Electromagnetic response of electrons in narrow-band-gap semiconductors with an energy-dependent relaxation time

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The effective conductivity tensor which includes the effects of both conduction and diffusion of carriers in electromagnetic fields is derived for charge carriers in narrow-band-gap semiconductors in the presence of an external magnetic field. The derivation uses an extension of the density-matrix formulation of Greene, Lee, Quinn, and Rodriquez to include the effects of the nonparabolicity of the energy-band structure and the possible energy dependence of the relaxation time. The resulting formulation is shown to be both gauge invariant and charge conserving. It is also shown that our theoretical expression reduces to those of other workers in the limits of either parabolic energy bands or a constant relaxation time.

I. INTRODUCTION

In a paper published in 1969, Greene $et \ al.^1$ developed a gauge-invariant formulation of the electromagnetic response of an electron gas with particular reference to the study of transport phenomena in metals. Using a density-matrix treatment in which the effects of collisions and a strong uniform magnetic field were considered, they calculated the current and charge densities of the electron gas to first order in the perturbing electromagnetic field. Moreover, their treatment also included the effect of the collision-drag current caused by moving impurities.

In this paper, we present a gauge-invariant formulation of the electromagnetic response of electrons in solids, taking into account the nonparabolicity of the energy bands and the possible energy dependence of the relaxation time. It is to be noted that this extension of the results of Greene et al. is of particular relevance to transport phenomena in narrow-band-gap semiconductors, especially in the presence of strong magnetic fields. Indeed, one of the most thoroughly investigated consequences of the strong coupling of the energy bands present in such semiconductors is that the effective mass of the electron is no longer constant, but increases with the applied magnetic field. Now because the transport properties in general depend on the density of states, which in turn is a function of the electronic effective mass, the transport properties themselves will also be affected by the strong coupling of the bands.

This extension also takes cognizance of the fact that many of the important interactions involving electrons in semiconductors depend on energy and cannot be represented by a constant relaxation time. Typical examples of interactions which are represented by an energy-dependent relaxation time include acoustic and optical deformation-potential scattering, piezoelectric scattering, and ionized-impurity scattering. Furthermore, since the interactions, in general, depend on various fundamental properties of both the electronic system and the system which interacts with it, their inclusion allows one to study the effect of these characteristic parameters on not only the electronic but also the other system as well. A rather important illustration of this occurs in the study of ultrasonic attenuation in semiconductors where the electron and phonon systems interact primarily through the piezoelectric or deformation-potential coupling mechanisms. Here, as is well known,² one finds that the absorption coefficient of the ultrasound and the change in the sound velocity of the material depend critically on the effective conductivity tensor of the electron system, which in turn is a function of the scattering mechanism via the energy-dependent relaxation time. Moreover, as we limit ourselves to semiconductors where piezoelectric coupling or deformation-potential coupling are the dominant modes of the electronphonon interaction, we can ignore the collisiondrag effect in our formulation.

To accomplish this extension, we use the twoband model of Lax³ to account for the nonparabolicity of the energy bands. This model which is derived from the Schrödinger equation of an electron in a solid is particularly appropriate to narrow-band-gap semiconductors. For in such a semiconductor, one reasonably expects those energy bands that are closely separated in energy to be strongly coupled and thus play a more significant role than the bands that are widely separated.

The effect of the energy-dependent relaxation time is included via a generalization of the usual relaxation-time ansatz. Specifically, we replace the single term of $(\rho - \rho_s)/\tau$ in the collision term with the anticommutator of $\rho - \rho_s$ and $1/\tau$. Al-

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though this replacement is strictly valid for the case of a constant relaxation time, we also assume its validity for the case of an energy-dependent relaxation time. While this form of the collision term was arrived at essentially by appealing to the correspondence principle, we should mention that the extensive calculations of Argyres⁴ and the somewhat later one of Arora and Peterson⁵ indicate that this assumption is indeed valid.

