

Dielectric matrix of band electrons with allowance for exchange-correlation effects

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The dielectric constant of electrons in a crystal is calculated in the form of a matrix in reciprocal-lattice vector space. A generalized self-consistent-field method is used, which reduces the problem to the solution of the single-particle problem of the behavior of an electron in an external field and in the crystal field of unscreened ions, as well as in the self-consistent field of other electrons, consisting of a Hartree potential and an exchange-correlation potential. A method is proposed for constructing the exchange-correlation potential and leads in the case of a homogeneous electron gas to the well known Toigo-Woodruff dielectric function. The equations obtained are used to determine the electron contribution to the dynamic oscillation matrix in simple metals, accurate to third order in the pseudopotential. It is shown that the obtained expressions obey some rules that connect the nonlinear polarizabilities of the electrons with their linear response.

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INTRODUCTION

It is known¹⁻³ that the dielectric constant of the electrons in a crystal is a matrix $\epsilon(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}', \omega)$ in the space of the reciprocal-lattice vectors $\{\mathbf{G}\}$ (here and elsewhere \mathbf{k} is the wave vector located within the first Brillouin zone). Knowledge of this matrix is necessary for a microscopic description of a great variety of phenomena in solids. Thus, e.g., the reciprocal dielectric matrix $\epsilon^{-1}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}', \omega)$ determines in the static limit $\omega = 0$ the adiabatic contribution of the electrons to the dynamic lattice-oscillation matrix, and exact calculations of $\epsilon^{-1}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}', 0)$ are extremely important for the understanding of the nature of various anomalies observed in phonon spectra of crystals. The quantity $\epsilon^{-1}(\mathbf{k}, \mathbf{k}, \omega)$ describes the long-wave limit $\mathbf{k} \rightarrow 0$ the optical properties of the crystal electrons, while $\text{Im} \epsilon^{-1}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}', \omega)$ describes the cross section for inelastic scattering for charged particles in a crystal and the resonances that appear in such spectra and are connected with excitation of plasmons, excitons, and others.

At the present status of the many-body theory, calculation of the dielectric matrix $\epsilon(\mathbf{q}, \mathbf{q}', \omega)$ and of its inverse $\epsilon^{-1}(\mathbf{q}, \mathbf{q}', \omega)$ is an extremely complicated problem. Practical success in its solution can be reached only by using very simple variants of the self-consistent-field approximation, which reduce it to a single-particle problem. In most papers $\epsilon(\mathbf{q}, \mathbf{q}', \omega)$ is actually calculated by using a generalized random-phase approximation, that takes into account only the band character of the wave functions and of the energies of the electron in the crystal, but neglects completely the exchange and correlation effects (see the reviews^{4,5}). It is well known, however, that in the case of a homogeneous electron gas the indicated approximation describes the properties of the system quite poorly at densities corresponding to the conduction-electron densities in real metals. The problem of correct allowance for exchange-correlation effects in a homogeneous electron gas is at present one of the most vital

ones in solid-state physics (see our recent review⁶). It is important here that it is precisely the exchange and the correlation (customarily called also the local-field effects) which give rise to many interesting phenomena in a system of interacting electrons.⁵ These include phase transitions in a state with a spin- or charge-density wave, the appearance of a negative static dielectric constant, and others. Allowance for local-field effects, as is well known, is most important also when it comes to describing the electromagnetic properties of crystals.⁷

In many studies of the dielectric matrix of band electrons,⁴ by local-field effects are mean effects connected with the existence of off-diagonal elements of the matrix $\epsilon(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}', \omega)$ with $\mathbf{G} \neq \mathbf{G}'$. As shown by Maksimov and Mazin,⁸ allowance for the off-diagonal elements of the dielectric matrix does not constitute allowance for the local-field effects in the sense used, e.g., in classical electrodynamics, meaning the difference between the microscopic field acting on the particles of the system and the average macroscopic field in the given medium. From the physical point of view, allowance for the local-field effect must of necessity include a contribution from the exchange-correlation interaction. And only a joint analysis of the off-diagonal elements of the dielectric matrix and of the exchange-correlation effects can lead to a correct description of the local-field effects in crystal systems.

Among the immense number of papers devoted to the calculation of the dielectric matrix of band electrons, one can find only a few in which attempts were made to take a consistent account of exchange-correlation effects. Mention should be made in this connection of the paper by Singhal and Callaway,⁹ who obtained the dielectric matrix within the framework of the single-particle self-consistent field method by using an exchange-correlation potential in the form

$$V_{xc}(\mathbf{r}, t) = -\frac{3}{2} \alpha e^2 \left[\frac{3}{\pi} n(\mathbf{r}, t) \right]^{1/2}, \quad (1.1)$$

where $n(\mathbf{r}, t) = n(\mathbf{r}) + n_{\text{ind}}(\mathbf{r}, t)$ is the average density of the Bloch electrons in the presence of an external perturbing potential, and α is an empirical parameter. Equation (1.1) is a generalization, of the known Slater $X\alpha$ potential¹⁰ to include the nonstationary case. A more consistent approach to the allowance for the contribution of the exchange-correlation effects to the dielectric matrix was developed by Stoddart and Hanks¹¹ within the framework of the density-functional method, but this method can be used only to calculate the static dielectric matrix at $\omega = 0$. Both these studies will be discussed in detail in later sections, and at present we wish to point out also a paper by Hanke and Sham,¹² in which exchange and correlation effects were taken into account in the calculation of the inverse dielectric matrix $\epsilon^{-1}(\mathbf{k}, \mathbf{k}, \omega)$ of covalent semiconductors in the long-wave limit as $k \rightarrow 0$. The methods used in that paper are valid, however, only in the case of crystals with strongly localized electrons and with negligibly small overlap integrals.

We have previously⁶ proposed a method of constructing a self-consistent exchange correlation potential $V_{xc}(\mathbf{r}, t)$, which in the case of a homogeneous electron gas leads to the well known dielectric function of Toigo and Woodruff,¹³ at present one of the best approximate dielectric functions with dynamic correction for the local field. In the present paper we generalize this method to include the case of Bloch electrons and obtain for $\epsilon(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}', \omega)$ an expression that goes over in the limit of a homogeneous electron gas into the equation of Toigo and Woodruff. This expression is then used to calculate the electron contribution to the dynamic lattice vibration matrix in metals with almost free electrons.

