yield at the limit of applicability of the linear approximation an additional conductivity $\Delta\sigma = 800\ \Omega^{-1}\,\mathrm{cm}^{-1}$, which amounts to 4% of the conductivity σ_n in the normal state. Using the result of Maki and Takayama,[9] that below H_{c2} the addition to the conductivity differs by a factor $\ln[L/\xi(T)]$, we obtain at $1-h=0.04$ the value $\Delta\sigma = 0.4\sigma_n$, i.e., the fluctuations should cause ρ_f to decrease to $0.7\rho_n$, in agreement with the experimental data.

It is useful to estimate the range of fields below H_{c2} in which fluctuations can occur. It is shown in Ref. 13 that the temperature range of the fluctuation region (the region where the fluctuations are large enough for their interaction to be taken into account) is

$$\frac{\Delta T}{T_c(H)} \approx 7\left(\frac{k_B}{8\pi\xi(0)^3\Delta C}\right)^{2/3}\left(t\frac{dh_{c2}}{dt}\right)^{1/3} h_{c2}^{2/3} \qquad (4)$$

[$h_{c2} = H_{c2}(t)/H_{c2}(0)$ and ΔC is the discontinuity of the heat capacity in the transition]. Substituting the parameters of V_3Ge and using for the estimate the heat-capacity discontinuity of $Ti_{84}Mo_{16}$ (Ref. 14), $\Delta C = 3\ \mathrm{mJ/cm^3\cdot K}$, we obtain $\Delta T/T_c(H) = 5\%$, or in terms of the magnetic field

$$\frac{\Delta H_{c2}}{H_{c2}(T)} = 2\frac{t^2}{h_{c2}}\frac{\Delta T}{T_c(H)} = 10\%, \qquad (a)$$

which is also close to the experimentally observed width of the $\rho_f(h)$ anomaly.

Estimates of the additional conductivity and of the width of the fluctuation region thus allow us to attribute the anomalies of $\rho_f(h)$ as $h \to 1$ to fluctuations.

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Self-consistent account of exchange-correlation effects in an electron gas

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A new approximation is obtained for the local-field correction $G(\mathbf{q},\omega)$ to the permittivity $\varepsilon(\mathbf{q},\omega)$ of a homogeneous interacting electron gas. The starting point is the exact equation derived by one of us [Gorobchenko, Sov. Phys. JETP **50**, 603 (1979)] as well as an estimate of the statistical expectation values of the second-quantization operators, obtained by the technique of the coupled equations of motion for the equal-time Green's functions. The result obtained for $G(\mathbf{q},\omega)$ is compared with other known approximations. The results of calculation of the static correction $G(\mathbf{q},0)$ for the local field and of the static structure factor $S(\mathbf{q})$ are presented.

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1. INTRODUCTION

One of the central problems of the theory of simple metals is allowance for the long-range Coulomb interaction between the conduction electrons. This problem is treated as a rule within the framework of the interacting-electron-gas model against the background of a uniformly distributed positive charge.[1] It is known that practically all the physical characteristics of such a model system are expressed in terms of its permittivity $\varepsilon(\mathbf{q},\omega)$, which is customarily expressed in the form

$$\varepsilon(\mathbf{q},\omega) = 1 + \frac{Q_0(\mathbf{q},\omega)}{1-G(\mathbf{q},\omega)Q_0(\mathbf{q},\omega)}, \qquad (1)$$

where $Q_0(\mathbf{q},\omega) = -v(\mathbf{q})\chi_0(\mathbf{q},\omega)$, $v(\mathbf{q}) = 4\pi e^2/q^2\Omega$ is the Fourier component of the Coulomb potential,

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$$\chi_0(q,\omega)=\sum_{k\sigma}\frac{n_{k\sigma}-n_{k+q\sigma}}{\hbar\omega-\varepsilon_{k+q}+\varepsilon_k+i\delta}, \tag{2}$$

and $G(q,\omega)$ is the so-called correction for the local field. In Eq. (2), $\varepsilon_k=\hbar^2k^2/2m$, $n_{k\sigma}=\langle c_{k\sigma}^+c_{k\sigma}\rangle$ are the mean occupation numbers of the single-electron states, and $c_{k\sigma}^+$ and $c_{k\sigma}$ are the electron creation and annihilation operators.

The main difficulty of the permittivity theory lies in the determination of the local-field correction that takes into account the local distortion of the density induced near the electron on account of exchange and correlation effects. In view of the long-range character of the Coulomb forces, the determination of $G(q,\omega)$ with guaranteed accuracy is an exceedingly complicated problem. And while this problem has been the subject of intensive theoretical research in recent years, it has found no satisfactory solution to this day (see the recent review[2]).

A new approach to the determination of the correction for the local field was developed in Ref. 3, where the following exact formula was obtained for $G(q,\omega)$:

$$-G(q,\omega)Q_0(q,\omega)=P(q,\omega)$$
$$=\frac{1}{NS(q)}\sum_{k\sigma}\frac{\langle\hat n(q)\hat B_{k\sigma}(q)\rangle}{\hbar\omega-\varepsilon_{k+q}+\varepsilon_k+i\delta}+\Delta P(q,\omega). \tag{3}$$

The angle brackets denote here statistical averaging, N is the total number of the electrons, $S(q)$ is the static structure factor, $\hat n(q)$ is the Fourier component of the electron-density operator, and $\hat B_{k\sigma}(q)$ is an operator connected with the commutator $[\hat V,c_{k+q\sigma}^+c_{k\sigma}]$, where $\hat V$ is the operator of the potential energy of the system. Here

$$\hat n(q)=\sum_{k\sigma}c_{k\sigma}^+c_{k+q\sigma}, \tag{4}$$

$$S(q)=\frac{1}{N}\langle\hat n(q)\hat n^+(q)\rangle, \tag{5}$$

$$\hat B_{k\sigma}(q)=\sum_{p\neq q}v(p)[c_{k+q\sigma}n^+(p)c_{k+p\sigma}-c_{k+q-p\sigma}^+\hat n^+(p)c_{k\sigma}]. \tag{6}$$

The quantity $\Delta P(q,\omega)$ is defined in Ref. 3. It is a very small correction, and within the framework of the approximation used in the present paper it can be neglected.

