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POLARIZABILITY OF A CRYSTAL WITH IMPURITIES*

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ABSTRACT

The expression for the complex frequency- and wavevector-dependent longitudinal electronic polarizability due to the presence of a weak static disorder (e.g. impurities) in a crystal with an arbitrary band structure is derived. The quantum kinetic equation in the self-consistent-field approximation is solved, expanding the one-particle density operator in powers of the screened static imperfection field and a weak perturbing electric field. The polarizability is determined by the induced electronic charge density quadratic in the imperfection field and linear in the perturbing field, averaged over the statistical distribution of imperfections. The obtained expression, which accounts properly for the collective effects in the electronic plasma, takes also into account the polar coupling of the plasma with longitudinal optical phonons. The conductivity in the optical limit ($\vec{q} \rightarrow 0$) is calculated, and the correspondence with one-band effective-mass approximation is established.

I. INTRODUCTION

For frequencies below the interband absorption edge the optical absorption in a crystal is predominantly given by the interaction of electrons with crystal imperfections (impurities, phonons). The calculation of the absorption thus requires the knowledge of the response function of the imperfect system. Below we shall consider the impurity-scattering contribution to the electronic polarizability.

In our previous paper [1] the expression for the high-frequency free-carrier polarizability (conductivity) due to the presence of static scatterers in a polar multivalley semiconductor was derived, and applied to lead chalcogenides [2], and also to zero-gap semiconductors [3]. The theory which accounted systematically for many-body, and in particular plasma effects, did not, however, allow to consider the details of the band structure. In particular it neglected the effects of the free-carrier band nonparabolicity and wave function mixing. It could also give only an approximate expression for the polarizability in zero gap semiconductors, not accounting exactly [3] for the influence of the interband (and also intraband) screening on impurity scattering. Until now, the exact account for the band structure on impurity-scattering was given only within one-electron approaches [e.g.4]. However, these approaches do not account for the dynamic screening of the scattering processes. Moreover, they totally neglect the collective absorption, which turned out to be of considerable importance in highly polar [2,5], as well as in zero-gap semiconductors [3,6].

In view of this, in the present paper we shall calculate the wavevector - and frequency- dependent polarizability due to the presence of a static disorder in a crystal with an arbitrary band structure. We account systematically for the electron-electron interaction and in particular for the plasma effects, as well as polar electron-phonon coupling. We use the kinetic equation approach, appropriately generalized as compared with the one developed in [1]. The self-consistent-field (SCF) kinetic-equation is solved expanding the one-particle density operator in powers of the weak screened imperfection field and a weak perturbing electric field. The corresponding induced charge densities are then calculated.

The unperturbed one-electron system is described in terms of Bloch functions and energies (including spin-orbit interaction), instead of the plane-wave representation used in the previous approach [1]. The complex longitudinal polarizability is determined by the charge density which is quadratic in the imperfection field and linear in the perturbing field, averaged over the statistical distribution of the imperfections. The expression for the polarizability is valid for all temperatures.

As we are especially interested in semiconductor applications, when deriving the expression for the polarizability we shall refer to semiconductor and impurities. However, the derivation presented below is valid in an arbitrary crystal with a weak static (charged or neutral) disorder.

In Sec. II the kinetic equation is solved and induced charge densities are determined. In Sec. III the polarizability is obtained, while in Sec. IV its dynamic ($\vec{q} \rightarrow 0$) form is established.

II. GENERAL FORMULATION

Let us consider a highly doped n-type^{*)} semiconductor of the volume V (subject to the periodic boundary conditions) consisting of N electrons of charge e ($e < 0$) and (free) mass m , originating from both the host-crystal and impurity atoms. The crystal is in contact with a heat bath of temperature T . The absence of an external constant magnetic field is assumed.

As the unperturbed system we shall consider the one consisting of N non-interacting electrons, each of them described by the Hamiltonian

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + eU(\vec{r}) + \frac{e\hbar}{2im^2c^2} \vec{\sigma} \cdot [\nabla U(\vec{r}) \times \hat{p}], \quad (1)$$

where \hat{p} and \hat{r} are the momentum and the position operators, respectively. The last term denotes the usual spin-orbit interaction, and $U(\vec{r})$ is the periodic potential given by

^{*)} The essentially analogous reasoning applies to p-type materials.

$$U(\vec{r}) = U_h(\vec{r}) + U_H(\vec{r}) + U_i \quad (2)$$

Here $U_h(\vec{r})$ is the potential due to the ideal (host) crystal nuclei, while $U_H(\vec{r})$ is the Hartree self-consistent potential due to all other $N-1$ electrons. U_i is the potential due to the positive uniform background with the charge density equal $N_i|e|/V$, where N_i is the number of excess electrons (as compared with the ideal host crystal) due to doping. We note that in the considered highly doped materials these electrons occupy the states in the conduction band (free-carrier plasma). The Hartree potential U_H is given by

$$U_H(\vec{r}) = \frac{e(N-1)}{NV} \int_V d^3r' \frac{1}{|\vec{r}-\vec{r}'|} \sum_{n\vec{k}} f_{n\vec{k}} |\psi_{n\vec{k}}(\vec{r}')|^2, \quad (3)$$

where $\psi_{n\vec{k}}(\vec{r}) = \langle n\vec{k} | \vec{r} \rangle$ represent the Bloch states satisfying the equation

$$H_0 |n\vec{k}\rangle = E_{n\vec{k}} |n\vec{k}\rangle \quad (4)$$

with \vec{k} belonging to the first Brillouin zone, and $f_{n\vec{k}} = [\exp\{E_{n\vec{k}} - \mu\}/k_0 T + 1]^{-1}$ are the Fermi-Dirac occupation functions which satisfy the condition $\sum_{n\vec{k}} f_{n\vec{k}} = N$. Hereafter the Bloch functions and energies, as well as sums over the band index contain a hidden spin variable running over two values. We observe that our Bloch energies $E_{n\vec{k}}$ differ from the usual one-electron energies by the constant term U_i .