In Sec. II, we solve the quantum Liouville equation to first order in the self-consistent electromagnetic field. With this solution, we then calculate the induced current and charge densities in Sec. III. In addition, we demonstrate that the electromagnetic response of the electron system is both charge conserving and gauge invariant. We then specialize and compare our results for the longitudinal effective-conductivity tensor with those derived in other papers in various limits. Finally, it should be noted that whereas in the main we have used the same conventions and notations as were employed by Greene et al., our treatment does differ in that we have utilized a different phase convention for the spatial and time variations; i.e., we have assumed that all such variations are of the form $\exp[i(\mathbf{q} \cdot \mathbf{r} - \omega t)]$.

II. SOLUTION OF THE QUANTUM LIOUVILLE EQUATION

We begin our analysis by introducing the quantum Liouville equation which includes the effects of the nonparabolicity, the electromagnetic field, and collisions on the electron system:

$$\frac{\partial \rho}{\partial t} + \frac{i}{\hbar} [H, \rho] = \left(\frac{\partial \rho}{\partial t}\right)_c.$$
(2.1)

Here *H* is the two-band Hamiltonian of the electron, which can be expressed succinctly in terms of the 2×2 unit matrix *I*, the Pauli spin matrices σ_x , σ_y , σ_z , and the two-band matrix elements $\bar{\pi}_{mn}$ as

$$H = \left[\frac{1}{2m}\left(\vec{\mathbf{p}} + \frac{e}{c}\vec{\mathbf{A}}\right)^2 - e\phi\right]I + \frac{\vec{\pi}_{12}}{m}\cdot\left(\vec{\mathbf{p}} + \frac{e}{c}\vec{\mathbf{A}}\right)\sigma_+ + \frac{\vec{\pi}_{21}}{m}\cdot\left(\vec{\mathbf{p}} + \frac{e}{c}\vec{\mathbf{A}}\right)\sigma_- + \frac{E_g\sigma_g}{2}, \qquad (2.2)$$

where

$$\sigma_{\star} = \frac{1}{2} (\sigma_{\star} + i\sigma_{y}) , \qquad (2.3)$$

$$\sigma_{-} = \frac{1}{2} (\sigma_{x} - i\sigma_{y}) , \qquad (2.4)$$

and

$$\bar{\pi}_{mn} = \frac{(2\pi)^3}{\Omega_0} \int u_{m0}^* \bar{p} u_{n0} d\bar{r}$$
(2.5)

for m, n = 1, 2. Here $\bar{\pi}_{mn}$ are the two-band matrix elements of the momentum operator \bar{p} in the

Bloch-function basis evaluated at $\vec{k} = 0$. In the above equations, we have introduced the freeelectron mass m, the energy gap $E_{\mathfrak{g}}$, and the volume of the unit cell Ω_0 . Also, we note that the vector and scalar potentials $\vec{A}(\vec{r},t)$ and $\phi(\vec{r},t)$, respectively, determine the electromagnetic fields \vec{E} and \vec{B} via the relations

$$\vec{\mathbf{E}} = -\nabla \phi - \frac{1}{c} \frac{\partial \vec{\mathbf{A}}}{\partial t}$$
 and $\vec{\mathbf{B}} = \nabla \times \vec{\mathbf{A}}$

As we have previously mentioned, we assume that the collision term $(\partial \rho / \partial t)_c$ in Eq. (2.1) can be expressed in the form

$$\left(\frac{\partial\rho}{\partial t}\right)_{c} = -\frac{1}{2} \left[(\rho - \rho_{s}), \frac{1}{\tau(H)} \right]_{*}, \qquad (2.6)$$

where $\rho_s(H)$ is the Fermi-Dirac distribution, $\tau(H)$ is the energy-dependent relaxation time, and $[,]_{*}$ is the anticommutator bracket.

We commence the analysis of the quantum Liouville equation by noting that for our purposes it is sufficient to consider the linear response of the system to the electromagnetic field $[\vec{A}(\vec{r},t), \phi(\vec{r},t)]$. Accordingly, we rewrite H as $H = H_0 + H_1$ and seek a solution of the form $\rho = \rho_s(H) + \rho_1$ such that $\rho_s(H) = \rho_{s0} + \rho_{s1}$, where the subscript denotes the corresponding order of the term in the electromagnetic field. Moreover, we assume all firstorder quantities to vary as $\exp[i(\vec{q} \cdot \vec{r} - \omega t)]$.