In accordance with (3), the problem reduces to finding for a system of interacting electrons expectation values of the form $\langle c_{k\sigma}^+c_{k\sigma}\rangle$, $\langle\hat n(q)\hat n^+(q)\rangle$, and $\langle\hat n(q)\hat B_{k\sigma}(q)\rangle$. A very simple approximation was used in Ref. 3 for these quantities, whereby they were calculated as in a system of noninteracting electrons of the same density. The calculation has shown that even so crude an approximation leads to a perfectly satisfactory result for the static correction $G(q,0)$, for the local field when compared with other known approximations of this quantity.

The purpose of the present paper is to develop further the method proposed in Ref. 3. In Sec. 2 we estimate average characteristics of the type $\langle\hat n(q)\hat B\rangle$ by the technique of coupled equations of motion of the equal-time Green's functions.[4] These characteristics can be expressed in term of the dielectric constant of the system, and this leads, when account is taken of (1) and (3), to the need for a self-consistent calculation of the functions $G(q,\omega)$ and $\varepsilon(q,\omega)$. A new formula for the correction for the local field is derived in Sec. 3, where a detailed comparison is made also of our approximation with the previously proposed approximations of Toigo and Woodruff,[5] Rajagopal and Jain,[6] and others,[7-9] as well as with the simplest approximation of Ref. 3. This formula, which initially contains a septuple integral, is recast in Sec. 4 in a form suitable for computer calculations. The calculation results are discussed in Sec. 5.

2. CORRELATION FUNCTIONS CONTAINING THE PARTICLE NUMBER DENSITY

We shall show how, knowing the dielectric function of the system, we can estimate statistical mean values of the form $\langle\hat n(q,t)\hat B\rangle$, where $\hat n(q,t)$ is the Fourier component of the particle-number density operator in the Heisenberg representation and $\hat B$ is a certain product of second-quantization operators. We use for this purpose the method of equal-time Green's functions[4] within the framework of which the calculation of correlation functions of the form $\langle\hat A(t)\hat B\rangle$ reduces to calculation of the Fourier transforms, with respect to time, of a retarded and advanced Green function

$$\langle\langle\hat A(t)\,|\,\hat B\rangle\rangle^{(r)}=-i\hbar^{-1}\theta(t)\langle[\hat A(t),\hat B]\rangle e^{-\delta t}, \tag{7a}$$

$$\langle\langle\hat A(t)\,|\,\hat B\rangle\rangle^{(a)}=i\hbar^{-1}\theta(-t)\langle[\hat A(t),\hat B]\rangle e^{\delta t}. \tag{7b}$$

Here $\theta(t)$ is the unit step functions, the square brackets denote a commutator, and the time constant $\delta\to+0$.

Taking into account the definition (4) of the operator $\hat n(q)$, we introduce into consideration, besides the Green's function $\langle\langle\hat n(q,t)\,|\,\hat B\rangle\rangle^{(r)}$ also its partial component $\langle\langle c_{k\sigma}^+(t)c_{k+q\sigma}(t)\,|\,\hat B\rangle\rangle^{(r)}$. The latter satisfies the equation of motion, which takes in the Fourier representation the form

$$(\hbar\omega-\varepsilon_{k+q}+\varepsilon_k+i\delta)\langle\langle c_{k\sigma}^+c_{k+q\sigma}|\hat B\rangle\rangle_\omega^{(r)}=\langle[c_{k\sigma}^+c_{k+q\sigma},\hat B]\rangle$$
$$+\sum_p v(p)\langle\langle c_{k\sigma}^+\hat n(p)c_{k+q-p\sigma}-c_{k+p\sigma}^+\hat n(p)c_{k+q\sigma}|\hat B\rangle\rangle_\omega^{(r)}. \tag{8}$$

The right-hand side of this equation contains a new Green's function of higher rank, stemming from the commutator of the operator $c_{k\sigma}^+c_{k+q\sigma}$ with the potential-energy operator of the system. In first-order approximation this Green's function can be estimated by retaining in the sum over p only the "coherent" contribution with $p=q$, and then carrying out the decoupling by pairing the creation and annihilation operators of electrons having equal momenta. As a result of this simplification, the second term in the right-hand side of (8) is replaced by the expression

$$v(q)(n_{k\sigma}-n_{k+q\sigma})\langle\langle\hat n(q)\,|\,\hat B\rangle\rangle_\omega^{(r)},$$

after which this equation can be easily solved for the Green's function $\langle\langle\hat n(q)\,|\,B\rangle\rangle_\omega^{(r)}$ of interest to us, for which we obtain the following approximate formula:

$$\langle\langle\hat n(q)\,|\,\hat B\rangle\rangle_\omega^{(r)}\cong\frac{1}{\varepsilon_{RPA}(q,\omega)}\sum_{k\sigma}\frac{\langle[c_{k\sigma}^+c_{k+q\sigma},\hat B]\rangle}{\hbar\omega-\varepsilon_{k+q}+\varepsilon_k+i\delta}. \tag{9}$$

Here

$$\varepsilon_{RPA}(q,\omega)=1-v(q)\chi_0(q,\omega) \tag{10}$$

is the permittivity in the random-phase approxima-

tion. We note that the explicit form of the operator $\hat{B}$ is no longer used anywhere after the derivation of (9).