There are two perturbations applied to the system. The first is the weak static field due to imperfections (placed on the uniform background with the charge density $-N_i|e|/V$) screened by all electrons and the lattice. We assume that the positions of the imperfections obey some statistical distribution (e.g. randomly distributed impurities) which gives the averaged bare (and screened) imperfection electric field vector equal to zero. The second perturbation is a weak probing electric field which (in $\vec{q} \rightarrow 0$ limit) can be caused e.g. by external radiation.

The electronic polarizability of the impured system can be inferred

from the induced charge density linear in probing field and, in the lowest order, bilinear in the imperfection field. A knowledge of the appropriate charge density linear in the imperfection field is insufficient as its average over the statistical distribution of imperfections vanishes.

The one-particle density operator $\hat{\rho}$ in the SCF approximation satisfies the following kinetic equation (comp. [7])

$$i\hbar \partial \hat{\rho}(t) / \partial t = [\hat{H}(t), \hat{\rho}(t)], \quad (5)$$

where the square bracket denotes the commutator. Here $H(t)$ is the one-electron Hamiltonian which can be written as

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t), \quad (6)$$

where \hat{H}_0 is given by (1), while

$$\hat{H}_1(t) = e\varphi(\vec{r}, t). \quad (7)$$

Here $\varphi(\vec{r}, t)$ is the total self-consistent potential of the field acting on a single electron. This field consists of the external perturbing fields and the self-consistent (i.e. averaged with the non-equilibrium^{*} part $\hat{\rho} - \hat{\rho}^{(0)}$, see Eq.(9) of the density operator ρ we look for) field produced by all other electrons and by the lattice. In the absence of the external perturbations we have $\varphi(\vec{r}, t) = 0$ which corresponds to the non-interacting particles.

In the presence of the weak probing and the imperfection fields the total self consistent potential can be written as (compare [1])

$$\varphi(\vec{r}, t) = \varphi^{(a)}(\vec{r}, t) + \varphi^{(b)}(\vec{r}) + \varphi^{(c)}(\vec{r}) + \varphi^{(e, b)}(\vec{r}, t) + \varphi^{(e, b^*)}(\vec{r}, t), \quad (8)$$

* The average with the equilibrium part $\hat{\rho}^{(0)}$, results in the potential $V_H(\vec{r})$ which was included in H_0 .

where $\varphi^{(e)}$ is the self-consistent potential of the linear-response theory due to the presence of probing field in the absence of imperfections. $\varphi^{(\delta)} + \varphi^{(\delta^2)}$ is the self-consistent (screened) potential due to the presence of imperfections in the absence of probing field; φ^δ is the potential of the linear response theory, while $\varphi^{(\delta^2)}$ is the correction bilinear in $\varphi^{(\delta)}$. The potentials $\varphi^{(e,\delta)}$ and $\varphi^{(e,\delta^2)}$ are responsible for the interaction of the probing field with imperfections (via electrons) and they are assumed to be of the order of $\varphi^{(\delta)}\varphi^{(e)}$ and $\varphi^{(\delta)}\varphi^{(\delta)}\varphi^{(e)}$, respectively.

According to the expansion of the potentials, we shall look for the solution of the kinetic equation in the form

$$\hat{G}(t) = \hat{G}^{(0)} + \hat{G}^{(e)}(t) + \hat{G}^{(\delta)} + \hat{G}^{(\delta^2)} + \hat{G}^{(e,\delta)}(t) + \hat{G}^{(e,\delta^2)}(t), \quad (9)$$

where $\hat{\rho}^{(0)}$ is the equilibrium density operator given by

$$\hat{G}^{(0)} = \frac{1}{N} \sum_{n\vec{k}} f_{n\vec{k}} |n\vec{k}\rangle \langle n\vec{k}|, \quad (10)$$

while the remaining operators correspond to the potentials defined by the indices, and are assumed to be of the order of the appropriate potentials.

Inserting the expansions (8) and (9) into the kinetic equation (5) we preserve only terms up to bilinear in $\varphi^{(\delta)}$ and linear in $\varphi^{(e)}$. We take the matrix elements of the equation between the states $\langle n'\vec{k} + \vec{q}|$ and $|n\vec{k}\rangle$ and integrate it with the initial condition $\hat{\rho}(t = -\infty) = \hat{\rho}^{(0)}$. The solution is then separated into the appropriate orders, and when Fourier transformed, results in

$$\langle n'\vec{k} + \vec{q} | \hat{G}^{(e)}(\omega) | n\vec{k} \rangle = K_{n\vec{k}}^{n'\vec{k} + \vec{q}}(\omega) \varphi^{(e)}(\vec{q}, \omega), \quad (11)$$

$$\begin{aligned} \langle n'\vec{k} + \vec{q} | \hat{G}^{(\delta)}(\omega) | n\vec{k} \rangle &= K_{n\vec{k}}^{n'\vec{k} + \vec{q}}(\omega) \varphi^{(\delta)}(\vec{q}) \delta(\omega) \\ &\equiv \langle n'\vec{k} + \vec{q} | \hat{G}^\delta | n\vec{k} \rangle \delta(\omega), \end{aligned} \quad (12)$$

$$\langle n'\vec{k} + \vec{q} | \hat{G}^{(\delta^2)}(\omega) | n\vec{k} \rangle = K_{n\vec{k}}^{n'\vec{k} + \vec{q}}(\omega) \varphi^{(\delta^2)}(\vec{q}, \omega) + \langle n'\vec{k} + \vec{q} | \hat{G}^{(e)}(\omega) | n\vec{k} \rangle \quad (13)$$

