960)].
[4] J. Lindhard, K. Dan. Vidensk. Selsk. Mat.-Fus. Medd. **28**, 8 (1954).
[5] F. Toigo and T. O. Woodruff, Phys. Rev. B **2**, 3858 (1970).
[6] D. N. Tripathy and S. S. Mandal, Phys. Rev. B **16**, 231 (1977).
[7] P. Vashishta and K. S. Singwi, Phys. Rev. B **6**, 875 (1972).
[8] D. J. W. Geldart and S. H. Vosko, Can. J. Phys. **44**, 2137 (1966).
[9] J. Hubbard, Proc. R. Soc. London, **A243**, 336 (1957).
[10] E. G. Brovman and Yu. Kagan, Usp. Fiz. Nauk **112**, 369 (1974) [Sov. Phys. Usp. **17**, 125 (1974)].

Translated by J. G. Adashko