We consider now the particular case when $\hat{B}=\hat{n}^+(\mathbf{q})$. It is known that the quantity

$$\chi(\mathbf{q},\omega)\equiv\langle\langle\hat{n}(\mathbf{q})|\hat{n}^+(\mathbf{q})\rangle\rangle_\omega^{(r)}=-\frac{i}{\hbar}\int_0^\infty dt\, e^{i(\omega+i\delta)t}\langle[\hat{n}(\mathbf{q},t),\hat{n}^+(\mathbf{q})]\rangle \qquad (11)$$

is the linear response of a system of interacting electrons to the introduction of a test charge, and is connected with the permittivity by the relation

$$\varepsilon^{-1}(\mathbf{q},\omega)=1+v(\mathbf{q})\chi(\mathbf{q},\omega). \qquad (12)$$

Recognizing that

$$[c_{\mathbf{k}\sigma}^+c_{\mathbf{k}+\mathbf{q}\sigma},\hat{n}^+(\mathbf{q})]=c_{\mathbf{k}\sigma}^+c_{\mathbf{k}\sigma}-c_{\mathbf{k}+\mathbf{q}\sigma}^+c_{\mathbf{k}+\mathbf{q}\sigma}, \qquad (13)$$

we obtain for $\chi(\mathbf{q},\omega)$ in accord with (9) and (2)

$$\chi(\mathbf{q},\omega)\approx\chi_0(\mathbf{q},\omega)/\varepsilon_{RPA}(\mathbf{q},\omega). \qquad (14)$$

Yet the exact formula for the response function is known to be (see, e.g., Ref. 2)

$$\chi(\mathbf{q},\omega)=\chi_0(\mathbf{q},\omega)/\tilde{\varepsilon}(\mathbf{q},\omega), \qquad (15)$$

where

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

is the so-called effective permittivity, which determines the screened interaction of an electron with an external charge, with account taken of the local distortion of the average induced density. Comparison of (14) and (15) suggests immediately a "prescription" for converting the approximation (9) into a perfectly exact result for the case when $\hat{B}=\hat{n}^+(q)$. It suffices to this end to substitute $\varepsilon_{\mathrm{RPA}}(\mathbf{q},\omega)$ by $\tilde{\varepsilon}(\mathbf{q},\omega)$ in (9).

It is clear from general considerations that the indicated change should improve the approximation (9) also in the case of an arbitrary operator $\hat{B}$, therefore to estimate the correlation function $\langle\hat{n}(\mathbf{q},t)\hat{B}\rangle$ we use just this improved approximation for $\langle\langle\hat{n}(\mathbf{q})|\hat{B}\rangle\rangle_\omega^{(r)}$.

The calculation of a correlation function of the form $\langle\hat{A}(t)\hat{B}\rangle$ reduces in the method of the equal-time Green's functions to evaluation of a Fourier integral:

$$\langle\hat{A}(t)\hat{B}\rangle=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\langle\hat{A}(t)\hat{B}\rangle_\omega=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{1-e^{-\hbar\omega/\tau}}\langle[\hat{A}(t),\hat{B}]\rangle_\omega, \qquad (17)$$

where the known relation

$$\langle\hat{B}\hat{A}(t)\rangle_\omega=e^{-\hbar\omega/\tau}\langle\hat{A}(t)\hat{B}\rangle_\omega.$$

is used in the course of the transformation. Taking into account the definition (7) of the Green's functions, we can also represent (17) in the form

$$\langle\hat{A}(t)\hat{B}\rangle=i\hbar\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{1-e^{-\hbar\omega/\tau}}[\langle\langle\hat{A}|\hat{B}\rangle\rangle_\omega^{(r)}-\langle\langle\hat{A}|\hat{B}\rangle\rangle_\omega^{(a)}]. \qquad (18)$$

In this case the Fourier transform of the advanced Green's function $\langle\langle\hat{A}|\hat{B}\rangle\rangle_\omega^{(a)}$ is obtained from $\langle\langle\hat{A}|\hat{B}\rangle\rangle_\omega^{(r)}$ by reversing the sign of the time constant δ.

In accordance with (18) we arrive at the following estimate for the correlation function of interest to us:

$$\langle\hat{n}(\mathbf{q},t)\hat{B}\rangle=-\frac{\hbar}{\pi}\sum_{\mathbf{k}\sigma}\langle[c_{\mathbf{k}\sigma}^+c_{\mathbf{k}+\mathbf{q}\sigma},\hat{B}]\rangle$$

$$\times\int_{-\infty}^{\infty}\frac{d\omega\, e^{-i\omega t}}{1-e^{-\hbar\omega/\tau}}\mathrm{Im}[\tilde{\varepsilon}(\mathbf{q},\omega)(\hbar\omega-\varepsilon_{\mathbf{k}+\mathbf{q}}+\varepsilon_{\mathbf{k}}+i\delta)]^{-1}. \qquad (19)$$

Setting the time argument t equal to zero, we can use this formula to calculate also ordinary statistical mean values of the form $\langle\hat{n}(\mathbf{q})\hat{B}\rangle$.

In particular, starting from (19), we obtain directly for the static structure factor (5), taking (2) and (12)–(14) into account,

$$S(\mathbf{q})=-\frac{\hbar}{\pi v(\mathbf{q})N}\int_{-\infty}^{\infty}\frac{d\omega}{1-e^{-\hbar\omega/\tau}}\mathrm{Im}\,\varepsilon^{-1}(\mathbf{q},\omega), \qquad (20)$$

which is a well known exact result.[1]

3. ANALYSIS OF EQUATION FOR THE CORRECTION FOR THE LOCAL FIELD

We shall use Eq. (19) to estimate the mean value of the operator $\hat{n}(\mathbf{q})\hat{B}_{\mathbf{k}\sigma}(\mathbf{q})$, which enters in (3) and contains products of six electron creation and annihilation operators. To this end it is necessary to turn to know the mean value of the commutator

$$[c_{\mathbf{k}'\sigma'}^+c_{\mathbf{k}'+\mathbf{q}\sigma'},\hat{B}_{\mathbf{k}\sigma}(\mathbf{q})]. \qquad (21)$$

The latter reduces to a product of only four second-quantization operators, and thus to simpler correlations between the particles. In first-order approximation these correlations can be taken into account within the framework of the ordinary Hartree-Fock decoupling scheme. In this approximation, the mean value of the commutator (21) reduces to

$$\langle[c_{\mathbf{k}'\sigma'}^+c_{\mathbf{k}'+\mathbf{q}\sigma'},\hat{B}_{\mathbf{k}\sigma}(\mathbf{q})]\rangle\approx\delta_{\sigma\sigma'}(n_{\mathbf{k}}-n_{\mathbf{k}+\mathbf{q}})$$

$$\times\Big[v(\mathbf{k}-\mathbf{k}')(n_{\mathbf{k}'}-n_{\mathbf{k}'+\mathbf{q}})-\delta_{\mathbf{k}\mathbf{k}'}\sum_{\mathbf{p}}v(\mathbf{k}-\mathbf{p})(n_{\mathbf{p}}-n_{\mathbf{p}+\mathbf{q}})\Big]. \qquad (22)$$

To permit a real calculation of the correction for the local field, we introduce at this stage the following two simplifications. First, we use for the mean value of the commutator (21) the approximate Hartree-Fock expression (22); second, we neglect both in the expression and in Eq. (2) for the function $\chi_0(\mathbf{q},\omega)$, the difference between the exact occupation numbers $n_{\mathbf{k}}$ of the single-electron states and the corresponding occupation numbers $f_{\mathbf{k}}$ in the free-electron system. By the same token we take $\chi_0(\mathbf{q},\omega)$ to mean the usual Lindhard formula.