for $(\cdot) = (\delta^2), (e, \delta), (e, \delta^2)$, where we have denoted

$$K_{n\vec{k}}^{n'\vec{k} + \vec{q}}(\omega) = \frac{e}{V^2} \frac{f_{n\vec{k}} - f_{n'\vec{k} + \vec{q}}}{\hbar\omega + E_{n\vec{k}} - E_{n'\vec{k} + \vec{q}} + i\eta} \langle n'\vec{k} + \vec{q} | n\vec{k} \rangle, \quad (14)$$

$$\langle n'\vec{k} + \vec{q} | \hat{G}^{(e,\delta)}(\omega) | n\vec{k} \rangle = \frac{1}{V} \sum_{m\vec{q}'} \chi_{nn'm}(\vec{k}, \vec{k} + \vec{q}, \vec{q}', 0, 0) \varphi^{(e)}(\vec{q}') \varphi^{(\delta)}(\vec{q} - \vec{q}') \delta(\omega), \quad (15)$$

$$\langle n'\vec{k} + \vec{q} | \hat{G}^{(e,\delta^2)}(\omega) | n\vec{k} \rangle = \frac{1}{V} \sum_{m\vec{q}'} \tilde{\chi}_{nn'm}(\vec{k}, \vec{k} + \vec{q}, \vec{q}', \omega, 0) \varphi^{(e)}(\vec{q}') \varphi^{(\delta^2)}(\vec{q} - \vec{q}', \omega), \quad (16)$$

$$\begin{aligned} \langle n'\vec{k} + \vec{q} | \hat{G}^{(e,\delta^2)}(\omega) | n\vec{k} \rangle &= \frac{1}{V} \sum_{m\vec{q}'} \tilde{\chi}_{nn'm}(\vec{k}, \vec{k} + \vec{q}, \vec{q}', \omega, 0) \varphi^{(e)}(\vec{q}') \varphi^{(\delta^2)}(\vec{q} - \vec{q}', \omega) \\ &+ \frac{e}{V^2} \frac{1}{\hbar\omega + E_{n\vec{k}} - E_{n'\vec{k} + \vec{q}} + i\eta} \sum_{m\vec{q}'} \sum_{m'\vec{q}''} \left[\langle n'\vec{k} + \vec{q} | m'\vec{k} + \vec{q}'' - \vec{q}' \rangle \tilde{\chi}_{nn'm'}(\vec{k}, \vec{k} + \vec{q} - \vec{q}', \vec{q}'', \omega, \omega) \right. \\ &- \left. (m'\vec{k} + \vec{q}'' | n\vec{k}) \tilde{\chi}_{nn'm'}(\vec{k} + \vec{q}', \vec{k} + \vec{q}, \vec{q}'', \omega, \omega) \right] \varphi^{(e)}(\vec{q}'', \omega) \varphi^{(\delta)}(\vec{q} - \vec{q}' - \vec{q}'') \varphi^{(\delta^2)}(\vec{q}') \\ &+ \frac{1}{V} \sum_{m\vec{q}'} \tilde{\chi}_{nn'm'}(\vec{k}, \vec{k} + \vec{q}, \vec{q}', \omega, \omega) \varphi^{(e)}(\vec{q}', \omega) \varphi^{(\delta^2)}(\vec{q} - \vec{q}') + \\ &+ \frac{e}{V^2} \frac{1}{\hbar\omega + E_{n\vec{k}} - E_{n'\vec{k} + \vec{q}} + i\eta} \sum_{m\vec{q}'} \sum_{m'\vec{q}''} \left[\langle n'\vec{k} + \vec{q} | m'\vec{k} + \vec{q}'' - \vec{q}' \rangle \chi_{nn'm}(\vec{k}, \vec{k} + \vec{q} - \vec{q}', \vec{q}'', 0, 0) \right. \\ &- \left. (m'\vec{k} + \vec{q}'' | n\vec{k}) \chi_{nn'm}(\vec{k} + \vec{q}', \vec{k} + \vec{q}, \vec{q}'', 0, 0) \right] \varphi^{(e)}(\vec{q}'', \omega) \varphi^{(\delta)}(\vec{q} - \vec{q}' - \vec{q}'') \varphi^{(\delta^2)}(\vec{q}') \end{aligned} \quad (17)$$

Here

$$\langle n' \vec{k}' + \vec{q} | n \vec{k} \rangle = \langle n' \vec{k}' + \vec{q}' | e^{i \vec{q}' \cdot \vec{r}} | n \vec{k}' \rangle, \quad (18)$$

$$\begin{aligned} \chi_{nm}(\vec{k}, \vec{k} + \vec{q}, \vec{q}', \omega, \omega') &= \frac{e}{i\omega + E_{n\vec{k}} - E_{m\vec{k} + \vec{q}} + i\eta} \\ &\times \left[K_{n\vec{k}}^{m\vec{k} + \vec{q}'}(\omega)(n' \vec{k}' + \vec{q}' | m \vec{k} + \vec{q}') - K_{n' \vec{k}' + \vec{q}'}^{m \vec{k} + \vec{q}}(\omega, \omega')(m \vec{k} + \vec{q}' | n \vec{k}') \right], \quad (19) \end{aligned}$$

$$\tilde{\chi}_{nm}(\vec{k}, \vec{k} + \vec{q}, \vec{q}', \omega, \omega') = \chi_{nm}(\vec{k}, \vec{k} + \vec{q}, \vec{q}', \omega, \omega') + \chi_{nm}(\vec{k}, \vec{k} + \vec{q}, \vec{q}' - \vec{q}, \omega, \omega'), \quad (20)$$

and $\eta \rightarrow 0^+$. Arriving at Eqs.(13) and (15)-(17) we inserted the expressions for the obtained lower order matrix elements. Thus, the matrix elements of all orders are expressed in terms of the potentials of the same or lower order. In the above formulas the Fourier components of the potentials $\varphi(\vec{q} + \vec{k}_m, \omega)$ with $\vec{k}_m \neq 0$ have been neglected, \vec{k}_m is the reciprocal lattice vector. This corresponds to the neglect of local field corrections (see e.g. [8]) which is justified in the case of perturbations varying slowly on a distance of a unit cell (see [9]).