If we substitute the above decompositions for H, ρ , and ρ_s in the quantum Liouville equation and retain terms of first order in H, we obtain

$$\langle \nu \left| \rho \right| \nu' \rangle = \rho_{\nu} \, \delta_{\nu\nu'} + \frac{i\hbar}{\tau_{\nu'\nu}} \frac{\langle \nu \left| \rho_{s1} \right| \nu' \rangle}{E_{\nu}' - E_{\nu} + \hbar\omega + i\hbar/\tau_{\nu\nu'}} + \frac{(\rho_{\nu}' - \rho_{\nu}) \langle \nu \left| H_{1} \right| \nu' \rangle}{E_{\nu}' - E_{\nu} + \hbar\omega + i\hbar/\tau_{\nu\nu'}},$$

$$(2.7)$$

where we have used the eigenstates of H_0 , which satisfy the H_1 equation:

$$H_0 | \nu \rangle = E_{\nu} | \nu \rangle . \tag{2.8}$$

In addition, we have defined the average relaxation time in the final and intial states as

$$\frac{1}{\tau_{\nu'\nu}} = \frac{1}{2} \left(\frac{1}{\tau_{\nu}} + \frac{1}{\tau_{\nu'}} \right), \qquad (2.9)$$

and for simplicity, have denoted the matrix elements of the equilibrium density operator $\rho_{s0}(E_{\nu})$ as ρ_{ν} . From Eq. (2.7) we see that to completely characterize the response of the electron system to the perturbation H_1 , we only need to substitute the known expressions for H_1 and ρ_{s1} . To find H_1 , we simply expand Eq. (2.2) to first order in the electromagnetic field. Expanding Eq. (2.2) we find the following explicit expressions for H_0 and H_1 :

$$H_{0} = \frac{1}{2m} \left(\vec{\mathbf{p}} + \frac{e}{c} \vec{\mathbf{A}}_{0} \right)^{2} I + \frac{\vec{\pi}_{12}}{m} \cdot \left(\vec{\mathbf{p}} + \frac{e}{c} \vec{\mathbf{A}}_{0} \right) \sigma_{\star} + \frac{\vec{\pi}_{21}}{m} \cdot \left(\vec{\mathbf{p}} + \frac{e}{c} \vec{\mathbf{A}}_{0} \right) \sigma_{\star} + \frac{E_{g}}{2} \sigma_{z} , \qquad (2.10)$$

$$H_{1} = \frac{1}{2} \left[\vec{\nabla}_{TB}, \frac{e}{c} \vec{A}_{1} I \right]_{+} - e \phi I$$
$$= \frac{e}{c} \vec{\nabla}(\vec{q}) \cdot \vec{A}_{10} e^{-i\omega t} - e \phi_{1} I , \qquad (2.11)$$

where

$$\vec{\mathbf{v}}_{TB} = \frac{1}{m} \left(\vec{\mathbf{p}} + \frac{e}{c} \vec{\mathbf{A}}_0 \right) I + \frac{\vec{\pi}_{12}}{m} \sigma_+ + \frac{\vec{\pi}_{21}}{m} \sigma_-$$
 (2.12)

and

$$\vec{\mathbf{V}}(\vec{\mathbf{q}}) = \frac{1}{2} [\vec{\mathbf{v}}_{\mathrm{TB}}, e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}} I].$$
(2.13)

Similarly, to determine ρ_{s0} and ρ_{s1} we use the expression for $\rho_s(H)$, which we write

$$\rho_s(H) = (1 + e^{\beta (H - \mu)})^{-1}, \qquad (2.14)$$

where $\beta = 1/k_B T$ and $\mu = \mu(\mathbf{\tilde{r}}, t)$ is the chemical potential. Expanding and retaining only first-order terms, we obtain the following matrix expression for $\rho_s(H)$:

$$\left\langle \nu \left| \rho_{s}(H) \right| \nu' \right\rangle = \rho_{\nu} \delta_{\nu\nu'} + \frac{\rho_{\nu} - \rho_{\nu}}{E_{\nu'} - E_{\nu}} \left\langle \nu \left| H_{1} - \mu_{1} \right| \nu' \right\rangle. \quad (2.15)$$