2. DERIVATION OF EQUATION FOR THE DIELECTRIC MATRIX

We consider the linear response of a model system of interacting electrons moving in a rigid ion lattice, to a test charge introduced from the outside. We use for this purpose a self-consistent field approximation and seek the perturbed single-electron wave functions by starting from the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi_{\lambda}(\mathbf{r}, t) = [H_0 + V_{\text{eff}}(\mathbf{r}, t)] \psi_{\lambda}(\mathbf{r}, t). \quad (2.1)$$

Here H_0 is the Hamiltonian that determines the electron band structure and includes the periodic potentials $V_{\text{el}}(\mathbf{r})$ and $V_{\text{e}}(\mathbf{r})$, respectively, of the interactions of the electron with the ion lattice and with the average self-consistent field due to the remaining electrons in the unperturbed system. [The potential $V_{\text{e}}(\mathbf{r})$ is a certain functional of the eigenstates $\psi_{\lambda}^{(0)}(\mathbf{r})$ of the Hamiltonian H_0 , and is responsible for the effective screening of the electron-ion interaction.] Next,

$$V_{\text{eff}}(\mathbf{r}, t) = V_{\text{ext}}(\mathbf{r}, t) + \delta V_{\text{e}}(\mathbf{r}, t) \quad (2.2)$$

is the total perturbation experienced by a Bloch electron when an external charge is introduced into the system. The effective potential (2.2) consists of the external potential $V_{\text{ext}}(\mathbf{r}, t)$ and of the correction $\delta V_{\text{e}}(\mathbf{r}, t)$ to the self-consistent field. This correction is a

result of the distortion of the electron density by the external perturbation, and ensures screening of the external potential. For the solutions $\psi_{\lambda}(\mathbf{r}, t)$ of Eq. (2.1) we retain the quantum numbers λ of those Bloch states $\psi_{\lambda}^{(0)}(\mathbf{r})$ into which these solutions go over as $t \rightarrow -\infty$, when the external perturbation is turned on adiabatically with a time constant $\delta \rightarrow +0$.

In the principal approximation in V_{eff} , the solutions of (2.1) are

$$\psi_{\lambda}(\mathbf{r}, t) = [\psi_{\lambda}^{(0)}(\mathbf{r}) + \psi_{\lambda}^{(1)}(\mathbf{r}, t)] \exp(-iE_{\lambda}t/\hbar), \quad (2.3)$$

where E_{λ} are the energy eigenvalues of the Hamiltonian H_0 , and

$$\psi_{\lambda}^{(1)}(\mathbf{r}, t) = \sum_{\mathbf{q}} \int \frac{d\omega}{2\pi} V_{\text{eff}}(\mathbf{q}, \omega) e^{-i(\omega+i\delta)t} \sum_{\lambda'} \frac{|\lambda'\rangle \langle \lambda'| e^{i\mathbf{q}\cdot\mathbf{r}} |\lambda\rangle}{\hbar\omega - E_{\lambda'} + E_{\lambda} + i\delta}. \quad (2.4)$$

Here $V_{\text{eff}}(\mathbf{q}, \omega)$ is the Fourier component of the effective potential (2.2) and has the property $V_{\text{eff}}^*(\mathbf{q}, \omega) = V_{\text{eff}}(-\mathbf{q}, -\omega)$, and the abbreviated notation $|\lambda\rangle = \psi_{\lambda}^{(0)}(\mathbf{r})$ has been introduced for the Bloch states.

Using (2.3) and (2.4) we can determine the average induced density

$$n_{\text{ind}}(\mathbf{r}, t) = 2 \sum_{\lambda} n_{\lambda} [|\psi_{\lambda}(\mathbf{r}, t)|^2 - |\psi_{\lambda}^{(0)}(\mathbf{r})|^2],$$

where n_{λ} are the Fermi occupation numbers of the band states. For the Fourier component $n_{\text{ind}}(\mathbf{q}, \omega)$ we obtain

$$n_{\text{ind}}(\mathbf{q}, \omega) = \sum_{\mathbf{q}'} \chi^{(0)}(\mathbf{q}, \mathbf{q}', \omega) V_{\text{eff}}(\mathbf{q}', \omega), \quad (2.5)$$

where the linear-response tensor is defined by

$$\chi^{(0)}(\mathbf{q}, \mathbf{q}', \omega) = 2 \sum_{\lambda\lambda'} \frac{n_{\lambda} - n_{\lambda'}}{\hbar\omega - E_{\lambda'} + E_{\lambda} + i\delta} \langle \lambda | e^{-i\mathbf{q}\cdot\mathbf{r}} | \lambda' \rangle \langle \lambda' | e^{i\mathbf{q}'\cdot\mathbf{r}} | \lambda \rangle. \quad (2.6)$$

The value of (2.6) differs from zero only if the difference $\mathbf{q} - \mathbf{q}'$ is equal to one of the reciprocal-lattice vectors, and constitutes in fact a matrix $\chi^{(0)}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}', \omega)$ with indices \mathbf{G} and \mathbf{G}' . In the intermediate calculations, to simplify the equations, we shall not use this circumstance explicitly.

To make the problem self-consistent it is necessary also to determine the potentials $V_{\text{e}}(\mathbf{r})$ and $\delta V_{\text{e}}(\mathbf{r}, t)$. We use for this purpose the method proposed by us⁶ for the construction of the self-consistent field. This method leads to the following expression for the gradient of the sum of these two quantities:

$$\begin{aligned} \nabla [V_{\text{e}}(\mathbf{r}) + \delta V_{\text{e}}(\mathbf{r}, t)] = \nabla \left[\sum_{\mathbf{q}} v(\mathbf{q}) n(\mathbf{q}, t) e^{i\mathbf{q}\cdot\mathbf{r}} \right] \\ - \frac{2i}{n(\mathbf{r}, t)} \sum_{\mathbf{q}} v(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}} \sum_{\lambda\lambda'} n_{\lambda} n_{\lambda'} \psi_{\lambda'}^*(\mathbf{r}, t) \psi_{\lambda}(\mathbf{r}, t) \int d^3\mathbf{r}' \psi_{\lambda'}^*(\mathbf{r}', t) e^{-i\mathbf{q}\cdot\mathbf{r}'} \psi_{\lambda}(\mathbf{r}', t). \end{aligned} \quad (2.7)$$

Here $v(\mathbf{q}) = 4\pi e^2/q^2\Omega$ is the Fourier component of the Coulomb potential, $n(\mathbf{r}, t)$ is the average electron density in the presence of the perturbation, and $n(\mathbf{q}, t)$ is its Fourier component with respect to the coordinate:

$$n(\mathbf{r}, t) = 2 \sum_{\lambda} n_{\lambda} |\psi_{\lambda}(\mathbf{r}, t)|^2 = \frac{1}{\Omega} \sum_{\mathbf{q}} n(\mathbf{q}, t) e^{i\mathbf{q}\cdot\mathbf{r}}.$$

The first term in the right-hand side of (2.7) is the Hartree self-consistent field, while the second de-

scribes the exchange-correlation potential of the electrons. Using (2.3) and (2.4) it is easy to separate from (2.7) in explicit form an equation for the potential $V_e(\mathbf{r})$, which should be used in the self-consistent calculation of the electron band structure, as well as an equation for the perturbed potential $\delta V_e(\mathbf{r}, t)$, which is needed to obtain the dielectric matrix of the system.