The induced charge densities can be calculated from the formula

$$S(\vec{r}, t) = eN \text{Tr} \left\{ \hat{g}(t) \delta(\vec{r} - \vec{r}') \right\}. \quad (21)$$

This leads to

$$S^{(e)}(\vec{q}, \omega) = -q^2 \alpha(\vec{q}, \omega)^0 \varphi^{(e)}(\vec{q}, \omega), \quad (22)$$

$$S^{(i)}(\vec{q}, \omega) = -q^2 \alpha(\vec{q}, \omega)^0 \varphi^{(i)}(\vec{q}, \omega), \quad (23)$$

$$S^{(e)}(\vec{q}, \omega) = -q^2 \alpha(\vec{q}, \omega)^0 \varphi^{(e)}(\vec{q}, \omega) + I^{(e)}(\vec{q}, \omega) \quad (24)$$

for $(.) = (\delta^2), (e, \delta), (e, \delta^2)$, where

$$\alpha(\vec{q}, \omega)^0 = \frac{e^2}{q^2 \epsilon} \sum_{n, n'} \sum_{\vec{k}} | \langle n' \vec{k}' + \vec{q}' | n \vec{k} \rangle |^2 \frac{f_{n' \vec{k}' + \vec{q}'} - f_{n \vec{k}}}{i\omega + E_{n \vec{k}} - E_{n' \vec{k}' + \vec{q}'} + i\eta} \quad (25)$$

is the Ehrenreich-Cohen[7] polarizability, $\alpha(\vec{q})^0 = \alpha(\vec{q}, 0)^0$, and

$$I^{(e)}(\vec{q}, \omega) = Ne \sum_{n, n'} \sum_{\vec{k}} \langle n' \vec{k}' + \vec{q}' | \mathcal{E}^{(e)}(\omega) | n \vec{k} \rangle \langle n \vec{k} | n' \vec{k}' + \vec{q}' \rangle \quad (26)$$

which shall be referred to as scattering densities.

In order to determine the induced charge densities completely, the potentials $\varphi^{(\delta^2)}, \varphi^{(e, \delta)}$ and $\varphi^{(e, \delta^2)}$ have to be expressed in terms of the linear-response potentials $\varphi^{(e)}$ and $\varphi^{(i)}$. This can be done with the use of the Poisson equation

$$\varphi(\vec{q}, \omega) = (4\pi/q^2) \left[S(\vec{q}, \omega) + S_{\text{ext}}(\vec{q}, \omega) \right] \quad (27)$$

which closes the self-consistent scheme. Here φ is given by Eq.(8), ρ_{ext} represents the external charge densities, while ρ is the full induced charge density consisting of electronic and (rigid) ionic contributions

$$S(\vec{q}, \omega) = \sum_{(\kappa)} S^{(\kappa)}(\vec{q}, \omega) = q^2 \alpha_{\text{ion}}(\vec{q}, \omega) \varphi(\vec{q}, \omega), \quad (28)$$

where $\alpha_{\text{ion}}(\vec{q}, \omega)$ is the ionic lattice polarizability, which can be assumed in the form $\alpha_{\text{ion}}(\vec{q}, \omega) = \frac{F \omega_{\text{TO}}^2}{\omega^2 - \omega_{\text{TO}}^2}$ [10].

The Poisson equation can now be separated into the appropriate orders. The external charge densities enter the equations for $\varphi^{(i)}$ and $\varphi^{(e)}$, while for the higher-order fields we obtain

$$\varphi^{(e)}(\vec{q}, \omega) = \frac{4\pi}{q^2 \epsilon(\vec{q}, \omega)^0} I^{(e)}(\vec{q}, \omega) \quad (29)$$

for $(.) = (\delta^2), (e, \delta), (e, \delta^2)$, where

$$\varepsilon(\vec{q}, \omega) = 1 + 4\pi\alpha_{\text{ion}}(\vec{q}, \omega) + 4\pi\alpha(\vec{q}, \omega) \quad (30)$$

is the longitudinal dielectric function of the system in the absence of imperfections.

Due to the formula (29) all the induced charge densities (24) can now be expressed by the lowest order potentials $\varphi^{(e)}$ and $\varphi^{(\delta)}$.