With this expression, we can relate ρ to H_1 and μ_1 :

$$\langle \nu \mid \rho \mid \nu' \rangle = \rho_{\nu} \delta_{\nu'\nu} + \frac{i\hbar}{\tau_{\nu'\nu}} \frac{\rho_{\nu} - \rho_{\nu}}{E_{\nu} - E_{\nu}} \frac{\langle \nu \mid H_{1} - \mu_{1} \mid \nu' \rangle}{E_{\nu} - E_{\nu} + \hbar\omega + i\hbar/\tau_{\nu'\nu}} + \frac{(\rho_{\nu} - \rho_{\nu}) \langle \nu \mid H_{1} \mid \nu' \rangle}{E_{\nu} - E_{\nu} + \hbar\omega + i\hbar/\tau_{\nu'\nu}}.$$

$$(2.16)$$

We obtain a more compact expression for $\langle \nu | \rho | \nu' \rangle$, if the notation of Greene *et al.* is modified to include an energy-dependent τ , i.e.,

$$\langle \nu \left| \rho \right| \nu' \rangle = \rho_{\nu} \delta_{\nu\nu} + \Lambda_{\nu\nu} \langle \nu \left| H_{1} - \mu_{1} \right| \nu' \rangle$$
$$+ \Lambda_{\nu\nu}^{1} \langle \nu \left| \mu_{1} \right| \nu' \rangle , \qquad (2.17)$$

where

$$\Lambda_{\nu\nu} = \frac{-i\omega\,\tau_{\nu\,\nu}}{1 - i\omega\,\tau_{\nu\,\nu}}\,\Lambda_{\nu\nu}^{1} + \frac{1}{1 - i\omega\,\tau_{\nu\,\nu}}\,\Lambda_{\nu\nu}^{2} \,, \qquad (2.18)$$

$$\Lambda^{1}_{\nu\nu} = \frac{\rho_{\nu} - \rho_{\nu}}{E_{\nu} - E_{\nu} + \hbar\omega + i\hbar/\tau_{\nu\nu}}, \qquad (2.19)$$

and

$$\Lambda_{\nu\nu}^{2} = \frac{\rho_{\nu} - \rho_{\nu}}{E_{\nu} - E_{\nu}}.$$
 (2.20)

Finally, to express the nonequilibrium density matrix ρ solely in terms of the perturbing electromagnetic potentials A_1 and ϕ_1 , we make use of the fact that the collision mechanism conserves the number of particles. Thus we must require the

$$\operatorname{Tr}\left[\delta(\mathbf{\vec{r}}-\mathbf{\vec{r}}_{0})I\left(\frac{\partial\rho}{\partial t}\right)_{c}\right]=0.$$
(2.21)

Using our expression for the collision term and the following representation of the Dirac δ function:

$$\delta(\mathbf{\tilde{r}} - \mathbf{\tilde{r}}_0) = V^{-1} \sum_{\mathbf{\tilde{q}}} e^{-i\mathbf{\tilde{q}} \cdot (\mathbf{\tilde{r}} - \mathbf{\tilde{r}}_0)} , \qquad (2.22)$$

we find that

$$\mu_{1}(\vec{\mathbf{q}},\omega) = \frac{1}{G} \sum_{\nu} \sum_{\nu'} \frac{\Lambda_{\nu'\nu}^{1}}{\tau_{\nu'\nu}} \langle \nu' \left| e^{-i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}} \right| \nu \rangle \left(\frac{e}{c} \langle \nu \left| \vec{\nabla}(\vec{\mathbf{q}}) \right| \nu' \rangle \vec{\mathbf{A}}_{1}(\vec{\mathbf{q}},\omega) - e \langle \nu \left| e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}} \right| \nu' \rangle \phi_{1}(\vec{\mathbf{q}},\omega) \right) \frac{\hbar\omega}{E_{\nu'} - E_{\nu}},$$
(2.23)

where

$$G = \sum_{\nu, \prime} \sum_{\nu} \frac{\Lambda_{\nu, \prime\nu}}{\tau_{\nu, \prime\nu}} |\langle \nu | e^{-i\bar{\mathfrak{q}}\cdot\vec{r}} | \nu \rangle|^2 \left(\frac{\hbar\omega}{E_{\nu, \prime} - E_{\nu}} + 1\right).$$
(2.24)