In accordance with the structure of (2.7), the potential $\delta V_e(\mathbf{r}, t)$ breaks up naturally into a sum of Hartree and exchange-correlation contributions

$$\delta V_e(\mathbf{r}, t) = \delta V_H(\mathbf{r}, t) + \delta V_{xc}(\mathbf{r}, t). \quad (2.8)$$

Using (2.5), we obtain for the Fourier component of the Hartree potential simply

$$\delta V_H(\mathbf{q}, \omega) = v(\mathbf{q}) n_{ind}(\mathbf{q}, \omega) = v(\mathbf{q}) \sum_{\mathbf{q}'} \chi^{(0)}(\mathbf{q}, \mathbf{q}', \omega) V_{eff}(\mathbf{q}', \omega). \quad (2.9)$$

Substituting next (2.3) and (2.4) in the second term of (2.7) and separating the contributions linear in V_{eff} , we obtain after simple algebraic transformations the following Fourier component of the exchange-correlation potential

$$\delta V_{xc}(\mathbf{q}, \omega) = - \sum_{\mathbf{q}'} P(\mathbf{q}, \mathbf{q}', \omega) V_{eff}(\mathbf{q}', \omega), \quad (2.10)$$

where the matrix $P(\mathbf{q}, \mathbf{q}', \omega)$ is given by

$$P(\mathbf{q}, \mathbf{q}', \omega) = 2v(\mathbf{q}) \sum_{\lambda, \lambda'} n_{\lambda} (n_{\lambda} - n_{\lambda'}) \left(\frac{1}{\hbar\omega - E_{\lambda'} + E_{\lambda} + i\delta} - \frac{1}{\hbar\omega - E_{\lambda} + E_{\lambda'} + i\delta} \right) \sum_{\mathbf{p}} \frac{q_{\mathbf{p}}}{p^2} \left[\frac{e^{i(\mathbf{p}-\mathbf{q})\mathbf{r}}}{\Omega n(\mathbf{r})} \right]_{\lambda, \lambda'} (e^{-i\mathbf{p}\mathbf{r}})_{\lambda, \lambda'} \quad (2.11)$$

$$\times (e^{i\mathbf{q}'\mathbf{r}})_{\lambda, \lambda'} - 2v(\mathbf{q}) \sum_{\lambda, \lambda'} n_{\lambda} n_{\lambda'} \sum_{\mathbf{p}} \frac{q_{\mathbf{p}}}{p^2} \left[\frac{e^{i(\mathbf{p}+\mathbf{p}'-\mathbf{q})\mathbf{r}}}{\Omega^2 n^2(\mathbf{r})} \right]_{\lambda, \lambda'} (e^{-i\mathbf{p}\mathbf{r}})_{\lambda, \lambda'} \chi^{(0)}(\mathbf{p}', \mathbf{q}', \omega).$$

It is easy to verify that this matrix also differs from zero only if the difference $\mathbf{q} - \mathbf{q}'$ coincides with one of the reciprocal-lattice vectors.

We can now express the components of the effective potential $V_{eff}(\mathbf{q}, \omega)$ in terms of $V_{ext}(\mathbf{q}, \omega)$. The corresponding relation is obtained from the definition (2.2) with account taken of (2.8)–(2.10), and takes the form

$$V_{eff}(\mathbf{q}, \omega) = \sum_{\mathbf{q}'} \bar{\epsilon}^{-1}(\mathbf{q}, \mathbf{q}', \omega) V_{ext}(\mathbf{q}', \omega), \quad (2.12)$$

where $\bar{\epsilon}^{-1}(\mathbf{q}, \mathbf{q}', \omega)$ is the inverse of the so-called effective dielectric matrix

$$\bar{\epsilon}(\mathbf{q}, \mathbf{q}', \omega) = \delta_{\mathbf{q}\mathbf{q}'} - v(\mathbf{q}) \chi^{(0)}(\mathbf{q}, \mathbf{q}', \omega) + P(\mathbf{q}, \mathbf{q}', \omega). \quad (2.13)$$

Substituting next (2.12) in (2.5), we obtain the induced electron density, and consequently also the linear-polarizability tensor $\chi(\mathbf{q}, \mathbf{q}', \omega)$, defined by the expression

$$n_{ind}(\mathbf{q}, \omega) = \sum_{\mathbf{q}'} \chi(\mathbf{q}, \mathbf{q}', \omega) V_{ext}(\mathbf{q}', \omega) \quad (2.14)$$

and connected with the inverse dielectric matrix by the well known relation

$$\bar{\epsilon}^{-1}(\mathbf{q}, \mathbf{q}', \omega) = \delta_{\mathbf{q}\mathbf{q}'} + v(\mathbf{q}) \chi(\mathbf{q}, \mathbf{q}', \omega). \quad (2.15)$$

By simple algebraic transformations we arrive at the following expression for the dielectric matrix of a system of Bloch electrons

$$\epsilon(\mathbf{q}, \mathbf{q}', \omega) = \delta_{\mathbf{q}\mathbf{q}'} - v(\mathbf{q}) \sum_{\mathbf{q}''} \chi^{(0)}(\mathbf{q}, \mathbf{q}'', \omega) \Lambda(\mathbf{q}'', \mathbf{q}', \omega), \quad (2.16)$$

where $\Lambda(\mathbf{q}, \mathbf{q}', \omega)$ is a vertex matrix defined by the equation

$$\Lambda^{-1}(\mathbf{q}, \mathbf{q}', \omega) = \delta_{\mathbf{q}\mathbf{q}'} + P(\mathbf{q}, \mathbf{q}', \omega). \quad (2.17)$$

Here $P(\mathbf{q}, \mathbf{q}', \omega)$ is the exchange-correlation matrix (2.11).