When (22) and (19) are taken into account [it is necessary to set $t=0$ in (19) and go to the limit as $T\to 0$] expression (3) for the correction for the local field is transformed into

$$P_{GK}(\mathbf{q},\omega)=\frac{2}{\hbar NS(\mathbf{q})}\sum_{\mathbf{kp}}v(\mathbf{k}-\mathbf{p})\left(\frac{1}{\omega-\Omega_{\mathbf{pq}}+i\delta}-\frac{1}{\omega-\Omega_{\mathbf{kq}}+i\delta}\right)$$

$$\times(f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}})(f_{\mathbf{p}}-f_{\mathbf{p}+\mathbf{q}})F(\mathbf{q},\Omega_{\mathbf{kq}}). \qquad (23)$$

Here $\Omega_{\mathbf{kq}}=(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})/\hbar$, and $F(\mathbf{q},\Omega)$ is defined by the expression

$$F(\mathbf{q},\Omega)=-\frac{1}{\pi}\mathrm{Im}\int_0^\infty\frac{d\omega}{\tilde{\varepsilon}(\mathbf{q},\omega)(\omega-\Omega+i\delta)}, \qquad (24)$$

where $\tilde{\varepsilon}(\mathbf{q},\omega)$ is the effective permittivity, which in accord with (16) is itself dependent on the sought correction for the local field. A self-consistent calculation is needed also for the static structure factor $S(q)$ in (23); this factor, as seen from (20) is given by

$$S(\mathbf{q})=-\frac{\hbar}{\pi v(\mathbf{q})N}\operatorname{Im}\int_0^\infty d\omega\,\varepsilon^{-1}(\mathbf{q},\omega)=-\frac{\hbar}{\pi N}\operatorname{Im}\int_0^\infty d\omega\,\frac{\chi_0(\mathbf{q},\omega)}{\tilde{\varepsilon}(\mathbf{q},\omega)}. \qquad (25)$$

It is of interest to track the connection between Eq. (23) and the simplest approximation for the local field, which follows from the exact formula (3) and is considered in Ref. 5. This approximation is obtained from (23) it we put in (24) and (25) $\tilde{\varepsilon}(\mathbf{q},\omega)=1$ or, equivalently [by virtue of (16)], if we use as the "bare" correction for the local field its Hartree-Fock value $G_{HF}(\mathbf{q},\omega)=1$. Then $S(\mathbf{q})$ becomes the static structure factor $S_0(q)$ of a non-interacting electron gas, and $F(\mathbf{q},\Omega)$ reduces to the unit step function $\theta(\Omega)$. Taking into consideration the obvious relation

$$(f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}})\theta(\Omega_{\mathbf{kq}})=f_{\mathbf{k}}-f_{\mathbf{k}}f_{\mathbf{k}+\mathbf{q}},$$

we obtain

$$P_G(\mathbf{q},\omega)=\frac{2}{\hbar NS_0(\mathbf{q})}\sum_{\mathbf{kp}}v(\mathbf{k}-\mathbf{p})\left(\frac{1}{\omega-\Omega_{\mathbf{pq}}+i\delta}-\frac{1}{\omega-\Omega_{\mathbf{kq}}+i\delta}\right)\times[f_{\mathbf{p}}f_{\mathbf{k}+\mathbf{q}}-(f_{\mathbf{p}}-f_{\mathbf{p}+\mathbf{q}})f_{\mathbf{k}}f_{\mathbf{k}+\mathbf{q}}]. \qquad (26)$$

Expression (26) differs from Eq. (22) of Ref. 3 only in notation.

It is useful to compare Eq. (23) also with other known approximate expressions for the dynamic correction for the local field. In this connection, we call attention first to the definite similarity of the structures of the integrals in (24) and (25) and note that in these integrals the reciprocal effective permittivity $\varepsilon^{-1}(\mathbf{q},\omega)$ serves as a sort of weighting factor for the frequency "averaging" of the functions $(\omega-\Omega_{\mathbf{kq}}+i\delta)^{-1}$ and $\chi_0(\mathbf{q},\omega)$. Without this averaging, Eq. (23) would take the form

$$P_{RJ}(\mathbf{q},\omega)=\frac{2}{\hbar^2\chi_0(\mathbf{q},\omega)}\sum_{\mathbf{kp}}v(\mathbf{k}-\mathbf{p})\left(\frac{1}{\omega-\Omega_{\mathbf{pq}}+i\delta}-\frac{1}{\omega-\Omega_{\mathbf{kq}}+i\delta}\right)\times(f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}})(f_{\mathbf{p}}-f_{\mathbf{p}+\mathbf{q}})\frac{1}{\omega-\Omega_{\mathbf{kq}}+i\delta}, \qquad (27)$$

which coincides exactly with the approximate expression first obtained by Rajagopal and Jain[6] for the correction for the local field, and later by a number of other workers using various methods.[2,7-9]

The numerical calculation, by Brosens *et al.*,[10] of the function $P_{RJ}(\mathbf{q},\omega)$ showed this function to have pathological singularities at the frequencies

$$\omega_s=\frac{\varepsilon_F}{\hbar}\left|\frac{q^2}{k_F^2}\pm\frac{2q}{k_F}\right|. \qquad (28)$$

These singularities were carefully investigated by Holas *et al.*,[8] who were able to prove analytically the existence of logarithmic divergences of $\mathrm{Re}P_{RJ}(\mathbf{q},\omega)$ and of jumplike discontinuities of $\mathrm{Im}P_{RJ}(\mathbf{q},\omega)$ at the characteristic frequencies (28). The character of the divergence of $\mathrm{Re}P_{RJ}(\mathbf{q},\omega)$ as $\omega\to\omega_s$ was established in explicit form in Ref. 11, In the opinion of the authors of Refs. 9 and 11 the nature of the indicated singularities of the correction (27) for the local field is due to the combined effect of the abrupt cutoff of the integration region by Fermi distribution functions and of the presence, in the integrand, of a second-order pole at $\omega=\Omega_{\mathbf{kq}}-i\delta$.