It is apparent that Eqs. (2.11), (2.17), and (2.23) allow us to relate the matrix elements of ρ to the electromagnetic potentials $\vec{A}_1(\vec{r}, t)$ and $\phi_1(\vec{r}, t)$. Moreover, we note that although we have only determined ρ in the linear response regime, it is also clear that because the Hamiltonian of the system incorporates the effects of the electromagnetic field via \vec{A}_1 and ϕ_1 , the fact that ρ = $\rho(A_1, \phi_1)$, will also persist for the nonlinear response. On the other hand, it is axiomatic in quantum theory that all measurable (observable) quantities must be gauge invariant under a transformation of the electromagnetic potentials. Consequently, since the measured quantities are computed using $\rho = \rho(\vec{A}_1, \phi_1)$, we deduce that the Hamiltonian cannot be arbitrary, but must be constrained to satisfy certain restrictions in any consistent formalism.

III. CURRENT AND CHARGE DENSITIES

With the expression for ρ given by equation, we can now evaluate the current density at the point $\dot{\mathbf{r}}_{o}$,

$$\mathbf{J}(\mathbf{\tilde{r}}_{0},t) = \mathbf{Tr}\left\{-\frac{1}{2}e\left[\mathbf{\tilde{v}},\delta(\mathbf{\tilde{r}}-\mathbf{\tilde{r}}_{0})I\right]_{+}\rho\right\},\tag{3.1}$$

to first order in the field, where

$$\vec{\mathbf{v}} = \vec{\mathbf{v}}_{\mathrm{TB}} + (e/mc)\vec{\mathbf{A}}_{\mathrm{I}}I.$$
(3.2)

Upon substituting the expression for $\langle \nu | H_1 | \nu' \rangle$, we see that $\mathbf{J}(\mathbf{q}, \omega)$, the Fourier transform of $\mathbf{J}(\mathbf{r}_0, t)$, can be written in the form

$$\vec{\mathbf{J}}(\vec{\mathbf{q}} \ \omega) = \frac{\omega_{\rho}^{2}}{4\pi c} \left(-\vec{\mathbf{A}}_{1}(\vec{\mathbf{q}}, \omega) - \vec{\mathbf{M}} \cdot \vec{\mathbf{A}}_{1}(\vec{\mathbf{q}}, \omega) + \vec{\mathbf{K}}\phi(\vec{\mathbf{q}}, \omega) + \frac{1}{e} (\vec{\mathbf{K}} - \vec{\mathbf{K}}_{1}) \ \mu_{1}(\vec{\mathbf{q}}, \omega) \right),$$
(3.3)

where

$$\vec{\mathbf{M}} = \frac{2m}{N} \sum_{\boldsymbol{\nu}\boldsymbol{\nu'}} \Lambda_{\boldsymbol{\nu'}\boldsymbol{\nu}} \langle \boldsymbol{\nu} \mid \vec{\nabla}(\vec{\mathbf{q}}) \mid \boldsymbol{\nu'} \rangle^* \langle \boldsymbol{\nu} \mid \vec{\nabla}(\vec{\mathbf{q}}) \mid \boldsymbol{\nu'} \rangle ,$$

$$(3.4)$$

$$\vec{\mathbf{K}} = \frac{2mc}{N} \sum_{\boldsymbol{\lambda}} \Lambda_{\boldsymbol{\nu'}\boldsymbol{\nu}} \langle \boldsymbol{\nu} \mid \vec{\nabla}(\vec{\mathbf{q}}) \mid \boldsymbol{\nu'} \rangle^* \langle \boldsymbol{\nu} \mid e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}} \mid \boldsymbol{\nu'} \rangle ,$$

$$\vec{\mathbf{K}}_{1} = \frac{2mc}{N} \sum_{\nu\nu'} \Lambda_{\nu'\nu'} \langle \nu | \mathbf{V}(\mathbf{q}) | \nu' \rangle^{*} \langle \nu | e^{i\mathbf{q}\cdot\mathbf{\vec{r}}} | \nu' \rangle ,$$
(3.6)

and

 $\omega_{p}^{2} = (4\pi e^{2}/m)(N/V)$.