In the limiting case of free electrons, Eq. (2.11) for the exchange-correlation matrix takes the form

$$P(\mathbf{q}, \mathbf{q}', \omega) = P(\mathbf{q}, \omega) \delta_{\mathbf{q}\mathbf{q}'}, \quad (2.18)$$

$$= \delta_{\mathbf{q}\mathbf{q}'} \frac{2v(\mathbf{q})}{N} \sum_{\mathbf{p}\mathbf{p}'} \frac{q(\mathbf{p}-\mathbf{p}')}{|\mathbf{p}-\mathbf{p}'|^2} (f_{\mathbf{p}} - f_{\mathbf{p}+\mathbf{q}}) \frac{f_{\mathbf{p}'} - f_{\mathbf{p}'+\mathbf{q}}}{\hbar\omega - \epsilon_{\mathbf{p}'+\mathbf{q}} + \epsilon_{\mathbf{p}'} + i\delta},$$

where $\epsilon_{\mathbf{p}} = \hbar^2 p^2 / 2m$, and $f_{\mathbf{p}} = f(\epsilon_{\mathbf{p}})$ is the Fermi distribution function. Formula (2.18) corresponds exactly to the correction for the local field

$$G(\mathbf{q}, \omega) = P(\mathbf{q}, \omega) / v(\mathbf{q}) \chi_0(\mathbf{q}, \omega) \quad (2.19)$$

in the theory of Toigo and Woodruff.¹³ Here $\chi_0(\mathbf{q}, \omega)$ is the known Lindhard function. In concluding this section, we compare our expression (2.16) for the dielectric matrix with the already mentioned results for $\epsilon(\mathbf{q}, \mathbf{q}', \omega)$ that follow from the generalized random-phase approximation and from Refs. 9 and 11. If exchange-correlation effects are neglected, i.e., the matrix $P(\mathbf{q}, \mathbf{q}', \omega)$ is set equal to zero, then Eq. (2.16) takes the form

$$\epsilon(\mathbf{q}, \mathbf{q}', \omega) = \delta_{\mathbf{q}\mathbf{q}'} - v(\mathbf{q}) \chi^{(0)}(\mathbf{q}, \mathbf{q}', \omega), \quad (2.20)$$

which coincides exactly with the widely used random-phase approximation.¹⁻⁴

Next, the equation obtained for $\epsilon(\mathbf{q}, \mathbf{q}', \omega)$ by Singhal and Callaway⁹ has formally the same form as Eq. (2.16), but their vertex matrix $\Lambda(\mathbf{q}, \mathbf{q}', \omega)$ is defined by the relation

$$\Lambda^{-1}(\mathbf{q}, \mathbf{q}', \omega) = \delta_{\mathbf{q}\mathbf{q}'} + v(\mathbf{q}) \sum_{\mathbf{q}''} G(\mathbf{q}, \mathbf{q}'') \chi^{(0)}(\mathbf{q}'', \mathbf{q}', \omega), \quad (2.21)$$

where $G(\mathbf{q}, \mathbf{q}')$ is the result of allowance for the local-field effects, and is given by

$$G(\mathbf{q}, \mathbf{q}') = \left(\frac{3}{8\pi} \right)^{1/2} \frac{\alpha e^2}{v(\mathbf{q}) \Omega^2} \int d^3 r n^{-3/2}(\mathbf{r}) \exp(-i(\mathbf{q}-\mathbf{q}')\mathbf{r}). \quad (2.22)$$

In our recent paper⁶ we have shown that if account is taken of exchange-correlation effects with the aid of a potential of the form (1.1) in the case of a homogeneous electron gas, a dielectric function $\epsilon(\mathbf{q}, \omega)$ is obtained with a static correction for the local field $G(\mathbf{q}) = 3\alpha q^2 / 8k_F^2$ [this result is obtained from (2.22) by putting in it $\mathbf{q} = \mathbf{q}'$ and $n(\mathbf{r}) = N/\Omega$]. Such a dielectric function distorts greatly the description of the correlations between the electrons at short distances. In addition, dielectric functions with static correction for the local field account poorly for the dynamic features of the system, particularly for the plasmon dispersion law. It is therefore quite clear that the approximation for $\epsilon(\mathbf{q}, \mathbf{q}', \omega)$ with a vertex matrix of the type (2.21) has a much more restricted applicability than the approximation obtained in the present paper.

Finally, Stoddart and Hanks¹¹ obtained for the static dielectric matrix an expression that reduces to (2.16) and (2.21) at $\omega = 0$, but the matrix of the corrections of

the local field has in their case the form

$$G(\mathbf{q}, \mathbf{q}') = -\frac{1}{v(\mathbf{q})\Omega^2} \int d^3r d^3r' \frac{\delta^2 E_{xc}(\{n(r)\})}{\delta n(r)\delta n(r')} \exp(i(\mathbf{q}\mathbf{r} - \mathbf{q}'\mathbf{r}')), \quad (2.23)$$

where $E_{xc}(\{n(r)\})$ is the exchange-correlation energy of the system and is a functional of the electron density. To use (2.23) it is necessary to make some assumption concerning the functional dependence of E_{xc} on $n(r)$, since the exact form of the exchange-correlation functional is unknown. In particular, this functional can be chosen such that at least at small \mathbf{q} and \mathbf{q}' the equations for the static dielectric matrix, obtained here and in Ref. 11, turn out to be identical.

3. THE CASE OF A METAL WITH ALMOST FREE ELECTRONS

The quantitative calculation of the dielectric matrix of band electrons in accord with the equations obtained in the preceding section is in the general case a rather complicated problem both from the point of view of obtaining the self-consistent Bloch wave functions $\psi_\lambda(\mathbf{r})$ and the corresponding energy eigenvalues E_λ , and during the stage of direct calculation of the linear-response tensor $\chi^{(0)}(\mathbf{q}, \mathbf{q}', \omega)$, the exchange-correlation matrix $P(\mathbf{q}, \mathbf{q}', \omega)$, and the subsequent inversion of the matrices $\Lambda^{-1}(\mathbf{q}, \mathbf{q}', \omega)$ and $\tilde{\epsilon}(\mathbf{q}, \mathbf{q}', \omega)$. This problem becomes much simpler in two limiting situations: in the case of simple metals with almost free conduction electrons, where the pseudopotential of the electron-ion interaction is relatively weak and the off-diagonal elements of the indicated matrices are correspondingly small, as well as in the case of dielectrics with weakly overlapping electron shells.