The approximation (23) obtained by us differs from $P_{RJ}(\mathbf{q},\omega)$ in that it contains in place of the complex and frequency-dependent functions $(\omega-\Omega_{\mathbf{kq}}+i\delta)^{-1}$ and $\chi_0(\mathbf{q},\omega)$ the real and frequency-independent quantities $F(\mathbf{q},\Omega_{\mathbf{kq}})$ and $S(\mathbf{q})$, in which the frequency dependence is averaged out with a weighting function $\tilde{\varepsilon}^{-1}(\mathbf{q},\omega)$. This one circumstance alone, which leads to the vanishing of the second-order poles in (23), eliminates completely the unphysical singularities of $P_{RJ}(\mathbf{q},\omega)$ even when distribution functions of the Fermi type are used (see Sec. 5). We note also that the appearance of the static structure factor $S(\mathbf{q})$ in the denominator of the right-hand side of (23) is not connected with any approximation whatever, and is stipulated by the exact formula (3), while the quantity

$$(f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}})(f_{\mathbf{p}}-f_{\mathbf{p}+\mathbf{q}})F(\mathbf{q},\Omega_{\mathbf{kq}})$$

does not depend on the frequency by definition, being an approximate value of the average of frequency-independent operator. Therefore, despite the formal similarity, the results (23) and (27) are qualitatively different.

We compare, finally, Eq. (23) with the expression for the correction obtained for the local field in the approximation of Toigo and Woodruff[5] and which transforms identically into

$$P_{TW}(\mathbf{q},\omega)=\frac{2}{\hbar N}\sum_{\mathbf{kp}}v(\mathbf{k}-\mathbf{p})\left(\frac{1}{\omega-\Omega_{\mathbf{pq}}+i\delta}-\frac{1}{\omega-\Omega_{\mathbf{kq}}+i\delta}\right)\times(f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}})(f_{\mathbf{p}}-f_{\mathbf{p}+\mathbf{q}})F_{TW}(\mathbf{q},\Omega_{\mathbf{kq}}), \qquad (29)$$

where

$$F_{TW}(\mathbf{q},\Omega_{\mathbf{kq}})=\frac{\mathbf{kq}}{q^2}=\frac{1}{2}\left(\frac{\hbar\Omega_{\mathbf{kq}}}{\varepsilon_{\mathbf{q}}}-1\right). \qquad (30)$$

The difference between (29) and (23) reduces to a replacement of the ratio $F(\mathbf{q},\Omega_{\mathbf{kq}})/S(\mathbf{q})$ by the function (30), which is real and does not depend on frequency. In this sense the approximation of Toigo and Woodruff is closer to our result than the approximation of Rajagopal and Jain.

The analysis above shows that Eq. (23) is quite universal and covers practically all those known free-field-correction approximations that do not require introduction of *a priori* assumptions in the theory (as is done, for example by Singwi *et al.*[12,13]). An important feature of the structure of this formula is that is gives a nonzero result for $P(\mathbf{q},\omega)$ only to the extent that $F(\mathbf{q},\Omega_{\mathbf{kq}})$ depends on k. Were there no such dependence, the expression under the summation sign in (23) would reverse sign upon permutation of k and p and the sum would be zero. Therefore the actual form of the dependence of $F(\mathbf{q},\Omega_{\mathbf{kq}})$ on the argument $\Omega_{\mathbf{kq}}$ is of primary importance.

We note that the function $F(\mathbf{q},\Omega)$ defined by (24) has the property

$$F(\mathbf{q},\Omega)+F(\mathbf{q},-\Omega)=1. \qquad (31)$$

Since $\tilde{\varepsilon}^*(\mathbf{q},\omega)=\tilde{\varepsilon}(\mathbf{q},-\omega)$ in a homogeneous electron gas, we can also rewrite (31) in the form

$$-\frac{1}{\pi}\operatorname{Im}\int_{-\infty}^{\infty}\frac{d\omega}{\tilde{\varepsilon}(\mathbf{q},\omega)(\omega-\Omega+i\delta)}=1, \qquad (32a)$$

from which it follows that

$$\mathrm{Re}\,\tilde{\varepsilon}^{-1}(\mathbf{q},\omega)=1-\frac{1}{\pi}\mathscr{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega'-\omega}\mathrm{Im}\,\tilde{\varepsilon}^{-1}(\mathbf{q},\omega'). \qquad (32b)$$

Thus, the property (31) is equivalent to the Kramers-Kronig relation (32b). The validity of the "sum rule" (32a) can be easily verified directly by using the following exact relations:

$$n_{k\sigma}-n_{k+q\sigma}=\langle[c_{k\sigma}^{+}c_{k+q\sigma},\hat{n}^{+}(q)]\rangle=-\frac{h}{\pi}\int_{-\infty}^{\infty}d\omega\,\mathrm{Im}\,\chi_{k\sigma}(q,\omega),$$

where $\chi_{k\sigma}(q,\omega)$ is a partial contribution to the response function (11) and is given by

$$\chi_{k\sigma}(q,\omega)\equiv\langle\langle c_{k\sigma}^{+}c_{k+q\sigma}|\hat{n}^{+}(q)\rangle\rangle_{\omega}^{(r)}=\frac{n_{k\sigma}-n_{k+q\sigma}}{\tilde{\varepsilon}(q,\omega)(\hbar\omega-\varepsilon_{k+q}+\varepsilon_{k}+i\delta)}.$$

The sum rule (31) can be effectively used to calculate the correction for the local field by formula (23). The actual value of the constant in the right-hand side of (31) plays no role whatever, so that this sum rule reflects in practice only the antisymmetry property of the function $f(q,\Omega)$ relative to the reversal of the sign of Ω. In this sense, the same property is possessed also by the function $F_{TW}(q,\Omega)$ [see Eq. (30)]. The function $F(q,\Omega)$ experiences at the point $\Omega=0$ a discontinuity whose size depends on the value of q and on the form of the function $\tilde{\varepsilon}(q,\omega)$. The largest discontinuity takes place at $\tilde{\varepsilon}=1$. In this case $F(q,\Omega)=\theta(\Omega)$. The function $F_{TW}(q,\omega)$ has no discontinuity at $\Omega=0$. As for the function $F(q,\Omega)$, which is obtained by a self-consistent solution of Eq. (23), its discontinuity at $\Omega=0$ is intermediate between these two extremal values.