We next consider the charge density at the point \vec{r}_0 :

$$\rho(\mathbf{\bar{r}}_{0},t) = -e \operatorname{Tr}\left[\delta(\mathbf{\bar{r}} - \mathbf{\bar{r}}_{0})I\rho\right].$$
(3.7)

Following the same procedure used in determining the current density, we obtain

$$\rho(\mathbf{\vec{q}},\omega) = \frac{\omega_p^2}{4\pi c} \left(-\left[\vec{\mathbf{K}}_1' - (\vec{\mathbf{K}}' - \vec{\mathbf{K}}_1') \right] \vec{\mathbf{A}}_1(\mathbf{\vec{q}},\omega) + L \phi_1(\mathbf{\vec{q}},\omega) + \frac{1}{e} (L - L_1) \mu_1(\mathbf{\vec{q}},\omega) \right).$$
(3.8)

Here the primed \vec{K} 's, \vec{K}' and \vec{K}_{l}' , are derived from the corresponding unprimed \vec{K} 's by carrying out the following operations: (a) write \vec{K} and $\vec{K} = \vec{f}(\omega + i\tau_{\nu}^{-1}{}_{\nu})$; (b) define an operator T which replaces $\omega + i\tau_{\nu}^{-1}{}_{\nu}$ in \vec{K} by $\omega - i\tau_{\nu}^{-1}{}_{\nu}$; (c) define an operator C which takes the complex conjugate of the result in (b). Thus, we have

$$\vec{\mathbf{K}}' = C(T(\vec{\mathbf{K}}))$$

$$= \frac{2mc}{N} \sum_{\nu} \sum_{\nu'} \Lambda_{\nu'\nu}^{*} (\omega - i\tau_{\nu'\nu}^{-1})$$

$$\times \langle \nu | e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}} | \nu' \rangle \langle \nu | \vec{\nabla}(\vec{\mathbf{q}}) | \nu' \rangle, \quad (3.9)$$

$$=\frac{2mc}{N}\sum_{\nu}\sum_{\nu^{\star}}\Lambda_{\nu^{\star}\nu}^{1*}\left(\omega-i\tau_{\nu^{\star}\nu}^{1}\right)$$

 $\vec{K}_1' = C(T(\vec{K}_1'))$

$$\times \langle \nu | e^{i\vec{q}\cdot\vec{r}} | \nu' \rangle \langle \nu | V(\vec{q}) | \nu' \rangle , \quad (3.10)$$

$$L = \frac{2mc^2}{N} \sum_{\nu} \sum_{\nu'} \Lambda_{\nu'\nu} \left| \left\langle \nu' \right| e^{-i\vec{q}\cdot\vec{r}} \left| \nu \right\rangle \right|^2, \quad (3.11)$$

and

$$L_{1} = \frac{2mc^{2}}{N} \sum_{\nu} \sum_{\nu'} \Lambda_{\nu'\nu}^{1} \left| \left\langle \nu' \right| e^{-i\vec{\mathfrak{q}}\cdot\vec{\mathfrak{r}}} \left| \nu \right\rangle \right|^{2}. \quad (3.12)$$

Upon examination of the expressions for the current density $\hat{J}(\vec{q}, \omega)$ and the charge density $\rho(\vec{q}, \omega)$, in accordance with our previous remarks, we observe that they are not manifestly gauge invariant. Nevertheless, we will show that the two-band Hamiltonian allows a gauge-invariant formulation of the electromagnetic response of the electron system. To this end, we first consider the expression for $\mu_1(\vec{q}, \omega)$. It is readily verified that the two-band Hamiltonian is such that the following relations hold:

$$[H_0, e^{i\vec{q}\cdot\vec{r}}I] = \hbar \vec{q} \cdot \vec{\nabla}(\vec{q})$$
(3.13)

and

(3.5)

$$\langle \nu \mid \vec{\mathbf{V}}(-\vec{\mathbf{q}}) \mid \nu' \rangle = \langle \nu' \mid \vec{\mathbf{V}}(\vec{\mathbf{q}}) \mid \nu \rangle^*.$$
 (3.14)