In this section we use the equations derived by us to estimate the electronic contribution to the dynamic lattice-vibration matrix in simple metals. On the one hand, this enables us to demonstrate that these equations, notwithstanding their complexity, can be used in actual calculations, and in this sense they are perfectly usable, and on the other hand the problem of calculating the electronic contribution to the lattice dynamics by a consistent account of the exchange-correlation effects is also of independent interest and has not been solved to this day.

The electronic contribution to the dynamic matrix of the lattice vibrations is described by the expression

$$D_e^{ab}(\mathbf{k}) = \frac{N_0}{M} \sum_{\mathbf{G}, \mathbf{G}'} (\mathbf{k} + \mathbf{G})^a V(\mathbf{k} + \mathbf{G}) \chi(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G}', 0) V(\mathbf{k} + \mathbf{G}') (\mathbf{k} + \mathbf{G}')^b \quad (3.1)$$

(for simplicity we consider the case of a monatomic crystal) where M is the ion mass, $V(\mathbf{q})$ is the Fourier component of the electron-ion pseudopotential, and $\chi(\mathbf{q}, \mathbf{q}', 0)$ is the matrix of the linear polarizability of the electrons in the static limit $\omega = 0$, and is given by

$$\chi(\mathbf{q}, \mathbf{q}', 0) = \sum_{\mathbf{q}''} \chi^{(0)}(\mathbf{q}, \mathbf{q}'', 0) \tilde{\epsilon}^{-1}(\mathbf{q}'', \mathbf{q}', 0). \quad (3.2)$$

We estimate the dynamic matrix (3.1) accurate to terms of third order in $V(\mathbf{q})$. To this end we rewrite first the matrices $\chi^{(0)}(\mathbf{q}, \mathbf{q}', 0)$ and $P(\mathbf{q}, \mathbf{q}', 0)$ and separate in them the small off-diagonal matrix elements

that are linear in $V(\mathbf{q})$:

$$\chi^{(0)}(\mathbf{q}, \mathbf{q}', 0) \approx \chi_0(\mathbf{q}) \delta_{\mathbf{q}\mathbf{q}'} + \chi_1(\mathbf{q}, \mathbf{q}') (1 - \delta_{\mathbf{q}\mathbf{q}'}), \quad (3.3)$$

$$P(\mathbf{q}, \mathbf{q}', 0) \approx P(\mathbf{q}) \delta_{\mathbf{q}\mathbf{q}'} + P_1(\mathbf{q}, \mathbf{q}') (1 - \delta_{\mathbf{q}\mathbf{q}'}). \quad (3.4)$$

Here $\chi_0(\mathbf{q})$ is the usual Lindhard function, which represents the static polarizability of a homogeneous non-interacting electron gas, and $P(\mathbf{q})$ is the correction for the local field and is given by (2.18) at $\omega = 0$. For the effective dielectric matrix $\tilde{\epsilon}(\mathbf{q}, \mathbf{q}', 0)$ in (3.2) we have approximately, in accordance with (2.13), (3.3), and (3.4),

$$\tilde{\epsilon}(\mathbf{q}, \mathbf{q}', 0) \approx \tilde{\epsilon}(\mathbf{q}) \delta_{\mathbf{q}\mathbf{q}'} - [v(\mathbf{q}) \chi_1(\mathbf{q}, \mathbf{q}') - P_1(\mathbf{q}, \mathbf{q}')] (1 - \delta_{\mathbf{q}\mathbf{q}'}), \quad (3.5)$$

where $\tilde{\epsilon}(\mathbf{q})$ is the effective dielectric function of a homogeneous interacting electron gas, for which the following equation holds

$$\tilde{\epsilon}(\mathbf{q}) = 1 - v(\mathbf{q}) \chi_0(\mathbf{q}) + P(\mathbf{q}). \quad (3.6)$$

For the approximate inversion of the matrix (3.5) we can use the matrix identity

$$(A+B)^{-1} = A^{-1} - A^{-1} B A^{-1} + A^{-1} B A^{-1} B A^{-1} - \dots$$

Accurate to terms of first order in the electron-ion pseudopotential, we then obtain

$$\tilde{\epsilon}^{-1}(\mathbf{q}, \mathbf{q}', 0) \approx \frac{\delta_{\mathbf{q}\mathbf{q}'}}{\tilde{\epsilon}(\mathbf{q})} + \frac{v(\mathbf{q}) \chi_1(\mathbf{q}, \mathbf{q}') - P_1(\mathbf{q}, \mathbf{q}')}{\tilde{\epsilon}(\mathbf{q}) \tilde{\epsilon}(\mathbf{q}')} (1 - \delta_{\mathbf{q}\mathbf{q}'}). \quad (3.7)$$

Substituting (3.3) and (3.7) in (3.2) we arrive at the following approximate expression for the linear electron-polarizability matrix

$$\chi(\mathbf{q}, \mathbf{q}', 0) \approx \frac{\chi_0(\mathbf{q})}{\tilde{\epsilon}(\mathbf{q})} \delta_{\mathbf{q}\mathbf{q}'} + \frac{1 - \delta_{\mathbf{q}\mathbf{q}'}}{\tilde{\epsilon}(\mathbf{q}) \tilde{\epsilon}(\mathbf{q}')} \{ [1 + P(\mathbf{q})] \chi_1(\mathbf{q}, \mathbf{q}') - \chi_0(\mathbf{q}) P_1(\mathbf{q}, \mathbf{q}') \}. \quad (3.8)$$

It remains now only to calculate the matrices $\chi_1(\mathbf{q}, \mathbf{q}')$ and $P_1(\mathbf{q}, \mathbf{q}')$ in the approximation linear in $V(\mathbf{q})$. At the indicated accuracy we have for the Bloch wave functions

$$\psi_\lambda(\mathbf{r}) \approx \frac{e^{i\mathbf{p}\mathbf{r}}}{\sqrt{\Omega}} \left[1 + N_0 \sum_{\mathbf{G} \neq \mathbf{0}} \frac{V(\mathbf{G}) e^{i\mathbf{G}\mathbf{r}}}{\tilde{\epsilon}(\mathbf{G}) (\epsilon_p - \epsilon_{\mathbf{p}+\mathbf{G}})} \right]. \quad (3.9)$$

The single-electron energies are $E_\lambda \approx \epsilon_p = \hbar^2 q^2 / 2m$, the corresponding occupation numbers are $n_\lambda \approx f(\epsilon_p)$, and the summation over λ in (2.6) and (2.11) reduces to summation over the wave vector \mathbf{p} in momentum space.