4. DERIVATION OF THE CALCULATION FORMULAS

We show now how the initial formula (23) for $P(q,\omega)$, which contains a septuple integral, can be recast in a form that lends itself to an effective self-consistent calculation.

We first replace k in the terms containing f_{k+q} by $-k-q$, and replace p in the terms with f_{p+q} by $-p-q$. As a result we get

$$P(q,\omega)=\frac{2}{\hbar NS(q)}\sum_{kp}f_{k}f_{p}\{v(k-p)[\Phi(\Omega_{pq},\Omega_{kq})F(\Omega_{kq})+\Phi(-\Omega_{pq},-\Omega_{kq})F(-\Omega_{kq})]-v(k+p+q)\times[\Phi(-\Omega_{pq},\Omega_{kq})F(\Omega_{kq})+\Phi(\Omega_{pq},-\Omega_{kq})F(-\Omega_{kq})]\},\quad(33)$$

where

$$\Phi(\Omega',\Omega)=\frac{1}{\omega-\Omega'+i\delta}-\frac{1}{\omega-\Omega+i\delta}\quad(34)$$

and we have left out for brevity the argument q on the function $F(q,\Omega)$.

We change next to dimensionless variables, in which the wave vectors k, p, and q are measured in units of k_F and the frequencies ω and Ω in units of $\varepsilon_F/\hbar$. The integrals with respect to k and p will be calculated in a cylindrical coordinate system with z axis along the vector $(-q)$. The coordinates k and p will be designated

$$k=(z,\ t^{1/2},\ \varphi),\quad p=(z',\ t'^{1/2},\ \varphi').\quad(35)$$

In this case we have

$$\Omega_{kq}=q^{2}-2qz\equiv\Omega,\quad\Omega_{pq}=q^{2}-2qz'\equiv\Omega',\quad(36)$$

$$|k-p|^{2}=t+t'-2(tt')^{1/2}\cos(\varphi-\varphi')+s_{1}(z,z'),$$
$$|k+p+q|^{2}=t+t'+2(tt')^{1/2}\cos(\varphi-\varphi')+s_{2}(z,z'),\quad(37)$$

where we have introduced the functions

$$s_{1}(z,z')=(z-z')^{2}=(\Omega-\Omega')^{2}/4q^{2},$$
$$s_{2}(z,z')=(z+z'-q)^{2}=(\Omega+\Omega')^{2}/4q^{2}.\quad(38)$$

The rule for changing from summation to integration in the coordinate system (35) is given by

$$\sum_{kp}f_{k}f_{p}\{\ldots\}=\left(\frac{3}{8}N\right)^{2}\int_{-1}^{1}dz\int_{-1}^{1}dz'\int_{0}^{1-z^{2}}dt\int_{0}^{1-z'^{2}}dt'\int_{0}^{2\pi}\frac{d\varphi}{2\pi}\int_{0}^{2\pi}\frac{d\varphi'}{2\pi}\{\ldots\}.\quad(39)$$

Taking (36)–(39) into account and changing in the integrals with respect to z and z′ to new variables Ω and Ω', defined by the relations in (36), we obtain

$$P(q,\omega)=\frac{3\alpha r_{s}}{16\pi}\frac{1}{q^{2}S(q)}\int_{-\omega_{1}}^{\omega_{2}}d\Omega\int_{-\omega_{1}}^{\omega_{2}}d\Omega'\{J_{1}(\Omega,\Omega')[\Phi(\Omega',\Omega)F(\Omega)+\Phi(-\Omega',-\Omega)F(-\Omega)]-J_{2}(\Omega,\Omega')[\Phi(-\Omega',\Omega)F(\Omega)+\Phi(\Omega',-\Omega)F(-\Omega)]\},\quad(40)$$

where $\omega_{1,2}=2q\mp q^{2}$, and $J_{1,2}(\Omega,\Omega')$ stands for the following triple integral:

$$J_{i}(\Omega,\Omega')\equiv J(T,T',s_{i})=\int_{0}^{T}dt\int_{0}^{T'}dt'\int_{0}^{2\pi}\frac{d\varphi}{2\pi}\frac{1}{t+t'+2(tt')^{1/2}\cos\varphi+s_{i}}.\quad(41)$$

Here, T, T′ and s_i are functions of Ω and Ω'. With this

$$T=T(\Omega)=1-z^{2}=1-(q^{2}-\Omega)^{2}/4q^{2},\quad T'=T(\Omega'),\quad(42)$$

and the relation $s_i(\Omega,\Omega')$ is determined by Eqs. (38). As for the numerical coefficient $3\alpha r_s/16\pi$ in (40), its origin can be easily understood if it is recognized that

$$Nv(k_F)/\varepsilon_F=8\alpha r_s/3\pi.$$

The functions $J_i(\Omega,\Omega')$, as can be seen directly from definition (41), are invariant to permutation of Ω and Ω'. A detailed calculation of these function is contained in Ref. 14, and we confine ourselves only to the result:

$$J(T,T',s)=T\ln|X|+T'\ln|Y|+{}^{1}/_{2}(W-B-s),\quad(43)$$

where

$$X=\frac{1}{2}\left(1+\frac{W+A}{s}\right),\quad Y=\frac{1}{2}\left(1+\frac{W-A}{s}\right),$$
$$W=(A^{2}+2sB+s^{2})^{1/2},\quad A=T'-T,\quad B=T'+T.$$