If we next substitute

$$\vec{\mathbf{A}}_{1}(\vec{\mathbf{q}},\omega) = \frac{ic \vec{\mathbf{E}}(\vec{\mathbf{q}},\omega)}{\omega} + \vec{\mathbf{q}} \frac{c}{\omega} \phi_{1}(\vec{\mathbf{q}},\omega)$$
(3.15)

and the above relations in the expression for $\mu_1(\hat{\mathbf{q}}, \omega)$, we obtain upon simplifying

$$\mu_1(\mathbf{\tilde{q}},\omega) + e\phi_1(\mathbf{\tilde{q}},\omega) = (eN/2mcG)(\mathbf{\tilde{K}}' - \mathbf{\tilde{K}}'_1)\mathbf{\tilde{E}}(\mathbf{\tilde{q}},\omega).$$
(3.16)

Upon substituting this expression in the equations for $\mathbf{J}(\mathbf{q}, \omega)$ and $\rho(\mathbf{q}, \omega)$, we find after considerable manipulation the following result:

$$\vec{\mathbf{J}}(\vec{\mathbf{q}},\omega) = \frac{\omega_p^2}{4\pi c} \left(i \ \frac{c}{\omega} \ (\vec{\mathbf{U}} + \vec{\mathbf{M}}) \cdot \vec{\mathbf{E}} + \frac{N}{2mcG} \right) \\ \times (\vec{\mathbf{K}} - \vec{\mathbf{K}}_1) (\vec{\mathbf{K}}' - \vec{\mathbf{K}}_1') \cdot \vec{\mathbf{E}}$$
(3.17)

and

$$\rho(\mathbf{\vec{q}},\omega) = \frac{\omega_{\rho}^{2}}{4\pi c^{2}} \left((2\mathbf{\vec{K}}_{1}' - \mathbf{\vec{K}}') \cdot \frac{ic\mathbf{\vec{E}}}{\omega} + \frac{N}{2mcG} \times (L - L_{1})(\mathbf{\vec{K}}' - \mathbf{\vec{K}}_{1}') \cdot \mathbf{\vec{E}} \right) , \quad (3.18)$$

where \overline{U} is the unit dyadic and for simplicity, the subscript on the field \vec{E} is dropped. Thus we see that both the current density $\overline{J}(\vec{q}, \omega)$ and the charge density $\rho(\vec{q}, \omega)$ have two contributions. In particular, $\overline{J}(\vec{q}, \omega)$ is the sum of two vectors, one involving the conductivity tensor σ and the other the diffusion tensor δ , where

$$\vec{\mathbf{J}}_{c} = \sigma \cdot \vec{\mathbf{E}} = \frac{\omega_{p}^{2}}{4\pi c} \left(\frac{ic}{\omega} \quad (\vec{\mathbf{U}} + \vec{\mathbf{M}}) \cdot E \right)$$
(3.19)

and

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$$\vec{\mathbf{J}}_{D} = \delta \cdot \vec{\mathbf{E}} = \frac{\omega_{p}^{2}}{4\pi c} \left(\frac{N}{2mcG} \left(\vec{\mathbf{K}} - \vec{\mathbf{K}}_{1} \right) \left(\vec{\mathbf{K}}' - \vec{\mathbf{K}}_{1}' \right) \cdot E \right).$$
(3.20)

Now as the above equations are clearly independent of the electromagnetic potentials \vec{A}_1 , and ϕ_1 , we can conclude that the two-band Hamiltonian permits a gauge-invariant description of the electromagnetic response of the system.