The scattering charge densities (26), entering the formula (24), can now be written as

$$P^{(\delta^2)}(\vec{q}) = \frac{1}{V} \sum_{\vec{q}'} \alpha(\vec{q}, \omega, \vec{q}', 0) \varphi^{(\delta)}(\vec{q}') \varphi^{(\delta)}(\vec{q} - \vec{q}'), \quad (31)$$

$$P^{(e, \delta)}(\vec{q}, \omega) = \frac{1}{V} \sum_{\vec{q}'} \tilde{\alpha}(\vec{q}, \omega, \vec{q}', 0) \varphi^{(\delta)}(\vec{q}') \varphi^{(e)}(\vec{q} - \vec{q}', \omega), \quad (32)$$

$$P^{(e, \delta^2)}(\vec{q}, \omega) = P^{(e, \delta^2), 1}(\vec{q}, \omega) + P^{(e, \delta^2), 2}(\vec{q}, \omega) \quad (33)$$

with

$$P^{(e, \delta^2), 1}(\vec{q}, \omega) = \frac{1}{V} \sum_{\vec{q}', \vec{q}''} \left\{ \frac{4\pi}{(\vec{q} - \vec{q}')^2 \varepsilon(\vec{q} - \vec{q}', \omega)} \tilde{\alpha}(\vec{q}, \omega, \vec{q}', 0) \tilde{\alpha}(\vec{q} - \vec{q}', \omega, \vec{q}'', \omega) + \tilde{\alpha}(\vec{q}, \omega, \vec{q}', 0, \vec{q}'', \omega) \right\} \varphi^{(\delta)}(\vec{q}') \varphi^{(\delta)}(\vec{q} - \vec{q}' - \vec{q}'') \varphi^{(e)}(\vec{q}'', \omega), \quad (34)$$

$$P^{(e, \delta^2), 2}(\vec{q}, \omega) = \frac{1}{V} \sum_{\vec{q}', \vec{q}''} \left\{ \frac{4\pi}{(\vec{q} - \vec{q}'')^2 \varepsilon(\vec{q} - \vec{q}'', 0)} \tilde{\alpha}(\vec{q}, \omega, \vec{q}', \omega) \tilde{\alpha}(\vec{q} - \vec{q}'', 0, \vec{q}'', 0) + \varphi(\vec{q}, \omega, \vec{q}'', \omega, \vec{q}', 0) \right\} \varphi^{(\delta)}(\vec{q}') \varphi^{(\delta)}(\vec{q} - \vec{q}' - \vec{q}'') \varphi^{(e)}(\vec{q}'', \omega). \quad (35)$$

Here

$$\tilde{\alpha}(\vec{q}, \omega, \vec{q}', \omega) = N e \sum_{n, n'} \sum_{m, m'} \langle \tilde{\alpha}_{n, n', m, m'}(\vec{q}, \omega, \vec{q}', \omega, \omega) \rangle \cdot n^i (n' \cdot \vec{q}), \quad (36)$$

$$\tilde{\varphi}(\vec{q}, \omega, \vec{q}', \omega', \vec{q}'', \omega'') = N e \sum_{n, n', m, m'} \langle \tilde{\varphi}_{n, n', m, m'}(\vec{q}, \omega, \vec{q}', \omega', \vec{q}'', \omega'') \rangle \times \left\{ (n^i \vec{q} + m^i \vec{q} - \vec{q}') \tilde{\gamma}_{n, n', m, m'}(\vec{q}, \vec{q}' - \vec{q}'', \vec{q}'', \omega - \omega', \omega'') - (m^i \vec{q}' + n^i \vec{q}) \tilde{\gamma}_{m, n', m', m'}(\vec{q}, \vec{q}' + \vec{q}'', \vec{q}'', \omega - \omega', \omega'') \right\}, \quad (37)$$

while $\alpha(\vec{q}, \omega, \vec{q}', \omega')$ and $\varphi(\vec{q}, \omega, \vec{q}', \omega', \vec{q}'', \omega'')$ are given by (36) and (37), respectively, with tildas dropped in $\tilde{\gamma}$ at the right-hand sides.

III. POLARIZABILITY

The longitudinal polarizability $\alpha(\vec{q}, \omega)$ of the system is defined by the following relation between averaged total potential and full induced charge density

$$\langle \varphi(\vec{q}, \omega) \rangle_{\delta} = -q^2 \alpha(\vec{q}, \omega) \langle \varphi(\vec{q}, \omega) \rangle_{\delta}. \quad (38)$$

The average, denoted by $\langle \dots \rangle_{\delta}$, is taken over the positions of static imperfections. We assume that the following relations are satisfied:

$$\langle \varphi^{(\delta)}(\vec{q}) \rangle_{\delta} = 0, \quad (39)$$

$$\langle \varphi^{(\delta)}(\vec{q}) \varphi^{(\delta)}(\vec{q}') \rangle_{\delta} = V \delta_{\vec{q}, -\vec{q}'} \langle \varphi^{(\delta)}(\vec{q}) \varphi^{(\delta)}(\vec{q}') \rangle_{\vec{q}}. \quad (40)$$

The second of them assumes a translationally invariant statistical distribution of imperfections, and $\langle \varphi^{(\delta)}(\vec{q}) \varphi^{(\delta)}(\vec{q}') \rangle_{\vec{q}}$ is the spectral density of the fluctuation of the potential $\varphi^{(\delta)}$. These relations hold, e.g. for randomly distributed ionized impurities placed on the compensating background, when we have

$$\langle \varphi^{(\delta)}(\vec{q}) \varphi^{(\delta)}(\vec{q}') \rangle_{\vec{q}} = \frac{4\pi N^2}{V q^4 \varepsilon^2(\vec{q})} \left[1 - \delta_{\vec{q}, \vec{q}'} \right] \left[\sum_{n, n'} \frac{1}{\varepsilon(\vec{q}, \omega)} \right] \langle \varphi^{(\delta)}(\vec{q}) \varphi^{(\delta)}(\vec{q}') \rangle_{\vec{q}}, \quad (41)$$

where N_i is the number of the impurities of charge e_s in the volume V . We observe that formula (41) accounts only for the Coulomb field due to the ionized impurities. In principle, the potential $\phi^\delta(\vec{r})$ includes also a short range part due to the difference between the impurity and host crystal core potentials. However, this rapidly varying (on the distance of a unit cell) part of the potential cannot be properly treated within our approach unless the local field effects, neglected for simplicity in our treatment, are included in the theory.