We note that the real and imaginary parts of the function $P(q,\omega)$ are connected by the dispersion relation

$$\mathrm{Re}\,P(q,\omega)=\frac{2}{\pi}\int_{0}^{\infty}d\omega'\frac{\omega'}{\omega'^{2}-\omega^{2}}\mathrm{Im}\,P(q,\omega'),\quad(44)$$

whose validity follows directly from the form of the initial formula (23) for the correction for the local field. It therefore suffices to calculate from (40) only $\mathrm{Im}P(q,\omega)$, and $\mathrm{Re}P(q,\omega)$ can then be found by using (44). This calculation procedure is convenient because for the imaginary part of the correction for the local field formula (40) admits a further simplification. By virtue of (34) we have

$$\mathrm{Im}\,\Phi(\Omega',\Omega)=\pi[\delta(\omega-\Omega)-\delta(\omega-\Omega')]$$

and after simple transformations we obtain ultimately

$$\mathrm{Im}\,P(q,\omega)=\frac{3\alpha r_{s}}{16}\frac{1}{q^{2}S(q)}\int_{-\omega_{1}}^{\omega_{2}}d\omega' f(\omega,\omega').\quad(45)$$

We have introduced here the function

$$f(\omega,\omega')=[F(\omega')-F(\omega)]g(\omega,\omega')+[F(-\omega')-F(\omega)]g(-\omega,\omega'),\quad(46)$$

where $g(\omega,\omega')$ is defined as follows

$$g(\omega,\omega')=\begin{cases} J_2(\omega',-\omega)-J_1(\omega',\omega), & |\omega|<\omega_1 \\ -J_1(\omega',\omega), & |\omega_1|<\omega<\omega_2 \end{cases},$$

$$g(\omega,\omega')=\begin{cases} J_2(\omega',-\omega), & -\omega_2<\omega<-|\omega_1| \\ 0, & |\omega|>\omega_2 \end{cases}.$$

The problem of finding the correction for the local field reduces thus the calculation of the single integrals (24), (25), (44), and (45). We note that the function (46) has logarithmic singularities of the derivative at the points $\omega'=\pm\omega$. This circumstance must be taken into account when evaluating the integral (45), but does not lead to substantial difficulties. In addition, the function $F(\omega')$ has a discontinuity at the point $\omega'=0$, and this can be easily taken into account by dividing at $q<2$ the region of integration in (45) into two parts, $(-\omega_1,0)$ and $(0,\omega_2)$. Finally, we note that in the numerical calculation of the real part of the correction for the local field it is convenient to use the following representation of the dispersion relation (44):

$$P_1(\omega)=\frac{1}{\pi}P_2(\omega)\ln\left|\frac{\omega_2^2-\omega^2}{\omega^2-\omega_0^2}\right|+\frac{2}{\pi}\int_{\omega_0}^{\infty}d\omega'\,\omega'\frac{P_2(\omega')-P_2(\omega)}{\omega'^2-\omega^2}, \qquad (47)$$

where $\omega_0=\max(0,-\omega_1)$, while $P_1(\omega)$ and $P_2(\omega)$ are shorthanded for the real and imaginary parts of the function $P(\mathbf{q},\omega)$.

5. RESULTS FOR THE CORRECTION FOR THE LOCAL FIELD AND FOR THE STATIC STRUCTURE FACTOR

Of greatest interest for the theory of simple metals is the static permittivity $\varepsilon(\mathbf{q},0)$, which can be easily found from Eq. (1) if one knows the static correction for the local field, $G(\mathbf{q},0)=-P(\mathbf{q},0)/Q_0(\mathbf{q},0)$. However, as seen from Eqs. (23)–(25), for a self-consistent calculation within the framework of the approximation considered in the present paper we must know the frequency dependence of the permittivity. The actual calculation was performed as follows. During the initial stage we used in the right-hand sides of (24) and (25) not $\tilde{\varepsilon}(\mathbf{q},\omega)$ but its value in the random-phase approximation [see Eq. (10)]. Next, Eqs. (45) and (47) were used to calculate the frequency dependence of $P(\mathbf{q},\omega)$, and this yielded a more accurate $\tilde{\varepsilon}(\mathbf{q},\omega)$. The latter was introduced into (24) and (25), and the procedure was repeated until a self-consistent solution was obtained. The convergence of this iteration procedure turned out to be very rapid—two or three iterations resulted usually in satisfactory accuracy.

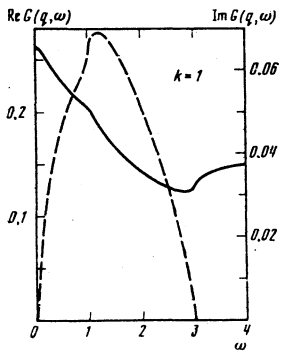

FIG. 1. Real and imaginary parts of the correction for the local field as functions of the frequency at $q=1$ and $r_s=1$, represented respectively by the solid and dashed curves [the frequency is in units of $\varepsilon_F/\hbar$ and the wave number in units of k_F, in which case the characteristic frequencies ω_s are, in accord with (28), equal to 1 and 3].

TABLE I. Static correction for the local field at $r_s=3$.

q	$G(q,0)$	q	$G(q,0)$	q	$G(q,0)$	q	$G(q,0)$
0.1	0.0025	1.1	0.3221	2.1	0.7954	3.1	0.5798
0.2	0.0100	1.2	0.3884	2.2	0.7349	3.2	0.5736
0.3	0.0226	1.3	0.4621	2.3	0.6962	3.3	0.5681
0.4	0.0403	1.4	0.5437	2.4	0.6683	3.4	0.5633
0.5	0.0632	1.5	0.6328	2.5	0.6470	3.5	0.5590
0.6	0.0916	1.6	0.7287	2.6	0.6301	3.6	0.5551
0.7	0.1254	1.7	0.8288	2.7	0.6163	3.7	0.5516
0.8	0.1651	1.8	0.9258	2.8	0.6049	3.8	0.5485
0.9	0.2109	1.9	1.0002	2.9	0.5952	3.9	0.5456
1.0	0.2631	2.0	0.9440	3.0	0.5870	4.0	0.5431

An idea of the frequency dependence of the function $G(\mathbf{q},\omega)$ can be gained from Fig. 1. The curves of this figure agree, in their general character, with the analogous curves calculated in the approximation of Toigo and Woodruff,[15] although there is of course no quantitative agreement. We note that neither $\mathrm{Re}G(\mathbf{q},\omega)$ nor $\mathrm{Im}G(\mathbf{q},\omega)$ shows even an indication of a divergence at the frequencies (28), in contrast to the situation in the approximation of Rajogapal and Jain (see the corresponding calculations in Refs. 9 and 11). Moreover, the curves calculated by us behave even far from ω_s quite differently than the corresponding curves of Refs. 9 and 11.