Substituting (3.9) in (2.6) we arrive after simple transformations to the following expression for the matrix $\chi_1(\mathbf{q}, \mathbf{q}')$:

$$\chi_1(\mathbf{q}, \mathbf{q}') = 2N_0 \frac{V(\mathbf{q} - \mathbf{q}') J^{(3)}(\mathbf{q}, \mathbf{q}')}{\tilde{\epsilon}(\mathbf{q} - \mathbf{q}')}. \quad (3.10)$$

Here $J^{(3)}(\mathbf{q}, \mathbf{q}')$ is the so-called "three-pole," the concrete expression for which is

$$J^{(3)}(\mathbf{q}, \mathbf{q}') = 2 \sum_{\mathbf{p}} f_p \left[\frac{1}{(\epsilon_p - \epsilon_{\mathbf{p}+\mathbf{q}}) (\epsilon_p - \epsilon_{\mathbf{p}+\mathbf{q}'})} + \frac{1}{(\epsilon_p - \epsilon_{\mathbf{p}+\mathbf{q}}) (\epsilon_p - \epsilon_{\mathbf{p}+\mathbf{q}-\mathbf{q}'})} + \frac{1}{(\epsilon_p - \epsilon_{\mathbf{p}+\mathbf{q}'} (\epsilon_p - \epsilon_{\mathbf{p}+\mathbf{q}-\mathbf{q}'}))} \right]. \quad (3.11)$$

To find the matrix $P_1(\mathbf{q}, \mathbf{q}')$ we substitute the approximate Bloch functions (3.9) in (2.11). Recognizing that in the case of a weak electron-ion pseudopotential we

have

$$\frac{1}{\Omega n(\mathbf{r})} \approx \frac{1}{N} - \frac{N_0}{N^2} \sum_{\mathbf{G}} \frac{\chi_0(\mathbf{G})}{\bar{\varepsilon}(\mathbf{G})} V(\mathbf{G}) e^{i\mathbf{G}\mathbf{r}},$$

we obtain after rather cumbersome but essentially straight-forward calculations

$$P_1(\mathbf{q}, \mathbf{q}') = -\frac{2N_0}{N} \frac{V(\mathbf{q}-\mathbf{q}')}{\bar{\varepsilon}(\mathbf{q}-\mathbf{q}')} \nu(\mathbf{q}) \chi_0(\mathbf{q}') \chi_0(\mathbf{q}-\mathbf{q}') \times \left[Q(\mathbf{q}, \mathbf{q}') + \frac{\mathbf{q}\mathbf{q}'}{2q'^2} G'(\mathbf{q}', 0) + \frac{\mathbf{q}(\mathbf{q}-\mathbf{q}')}{2|\mathbf{q}-\mathbf{q}'|^2} G(\mathbf{q}-\mathbf{q}', 0) \right]. \quad (3.12)$$

Here $G(\mathbf{q}, 0)$ is the static correction for the local field, defined by (2.19) in which we must put $\omega = 0$, while $Q(\mathbf{q}, \mathbf{q}')$ is given by

$$\chi_0(\mathbf{q}') \chi_0(\mathbf{q}-\mathbf{q}') Q(\mathbf{q}, \mathbf{q}') = 2 \sum_{\mathbf{p}\mathbf{p}'} \frac{\mathbf{q}(\mathbf{p}'-\mathbf{p})}{|\mathbf{p}'-\mathbf{p}|^2} \left[\frac{(f_{\mathbf{p}'}-f_{\mathbf{p}+\mathbf{q}'}) (f_{\mathbf{p}'}-f_{\mathbf{p}+\mathbf{q}-\mathbf{q}'})}{(\varepsilon_{\mathbf{p}'}-\varepsilon_{\mathbf{p}+\mathbf{q}'}) (\varepsilon_{\mathbf{p}'}-\varepsilon_{\mathbf{p}+\mathbf{q}-\mathbf{q}'})} + \frac{f_{\mathbf{p}'}-f_{\mathbf{p}+\mathbf{q}}}{\varepsilon_{\mathbf{p}'}-\varepsilon_{\mathbf{p}+\mathbf{q}}} \left(\frac{f_{\mathbf{p}}-f_{\mathbf{p}+\mathbf{q}'}}{\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}+\mathbf{q}'}} + \frac{f_{\mathbf{p}}-f_{\mathbf{p}+\mathbf{q}-\mathbf{q}'}}{\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}+\mathbf{q}-\mathbf{q}'}} \right) \right]. \quad (3.13)$$

Taking (3.1), (3.8), (3.10), and (3.12) into account, we arrive at the following expression for the electronic contribution to the dynamic lattice-vibration matrix of a metal with almost free conduction electrons:

$$D_e^{\alpha\beta}(\mathbf{k}) \approx \frac{N_0}{M} \sum_{\mathbf{G}} (\mathbf{k}+\mathbf{G})^\alpha (\mathbf{k}+\mathbf{G})^\beta \chi_0(\mathbf{k}+\mathbf{G}) \frac{V^2(\mathbf{k}+\mathbf{G})}{\bar{\varepsilon}(\mathbf{k}+\mathbf{G})} + \frac{2N_0^2}{M} \sum_{\mathbf{G}=\mathbf{G}'} (\mathbf{k}+\mathbf{G})^\alpha (\mathbf{k}+\mathbf{G}')^\beta J^{(3)}(\mathbf{k}+\mathbf{G}, \mathbf{k}+\mathbf{G}') \times \frac{V(\mathbf{k}+\mathbf{G})}{\bar{\varepsilon}(\mathbf{k}+\mathbf{G})} \frac{V(\mathbf{G}-\mathbf{G}')}{\bar{\varepsilon}(\mathbf{G}-\mathbf{G}')} \frac{V(\mathbf{k}+\mathbf{G}')}{\bar{\varepsilon}(\mathbf{k}+\mathbf{G}')}. \quad (3.14)$$