Averaging Eq.(28) we get: $\langle P^{(e,\delta)} \rangle_\delta = 0$ and thus $\langle \varphi^{(e,\delta)} \rangle_\delta = 0$ and $\langle \rho^{(e,\delta)} \rangle_\delta = 0$, also $\langle P^{(e^2)} \rangle_\delta = \langle \rho^{(\delta^2)} \rangle_\delta = 0$ and $\langle \varphi^{(\delta^2)} \rangle_\delta = 0$. Averaging $\rho^{(e,\delta^2)}$ we obtain

$$\langle P^{(e,\delta^2)}(\vec{q},\omega) \rangle_\delta = -q^2 \alpha(\vec{q},\omega)^\delta \varphi^{(e)}(\vec{q},\omega), \quad (42)$$

where

$$\alpha(\vec{q},\omega)^\delta = -\frac{1}{Vq^2} \sum_{\vec{q}'} \left\{ \frac{4\pi \tilde{\alpha}(\vec{q},\omega,\vec{q}',0) \tilde{\alpha}(\vec{q}-\vec{q}',\omega,\vec{q},\omega)}{(\vec{q}-\vec{q}')^2 \epsilon(\vec{q}-\vec{q}',\omega)^\delta} + \tilde{\varphi}(\vec{q},\omega,\vec{q},0,\vec{q},\omega) + \varphi(\vec{q},\omega,\vec{q},\vec{q},0) \right\} / \varphi^{(\delta)} / \varphi^{(\delta)} / -\vec{q}'. \quad (43)$$

Here we observed that when averaged, the first term in (35) vanishes as it is proportional to $\varphi^{(\delta^2)}$.

The average of the Eq. (28) can thus be written as

$$\langle \rho(\vec{q},\omega) \rangle_\delta = -q^2 \left[\alpha_{ion}(\vec{q},\omega) + \alpha(\vec{q},\omega)^\delta \right] \times \left[\varphi^{(e)}(\vec{q},\omega) + \varphi^{(e,\delta^2)}(\vec{q},\omega) \right] + O(\delta^4). \quad (44)$$

Comparing this equation with (38) we obtain the full polarizability of the system up to the lowest non-vanishing order in the imperfection field

$$\alpha(\vec{q},\omega) = \alpha_{ion}(\vec{q},\omega) + \alpha(\vec{q},\omega)^0 + \alpha(\vec{q},\omega)^\delta, \quad (45)$$

where $\alpha^\delta(\vec{q},\omega)$ and $\alpha(\vec{q},\omega)^0$ are given by Eqs. (43) and (25) respectively. The formula (43) represents our principle result for the wavevector- and frequency-dependent electronic polarizability of a crystal with a static disorder. The result accounts systematically for electron-electron interaction and is valid for arbitrary temperatures.

IV. DYNAMICAL LIMIT

Let us now consider the dynamical polarizability $\alpha(\omega)^\delta = \lim_{\vec{q} \rightarrow 0} \alpha(\vec{q},\omega)^\delta$ which is useful for the interpretation of the optical data.

For $\vec{q} \rightarrow 0$ both of the $\tilde{\alpha}$ functions entering (43) are at least of the order of \vec{q} , and thus expansion of $\tilde{\alpha}$ functions in (43) up to terms linear in \vec{q} is sufficient. With the use of the identities

$$(n\vec{k}' | n'\vec{k} + \vec{q}) (E_{n\vec{k}+\vec{q}} - E_{n\vec{k}'}) = \frac{\hbar}{m} \vec{q} \cdot (n\vec{k}' | \hat{P} + \hbar\vec{k}' + \hbar\vec{q} / 2 | n'\vec{k} + \vec{q}), \quad (44)$$

$$(n-\vec{k}' | n'-\vec{k}' - \vec{q}) = (n'\vec{k}' + \vec{q} | n\vec{k}'), \quad (45)$$

$$(n-\vec{k}' | \hat{P} | n'-\vec{k}' - \vec{q}) = - (n'\vec{k}' + \vec{q} | \hat{P} | n\vec{k}'), \quad (46)$$

where

$$\hat{P} = \hat{p} + \frac{\hbar e^2}{4\pi m c^2} [\vec{\sigma} \times \nabla(T(\vec{r}))] \quad (47)$$

we obtain, up to terms linear in \vec{q}

$$\tilde{\alpha}(\vec{q},\omega,\vec{q}',0) = \frac{e^3}{m\omega V} \vec{q} \cdot \sum_{n,n'} \sum_{\vec{k},\vec{k}'} (n\vec{k}' | \hat{P} + \hbar\vec{k}' | n\vec{k}') (n'\vec{k}' | m\vec{k}' + \vec{q}') (m\vec{k}' + \vec{q}' | n\vec{k}') \times \left\{ \frac{1}{\hbar\omega + E_{n\vec{k}'} - E_{n\vec{k}'} + i\eta} \left[\frac{f_{m\vec{k}'} - f_{n\vec{k}'}}{E_{m\vec{k}'} - E_{n\vec{k}'} + i\eta} - \frac{f_{n\vec{k}'} - f_{m\vec{k}'} + \vec{q}'}{\hbar\omega + E_{n\vec{k}'} - E_{m\vec{k}'} + i\eta} \right] + \frac{1}{\hbar\omega + E_{n\vec{k}'} - E_{n\vec{k}'} + i\eta} \left[\frac{f_{n\vec{k}'} - f_{m\vec{k}'} + \vec{q}'}{E_{n\vec{k}'} - E_{m\vec{k}'} + i\eta} - \frac{f_{m\vec{k}'} - f_{n\vec{k}'}}{\hbar\omega + E_{m\vec{k}'} - E_{n\vec{k}'} + i\eta} \right] \right\}, \quad (48)$$