Finally, we show that not only are the expressions for $\vec{J}(\vec{q}, \omega)$ and $\rho(\vec{q}, \omega)$ gauge invariant, but they also satisfy charge conservation. If we form the scalar product of q and $\vec{J}(\vec{q}, \omega)$, we get

$$\vec{\mathbf{q}} \cdot \vec{\mathbf{J}}(\vec{\mathbf{q}}, \omega) = \frac{\omega_p^2}{4\pi c} \left(i \vec{\mathbf{K}}_1' \cdot \vec{\mathbf{E}} - i (\vec{\mathbf{K}}' - \vec{\mathbf{K}}_1') \cdot \vec{\mathbf{E}} + \frac{\omega N}{2mcG} (L - L_1) (\vec{\mathbf{K}}' - \vec{\mathbf{K}}_1') \cdot \vec{\mathbf{E}} \right).$$
(3.21)

Comparing this expression with $\rho({\bf \bar q},\omega),$ we see that

$$\mathbf{\dot{q}} \cdot \mathbf{J}(\mathbf{\ddot{q}}, \omega) = \omega \,\rho(\mathbf{\ddot{q}}, \omega) \,.$$
 (3.22)

Hence, the two-band Hamiltonian is also consistent with charge conservation.

IV. EFFECTIVE CONDUCTIVITY TENSORS

Having demonstrated the gauge invariance of the electromagnetic response of the electron system, we now limit ourselves to a consideration of a longitudinal electric field. This case is of extreme importance for those semiconductors in which the principal electron-phonon interaction is via either the piezoelectric or deformation-potential coupling mechanisms; for in these semiconductors the interaction of the charge carriers and the piezoelectric or deformation-potential fields is known to be strongest for longitudinal electric fields. Accordingly, we need only consider the longitudinal component of the diffusion and conductivity tensors. The effective longitudinal conductivity tensor, which combines the phenomena of conduction and diffusion, follows immediately from our expression for $\mathbf{q} \cdot \mathbf{J}(\mathbf{q}, \omega)$.

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Using this expression we find that the effective longitudinal conductivity is given by

$$\sigma_{\scriptscriptstyle \parallel}^{e} = \hat{q} \cdot (\sigma + \delta) \cdot \hat{q} = \frac{i\omega\omega_{p}^{2}}{4\pi c^{2}q^{2}} \left(\frac{LM_{1} - i\omegaL_{1}(L - L_{1})}{M_{1} - i\omega(L - L_{1})} \right),$$
(4.1)

where \hat{q} is a unit vector in the direction of q and

$$M_{1} = \frac{2mc^{2}}{N} \sum_{\nu} \sum_{\nu'} \frac{\Lambda^{1}_{\nu'\nu}}{\tau_{\nu'\nu}} \left| \left\langle \nu' \right| e^{-i\vec{\mathfrak{q}}\cdot\vec{\mathfrak{r}}} \left| \nu \right\rangle \right|^{2}. \quad (4.2)$$

With the derivation of the above expression, which is valid for an energy-dependent relaxation time $\tau(E)$ we now consider two important limiting cases.

In the case of a constant relaxation time, we find that Eq. (4.1) reduces to

$$\sigma_{\parallel}^{e} = \frac{\omega_{p}^{e} \tau \omega \overline{\omega}}{4\pi q^{2} c^{2}} \frac{L_{1}L_{2}}{L_{1} - i\omega\tau L_{2}}$$
(4.3)

where

$$L_2 = L_1 \Big|_{\overline{\omega}=0} \tag{4.4}$$

and

$$\overline{\omega} = \omega + i\tau^{-1} \,. \tag{4.5}$$

For the case of no collisions, i.e., an infinite collision time, Eq. (4.3) simplifies to the following expression:

$$\sigma_{\parallel}^{e} = \frac{i\omega_{\rho}^{2}\omega}{4\pi q^{2}c^{2}} L_{3}, \qquad (4.6)$$

where

$$L_3 = L_1 | 1/\tau = 0. \tag{4.7}$$

In conclusion, we should mention that the expression for σ_{\parallel}^{e} in Eq. (4.3) agrees with the formal expression of Greene *et al.* when it is evaluated for a nondegenerate semiconductor. It also agrees with the corresponding expression derived by Spector⁶ on the basis of a Boltzmann-equation formulation. Finally, we note that Eq. (4.6) is identical to the expression derived previously by Wu and Spector.⁷ For a detailed application of the above expressions, we defer to a later paper, which will investigate magnetoacoustic phenomena in semiconductors.⁸

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