$\bar{J}^{(3)}(\mathbf{q}, \mathbf{q}')$ denotes here the effective "three-pole" renormalized on account of the exchange-correlation effects:

$$J^{(3)}(\mathbf{q}, \mathbf{q}') = [1+P(\mathbf{q})] J^{(3)}(\mathbf{q}, \mathbf{q}') + \frac{1}{N} \nu(\mathbf{q}) \chi_0(\mathbf{q}) \times \chi_0(\mathbf{q}') \chi_0(\mathbf{q}-\mathbf{q}') \left[Q(\mathbf{q}, \mathbf{q}') + \frac{\mathbf{q}\mathbf{q}'}{2q'^2} G(\mathbf{q}', 0) + \frac{\mathbf{q}(\mathbf{q}-\mathbf{q}')}{2|\mathbf{q}-\mathbf{q}'|^2} G(\mathbf{q}-\mathbf{q}', 0) \right]. \quad (3.15)$$

The first term in (3.14) is of second order of smallness in the pseudopotential and describes the contribution of the free electrons to the paired inter-ion interaction. The second term is of third order in $V(\mathbf{q})$. It is usually referred to as the electron contribution, corresponding to unpaired three-particle interaction forces between the ions, to the lattice dynamics. As first shown by Brovman and Kagan,¹⁴ allowance for terms of this kind in the dynamic matrix is extremely important for a correct description of the entire lattice dynamics of simple metals. Even if we disregard the fact that in the polyvalent simple metals the contribution of the three-particle forces to the dynamics of the lattice turns out to be not small from the purely quantitative viewpoint, allowance for these forces is of fundamental importance in the analysis of the Cauchy relations for the elastic moduli, as well as for a consistent description of the static and the dynamic compressibility moduli even in the case of alkali metals.

To compare the expression obtained by us for the dynamic matrix with those already given in the literature, we rewrite first Eq. (3.14) and neglect in it all the exchange-correlation corrections:

$$D_e^{\alpha\beta}(\mathbf{k}) \approx \frac{N_0}{M} \sum_{\mathbf{G}} (\mathbf{k}+\mathbf{G})^\alpha (\mathbf{k}+\mathbf{G})^\beta \chi_0(\mathbf{k}+\mathbf{G}) \frac{V^2(\mathbf{k}+\mathbf{G})}{\varepsilon_0(\mathbf{k}+\mathbf{G})} + \frac{2N_0^2}{M} \sum_{\mathbf{G}=\mathbf{G}'} (\mathbf{k}+\mathbf{G})^\alpha (\mathbf{k}+\mathbf{G}')^\beta J^{(3)}(\mathbf{k}+\mathbf{G}, \mathbf{k}+\mathbf{G}') \times \frac{V(\mathbf{k}+\mathbf{G})}{\varepsilon_0(\mathbf{k}+\mathbf{G})} \frac{V(\mathbf{G}-\mathbf{G}')}{\varepsilon_0(\mathbf{G}-\mathbf{G}')} \frac{V(\mathbf{k}+\mathbf{G}')}{\varepsilon_0(\mathbf{k}+\mathbf{G}')}. \quad (3.16)$$

Here $\varepsilon_0(\mathbf{q})$ is the static dielectric function of the homogeneous electron gas in the random-phase approximation,

$$\varepsilon_0(\mathbf{q}) = 1 - \nu(\mathbf{q}) \chi_0(\mathbf{q}). \quad (3.17)$$

We note immediately that Eq. (3.16) for the dynamic matrix is not suitable for an exact description of the phonon spectra of a simple metal is played, besides the Coulomb repulsion between the ions, by their indirect attraction, quadratic in the pseudopotential, to one another via the conduction electrons. The corresponding electronic contribution to the dynamic matrix is represented by the first term of (3.16), and such an approximation for this term, with no account taken of the exchange-correlation effects, turns out to be too rough.^{15,16} Fortunately, these effects can be easily included in the contribution, quadratic in the pseudopotential, to the dynamic matrix. To this end it suffices only to replace in the first term in expression (3.16) for $D_e^{\alpha\beta}(\mathbf{k})$ the quantity $\chi_0(\mathbf{q})/\varepsilon_0(\mathbf{q})$ by the exact value of the polarizability of the homogeneous interacting electron gas

$$\gamma(\mathbf{q}) = \chi_0(\mathbf{q})/\bar{\varepsilon}(\mathbf{q}), \quad (3.18)$$

where the function $\bar{\varepsilon}(\mathbf{q})$ is defined by (3.6). Generally speaking, it is necessary here to use the exact value of $P(\mathbf{q})$. Since this is of course, unknown, in the actual calculations for $P(\mathbf{q})$ one used various approximate formulas, including Eq. (2.18) of Toigo and Woodruff.

As for the contribution made to the dynamic matrix by the terms of third order in $V(\mathbf{q})$, in most papers in which such a contribution was taken into account its calculation was carried out in the random-phase approximation, i.e., in accord with Eq. (3.16) (see the review¹⁵). In certain papers the function $\varepsilon_0(\mathbf{q})$ in the second term of (3.16), just as in the contribution quadratic in the $V(\mathbf{q})$, was simply replaced by $\bar{\varepsilon}(\mathbf{q})$. In a recent paper, Paasch and Heinrich¹⁷ have attempted to justify precisely such a procedure for taking into account exchange-correlation effects in the calculation of the contribution of three-particle forces to the lattice dynamics. However, as see from (3.14), such an approach is in fact not self-consistent. The influence of the exchange and correlation effects does not reduce nearly to replacement of $\varepsilon_0(\mathbf{q})$ by the effective dielectric function $\bar{\varepsilon}(\mathbf{q})$, but leads also to a renormalization of the three-pole.