$$\tilde{\alpha}(\vec{q}-\vec{q}', \omega, \vec{q}, \omega) = \frac{e^3}{m\omega V} \vec{q} \cdot \sum_{n'n} \sum_{\vec{k}} (n\vec{k} | \hat{P} + \hbar\vec{k} | n'\vec{k}') (n'\vec{k}' | m\vec{k} + \vec{q}' | m\vec{k} + \vec{q} | n\vec{k}) \times \left\{ \frac{1}{\hbar\omega + E_{n\vec{k}} - E_{n'\vec{k}'} + i\eta} \left[\frac{f_{m\vec{k}+\vec{q}'} - f_{n'\vec{k}'}}{E_{m\vec{k}+\vec{q}'} - E_{n'\vec{k}'} - i\eta} - \frac{f_{n\vec{k}} - f_{m\vec{k}+\vec{q}}}{\hbar\omega + E_{n\vec{k}} - E_{m\vec{k}+\vec{q}} + i\eta} \right] + \frac{1}{\hbar\omega + E_{n'\vec{k}'} - E_{n\vec{k}} + i\eta} \left[\frac{f_{n\vec{k}} + f_{m\vec{k}+\vec{q}}}{E_{n'\vec{k}'} - E_{m\vec{k}+\vec{q}} - i\eta} - \frac{f_{m\vec{k}+\vec{q}'} - f_{n'\vec{k}'}}{\hbar\omega + E_{m\vec{k}+\vec{q}'} - E_{n'\vec{k}'}} + i\eta} \right] \right\}. \quad (49)$$

Up to the required q^2 -accuracy, for $\vec{\varphi} + \varphi$ entering (43), we get after a tedious calculation:

$$\hat{\varphi}(\vec{q}, \omega, \vec{q}', \omega', \vec{q}, \omega) + \varphi(\vec{q}, \omega, \vec{q}, \omega, \vec{q}', \omega') = \frac{e^4}{\sqrt{m^2 \omega^2}} \sum_{n'n'mm'} \sum_{\vec{k}} \vec{q} \cdot (n\vec{k} | \hat{P} + \hbar\vec{k} | n'\vec{k}') \times \left\{ \frac{(n'\vec{k}' | m\vec{k} - \vec{q}') [\vec{q} \cdot (m\vec{k} - \vec{q}') \hat{P} + \hbar\vec{k} \cdot \hbar\vec{q}' | m\vec{k} - \vec{q}' | n\vec{k}]}{\hbar\omega + E_{n'\vec{k}'} - E_{m\vec{k} - \vec{q}'} + i\eta} \left[\frac{f_{n\vec{k}} - f_{m\vec{k} - \vec{q}'}}{E_{n'\vec{k}'} - E_{m\vec{k} - \vec{q}'} + i\eta} - \frac{f_{n\vec{k}} - f_{m\vec{k} - \vec{q}'}}{\hbar\omega + E_{n\vec{k}} - E_{m\vec{k} - \vec{q}'} + i\eta} \right] - \frac{(n'\vec{k}' | m\vec{k} - \vec{q}') (m\vec{k} - \vec{q}' | m\vec{k}') [\vec{q} \cdot (m\vec{k}') \hat{P} + \hbar\vec{k}' | n\vec{k}]}{\hbar\omega + E_{n'\vec{k}'} - E_{m\vec{k}'} + i\eta} \left[\frac{f_{m\vec{k}'} - f_{m\vec{k} - \vec{q}'}}{E_{n'\vec{k}'} - E_{m\vec{k} - \vec{q}'} + i\eta} - \frac{f_{n\vec{k}} - f_{m\vec{k} - \vec{q}'}}{\hbar\omega + E_{n\vec{k}} - E_{m\vec{k} - \vec{q}'} + i\eta} \right] - \frac{[\vec{q} \cdot (n'\vec{k}') \hat{P} + \hbar\vec{k}' | m\vec{k}]}{\hbar\omega + E_{n\vec{k}} - E_{n'\vec{k}'} + i\eta} \left[\frac{f_{m\vec{k} + \vec{q}'} - f_{n'\vec{k}'}}{E_{m\vec{k} + \vec{q}'} - E_{n'\vec{k}'} + i\eta} - \frac{f_{m\vec{k} + \vec{q}'} - f_{n'\vec{k}'}}{\hbar\omega + E_{m\vec{k} + \vec{q}'} - E_{n'\vec{k}'}} + i\eta} \right] + \frac{(n'\vec{k}' | m\vec{k} + \vec{q}') [\vec{q} \cdot (m\vec{k} + \vec{q}') \hat{P} + \hbar\vec{k}' | m\vec{k} + \vec{q}' | n\vec{k}]}{\hbar\omega + E_{n'\vec{k}'} + E_{m\vec{k} + \vec{q}'} - E_{n\vec{k}} + i\eta} \left[\frac{f_{m\vec{k} + \vec{q}'} - f_{n'\vec{k}'}}{E_{m\vec{k} + \vec{q}'} - E_{n'\vec{k}'} + i\eta} - \frac{f_{m\vec{k} + \vec{q}'} - f_{n'\vec{k}'}}{\hbar\omega + E_{m\vec{k} + \vec{q}'} - E_{n'\vec{k}'}} + i\eta} \right] \right\} + \frac{e^4}{\sqrt{m^2 \omega^2}} \sum_{n'n'mm'} \sum_{\vec{k}} \vec{q} \cdot (n\vec{k} | \hat{P} + \hbar\vec{k} | n'\vec{k}') \times \left\{ \frac{[\vec{q} \cdot (n'\vec{k}') \hat{P} + \hbar\vec{k}' | n\vec{k}]}{E_{n'\vec{k}'} - E_{n\vec{k}} + i\eta} \left[\frac{f_{n\vec{k}} - f_{m\vec{k} + \vec{q}'}}{\hbar\omega + E_{n\vec{k}} - E_{m\vec{k} + \vec{q}'} + i\eta} - \frac{f_{m\vec{k} + \vec{q}'} - f_{n'\vec{k}'}}{\hbar\omega + E_{m\vec{k} + \vec{q}'} - E_{n'\vec{k}'}} + i\eta} \right] + \frac{(n'\vec{k}' | m\vec{k} - \vec{q}') (m\vec{k} - \vec{q}' | m\vec{k}') [\vec{q} \cdot (m\vec{k}') \hat{P} + \hbar\vec{k}' | n\vec{k}]}{E_{m\vec{k} - \vec{q}'} - E_{n'\vec{k}'} + i\eta} \left[\frac{f_{m\vec{k} - \vec{q}'}}{\hbar\omega + E_{m\vec{k} - \vec{q}'} - E_{n'\vec{k}'}} + i\eta} - \frac{f_{m\vec{k} - \vec{q}'}}{\hbar\omega + E_{m\vec{k} - \vec{q}'}} - E_{n'\vec{k}'} + i\eta} \right] \right\}. \quad (50)$$