As seen from Eqs. (23)–(25), the correction for the local field is in our approximation a function of r_s. The actual calculations show, however, that in the static limit $\omega=0$ the function $G(\mathbf{q},0)$ depends on r_s very little, and therefore we list in Table I complete data for $G(\mathbf{q},0)$ at only one value $r_s=3$. It is seen from this table that at small wave numbers we have $G(\mathbf{q},0)\approx q^2/4$. At large q, on the other hand, the function $G(\mathbf{q},0)$ behaves exactly as the static correction for the local field in the simplest approximation of Ref. 3 [see formula (26)]. The last circumstance is easy to understand if it is recalled that the approximation (26) is obtained from (23)–(25) by putting in them $\tilde{\varepsilon}(\mathbf{q},0)=1$. This substitution is fully justified in the limit as $q\to\infty$. The dependence of $G(\mathbf{q},0)$ on r_s manifests itself most noticeably in the wave-number region $1.1\leq q\leq 2.1$. The values of the function $G(\mathbf{q},0)$ in this region of q, for different values of r_s in the metallic-density range, are listed in Table II.

We note that the procedure for the self-consistent

TABLE II. Dependence of the function $G(\mathbf{q},0)$ on the parameter r_s.

q	r_s					
	1	2	3	4	5	6
1.1	0.3242	0.3230	0.3221	0.3214	0.3207	0.3201
1.2	0.3909	0.3895	0.3884	0.3873	0.3864	0.3857
1.3	0.4652	0.4635	0.4621	0.4608	0.4597	0.4587
1.4	0.5471	0.5453	0.5437	0.5421	0.5408	0.5396
1.5	0.6365	0.6346	0.6328	0.6311	0.6297	0.6283
1.6	0.7323	0.7305	0.7287	0.7270	0.7255	0.7240
1.7	0.8317	0.8302	0.8288	0.8273	0.8258	0.8244
1.8	0.9280	0.9269	0.9258	0.9246	0.9235	0.9224
1.9	1.0018	1.0010	1.0002	0.9995	0.9987	0.9979
2.0	0.9451	0.9445	0.9440	0.9434	0.9429	0.9423
2.1	0.7957	0.7955	0.7954	0.7952	0.7951	0.7949

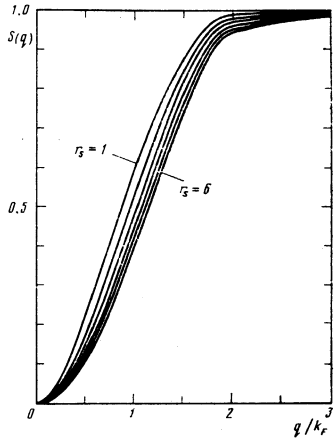

FIG. 2. Behavior of the static structure factor of an interacting electron gas in the metallic-density range.

solution of the system of Eqs. (23)–(25) at each iteration stage includes as a required element the recalculation of the static structure factor $S(\mathbf{q})$. This quantity is, as is well known, also of independent interest, since many physical characteristics of a system of interacting electrons are expressed by functionals of $S(\mathbf{q})$. We show therefore in Fig. 2 the results of the calculation of $S(\mathbf{q})$ for a number of values of the parameter r_s. In the limit of small q, the curves in Fig. 2 tend to an asymptotically correct relation (as $q \to 0$)

$$S(\mathbf{q}) \to q^2/2\alpha^2(3r_s)^{1/2},$$

while as $q \to \infty$ they are approximated by the formula

$$S(\mathbf{q}) \to 1 - 4\alpha r_s/3\pi q^4.$$

We note that in the approximation of Rajagopal and Jain the static structure factor has also the same asymptotic behavior (see Ref. 9 for the proof).

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Mode dependence of resonant absorption of ballistic phonons in CaF_2:Eu^{2+} crystals

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The anisotropy of absorption of longitudinal and transverse acoustic phonons in the 3×10^{11} band in a CaF_2:Eu^{2+} crystal is investigated experimentally and theoretically in the case of resonant interaction of the phonons with the electronic state $4f^65d(\Gamma_8^+)$ of the Eu^{2+} ion, split into a doublet by uniaxial compression of the crystal. The anisotropy agrees with the selection rules for transitions induced by dynamic deformation of a lattice in the field of a hypersound wave.

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Experiments have been recently performed[1–3] on the behavior of nonequilibrium monochromatic terahertz acoustic phonons in uniaxially stressed CaF_2 and SrF_2 crystals activated with Eu^{2+} ions. The Eu^{2+} ions are situated in the lattices of these crystals in a cubic field of high symmetry O_h and some of the Eu^{2+} levels have orbital degeneracy. Use is made in Refs. 1–3 of the fact[4] that uniaxial deformation splits the orbitally degenerate radiative level Γ_8^+ of the excited $4f^65d$ configuration of Eu^{2+} into two, and the magnitude of the doublet splitting can vary smoothly in a range of several dozen reciprocal centimeters.[1,4] The existence of resonant single-phonon transitions between the components of the deformation doublet has made it possible to effect both fluorescent detection[1,2] of nonequilibrium monochromatic phonons with frequencies up to 2.4 THz [piezospectroscopic phonon detector (PPD)], as well as their generation in nonradiative relaxation of the optically excited ions.[1,3]

The ballistic character of the propagation of transverse phonons with $\nu \approx 0.5$ THz was demonstrated in

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