As shown by Brovman and Kagan,¹⁴ and also by Pe-thick,¹⁸ the response functions in the expression for the electronic part of the dynamic matrix should satisfy definite sum rules that actually connect the nonlinear polarizabilities of the homogeneous electron gas with the derivatives of the linear polarizability (3.18) with respect to the density $n = N/\Omega$. In the notation of the present paper, the corresponding sum rule for

$\bar{J}^{(3)}(\mathbf{q}, \mathbf{q}')$ is written as follows:

$$\frac{J^{(3)}(0, \mathbf{q}')}{\varepsilon^2(\mathbf{q}')} = \frac{1}{2} \chi_0(0) \frac{d}{dn} \left[\frac{\chi_0(\mathbf{q}')}{\Omega \varepsilon(\mathbf{q}')} \right]. \quad (3.19)$$

In accord with (3.15), we represent the function $\bar{J}^{(3)}(0, \mathbf{q}')$ in the form

$$J^{(3)}(0, \mathbf{q}') = J^{(3)}(0, \mathbf{q}')^{-1/2} \chi_0(0) \chi_0^2(\mathbf{q}') \varphi(0, \mathbf{q}'), \quad (3.20)$$

where $\varphi(0, \mathbf{q}')$ denotes the quantity

$$\begin{aligned} \varphi(0, \mathbf{q}') = & -\frac{2}{N} \lim_{q \rightarrow 0} v(q) \left[Q(\mathbf{q}, \mathbf{q}') + \frac{q^2}{2q'} G(\mathbf{q}') \right] \\ & - \frac{2J^{(3)}(0, \mathbf{q}')}{\chi_0^2(\mathbf{q}')} \lim_{q \rightarrow 0} v(q) G(\mathbf{q}). \end{aligned} \quad (3.21)$$

Recognizing that the renormalized function $J^{(3)}(0, \mathbf{q}')$ satisfies¹⁴ a sum rule of the form

$$\frac{J^{(3)}(0, \mathbf{q}')}{\varepsilon_0^2(\mathbf{q}')} = \frac{1}{2} \chi_0(0) \frac{d}{dn} \left[\frac{\chi_0(\mathbf{q}')}{\Omega \varepsilon_0(\mathbf{q}')} \right], \quad (3.22)$$

where $\varepsilon_0(\mathbf{q})$ is given by (3.17), it can be shown that the quantity $\varphi(0, \mathbf{q}')$ should satisfy the following sum rule:

$$\varphi(0, \mathbf{q}') = \frac{1}{\Omega^2} \frac{d}{dn} [v(q') G(\mathbf{q}') \Omega]. \quad (3.23)$$

Using (3.13) and (2.29) we can verify by direct calculation that the function $\varphi(0, \mathbf{q}')$, defined by Eq. (3.21), actually satisfies the sum rule (3.23). Thus, the method proposed in the present paper for taking into account the exchange-correlation effects does not violate the sum rule for the nonlinear polarizabilities, and by the same token does not introduce additional errors in the calculations of the phonon spectra. On the other hand, as seen from (3.23), any approximation that takes into account exchange-correlation effects by introducing corrections for the local field $G(\mathbf{q})$ in the function $\bar{\varepsilon}(\mathbf{q})$, but ignores the renormalization of the effective three-pole (when $\varphi = 0$) certainly violates the sum rule (3.19). A similar conclusion that it is necessary to renormalize the three-pole on account of the exchange in correlation was recently arrived at by Zarochentsev and Teplov.¹⁹ They used in fact relation (3.23) to determine the renormalization of the three-pole by replacing the function $\varphi(\mathbf{q}, \mathbf{q}')$ at all \mathbf{q} by its value $\varphi(0, \mathbf{q}')$. As is clear from our present results, such a replacement is generally speaking not valid, since $\varphi(\mathbf{q}, \mathbf{q}')$ with nonzero wave vectors \mathbf{q} , in no way coincides with $\varphi(0, \mathbf{q}')$.

The renormalization of the three-pole may turn out to be significant in the analysis of the anomalies of phonon spectra. It is known¹⁵ that the singularities of the function $J^{(3)}(\mathbf{q}, \mathbf{q}')$ lead to the appearance of additional anomalies in the phonon spectra, which differ from the ordinary Kohn singularities. The latter are connected with the singularity of the effective dielectric function of $\bar{\varepsilon}(\mathbf{q})$ and appear already in the contribution of second order in the potential to the dynamic matrix. It is not excluded that correct allowance for the renormalization of the three-pole can substantially modify these additional anomalies in the phonon spectra. This question, however, calls for a special investigation.

Thus, from the fundamental point of view, the need for taking into account the renormalization of the three-pole is subject to no doubt. The question is:

what is the quantitative contribution of this renormalization? To answer this question we estimate first the unrenormalized function $J^{(3)}(0, \mathbf{q}')$. Using (3.22), we obtain

$$J^{(3)}(0, \mathbf{q}') = \frac{\Omega m^2}{2\pi^2 q'} \ln \left| \frac{q' + 2k_F}{q' - 2k_F} \right|. \quad (3.24)$$

Next, in the limit of small wave numbers, we have for the correction for the local field (2.19) (Ref. 6)

$$G(\mathbf{q}') \approx (q'/2k_F)^2. \quad (3.25)$$

Using (3.25), we obtain from the sum rule (3.23) the following estimate for $\varphi(0, \mathbf{q}')$:

$$\varphi(0, \mathbf{q}')|_{q' \rightarrow 0} \approx -\frac{2\pi e^2}{3nk_F^2 \Omega^2}. \quad (3.26)$$

Taking (3.24), (3.26), and (3.20) into account, we arrive at the following expression, valid at $q' \ll 2k_F$, for the total renormalized function $\bar{J}^{(3)}(0, \mathbf{q}')$:

$$J^{(3)}(0, \mathbf{q}') \approx \frac{\Omega m^2}{2\pi^2 k_F} (1 - \alpha). \quad (3.27)$$

Here α is the effective Coulomb-interaction constant,

$$\alpha = e^2 / \pi \hbar v_F, \quad (3.28)$$

which is precisely a measure of the renormalization of the three-pole. In simple metals, α ranges from 0.37 for tin to 0.83 for potassium. It is clear therefore that at small q' allowance for the renormalization of the three-pole is very important also from the quantitative viewpoint. If we use the estimate (3.25) for the correction for the local field also at large wave numbers ($q' > 2k_F$), then we obtain for the function $\bar{J}^{(3)}(0, \mathbf{q}')$

$$J^{(3)}(0, \mathbf{q}') \approx \frac{2\Omega m^2 k_F}{\pi^2 q'^2} \left[1 - \frac{\alpha}{2} \left(\frac{2k_F}{q'} \right)^2 \right]. \quad (3.29)$$

The second term in the square brackets, which characterizes the renormalization of the three-pole, turns out to be small in this case.

In the calculation of physical quantities, the function $\bar{J}^{(3)}(0, \mathbf{q}')$ appears only for a wave vectors \mathbf{q}' that coincide with one of the reciprocal-lattice vectors. It is clear therefore that allowance for its renormalization is particularly important for polyvalent metals, where there are reciprocal-lattice vectors smaller than $2k_F$.

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