In this expression we have dropped the terms of the form $\{F(\vec{q}') - F(-\vec{q}')\}$ which do not contribute to the polarizability if the relation $\langle \varphi^{(\delta)} | \varphi^{(\delta)} \rangle_{-\vec{q}'} = \langle \varphi^{(\delta)} | \varphi^{(\delta)} \rangle_{\vec{q}'}$, assumed here, is satisfied.

The expressions (48)-(50) when inserted into (43) give the required dynamical polarizability $\alpha(\omega)^\delta$, which in general depends on the direction of the wavevector \hat{q} . For cubic crystals $\alpha(\omega)^\delta$ is, however, independent of \hat{q} .

The obtained expression for $\alpha(\omega)^\delta$ is still very complicated, and its use for any particular band structure requires a special and careful treatment.

Here we shall consider $\alpha(\omega)^\delta$ in the simplest one (n-th)-band approximation, in which we obtain

$$\tilde{\alpha}(\vec{q}, \omega, \vec{q}', 0)_{1b} = \tilde{\alpha}(\vec{q}, \vec{q}', \omega, \vec{q}', \omega)_{1b} = \frac{e^4}{\hbar^2 \omega^2 V} \vec{q} \cdot \sum_{\vec{k}} |(n\vec{k} | n\vec{k} + \vec{q}')|^2 \left[\frac{\partial E_{n\vec{k}}}{\partial \vec{k}} - \frac{\partial E_{n\vec{k}'}}{\partial \vec{k}'} \right]_{\vec{k}, \vec{q}'} \times \left\{ \frac{f_{n\vec{k} + \vec{q}'} - f_{n\vec{k}}}{\hbar\omega + E_{n\vec{k}} - E_{n\vec{k} + \vec{q}'} + i\eta} - \frac{f_{n\vec{k} + \vec{q}'} - f_{n\vec{k}}}{E_{n\vec{k}} - E_{n\vec{k} + \vec{q}'} + i\eta} \right\}, \quad (51)$$

$$\hat{\varphi}(\vec{q}, \omega, \vec{q}', 0, \vec{q}, \omega) + \varphi(\vec{q}, \omega, \vec{q}, \omega, \vec{q}', 0)_{1b} = -\frac{e^4}{\hbar^2 \omega^2 V} q_i q_j \sum_{\vec{k}} |(n\vec{k} | n\vec{k} + \vec{q}')|^2 \left[\frac{\partial E_{n\vec{k}}}{\partial k_i} - \frac{\partial E_{n\vec{k}'}}{\partial k_i'} \right]_{\vec{k}, \vec{q}'} \left[\frac{\partial E_{n\vec{k}}}{\partial k_j} - \frac{\partial E_{n\vec{k}'}}{\partial k_j'} \right]_{\vec{k}, \vec{q}'} \times \left\{ \frac{f_{n\vec{k} + \vec{q}'} - f_{n\vec{k}}}{\hbar\omega + E_{n\vec{k}} - E_{n\vec{k} + \vec{q}'} + i\eta} - \frac{f_{n\vec{k} + \vec{q}'} - f_{n\vec{k}}}{E_{n\vec{k}} - E_{n\vec{k} + \vec{q}'} + i\eta} \right\}. \quad (52)$$

These formulas when inserted into (45) and applied to the conduction band (n=c) supply the expression for free-carrier polarizability on n-type doped semiconductor. The expression accounts for the non polarizability of the conduction band and its true wave functions. For $\hbar\omega \ll E_g$, when E_g

is the energy gap, the considered free-carrier polarizability can be shown to represent, within a good accuracy, the total electronic polarizability $\alpha(\omega)^d$ due to the impurity scattering.

Let us finally establish the effective-mass approximation (for the parabolic band) in expressions (51) and (52), in the case of the multivalley semiconductor considered in [1]. If the sum over \vec{k} is divided (due to differences of the occupation functions) into sums over wavevectors \vec{k}^i measured from the a -th minimum of conduction band, and we then put

$$\frac{\partial E_{c\vec{k}}}{\partial \vec{k}} = \hbar^2 \frac{\langle \vec{v} \rangle}{m_a} \cdot \vec{k}^i$$

and

$$|\langle c\vec{k}^i | c\vec{k}^i + \vec{q} \rangle|^2 \approx 1$$

we arrive at the expression which is in complete agreement with the result obtained in [1].

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