Nonequilibrium total-dielectric-function approach to the electron Boltzmann equation for inelastic scattering in doped polar semiconductors

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This paper describes a simple and general method for deriving the inelastic collision term in the electron Boltzmann equation for scattering from a coupled electron-phonon system and applies the method to the case of doped polar semiconductors. In the Born approximation, the inelastic differential scattering rate W^{inel} can be expressed in terms of the nonequilibrium total dynamic dielectric function, which includes both electronic and lattice contributions. Within the random-phase approximation W^{inel} separates into two components: an electron-electron interaction containing the nonequilibrium distribution function for excitations of the electron gas and a Fröhlich interaction including the phonon distribution function and self-energy due to polarization of the electrons. Each of these two interactions is screened by only the electronic part of the total dielectric function, which contains the high-frequency dielectric constant, unlike commonly used expressions that contain the static dielectric constant. The detailed balance between plasmons and electron-hole pairs in steady state is used to eliminate the nonequilibrium plasmon distribution from the Boltzmann equation, resulting in a dynamically screened electron-electron collision term. The phonon self-energy modifies the longitudinal optical-phonon dispersion so that two hybrid normal modes contribute to the electron-phonon collision term.

I. INTRODUCTION

The electron Boltzmann equation for inelastic scattering in solids is usually established either by making approximations to more general equations derived with powerful nonequilibrium Green's function techniques[1-4] or simply by ansatz with the aid of analogy to simpler physical systems. An alternative method described here proceeds by using time-dependent perturbation theory to determine the inelastic collision term from the total dynamic dielectric function for the nonequilibrium coupled electron-phonon system. This paper treats the case of a system of polar optical phonons in the presence of conduction electrons and Coulomb interactions, though the method is more generally applicable. Except for the nonequilibrium character of the Boltzmann problem, the approach is similar to Van Hove's correlation function method[5] applied to doped polar semiconductors[6] to determine the inelastic lifetime of a quasiparticle excitation of an equilibrium system. In addition to providing physical insight, the total dielectric function approach is a systematic way to include scattering against coupled electron-phonon modes in the Boltzmann equation, so that the influence of mode coupling on mobility can be studied. Numerical results for mobility in n-type GaAs are presented in Ref. 7.

In the Born approximation, the interaction between a conduction electron and a coupled electron-phonon system can be represented as an effective electron-electron interaction screened by the total dynamic longitudinal dielectric function $\epsilon_T(\mathbf{q}, \omega)$, which includes contributions from both electrons and phonons.[8-10] In this context, ϵ_T describes the linear response of the electron-phonon

gas not to an externally applied potential, but to the *internal* potential due to the probe electron plus the induced density fluctuations of the gas itself. The effective interaction has the form of a total density autocorrelation function. Unlike the lifetime problem,[6] the entire electron-phonon gas is away from equilibrium in the dc transport case and the correlation function must be evaluated for the *nonequilibrium* ensemble. It follows that the effective electron-electron interaction is screened by the nonequilibrium total dielectric function in this case. In fact, taking account of the nonequilibrium character of the interaction is essential to obtaining the correct form of the inelastic collision term, which contains nonequilibrium distribution functions for the system's excitations. Thus this paper generalizes previous work[6,11,12] that used the total dielectric function to study the scattering of excited electrons from coupled electron-polar-phonon systems in equilibrium.

The effective electron-electron interaction can be separated into a purely electron-electron term and a screened electron-phonon interaction. In the random-phase approximation (RPA), the electron-phonon part contains a phonon self-energy that arises from the polarization of the electron gas.[10] The self-energy correction modifies the longitudinal-optical (LO) –phonon dispersion in doped polar semiconductors, producing two hybrid normal modes with phonon strength in both. This paper determines the inelastic differential scattering rate W^{inel} for the nonequilibrium case in the RPA Born approximation. The result consists of an electron-electron component containing the nonequilibrium distribution function for excitations of the electron gas and an electron-phonon component containing the phonon self-energy and dis-

tribution function. Each of these two interactions is screened by *only* the electronic part of the total dielectric function, which contains the high-frequency dielectric constant ϵ_∞. Thus the RPA Born result differs from commonly used expressions for screened interactions in doped polar semiconductors, which contain the static dielectric constant ϵ_0. Examples using ϵ_0 rather than ϵ_∞ for n-type GaAs include a calculation of dynamically screened electron-electron scattering,[13] as well as static screening approximations for electron–LO-phonon scattering[14] and electron-electron scattering.[15] For more strongly polar doped semiconductors (where $\epsilon_0 \gg \epsilon_\infty$), it is essential to treat this aspect of the screening problem correctly.

The collective modes have a finite lifetime for decay into electron-hole pairs. This Landau damping process provides an indirect mechanism for single-particle electron-electron scattering. For the electronic system in steady state, Landau damping creates a detailed balance relation between plasmons and electron-hole pairs that can be used to eliminate the nonequilibrium plasmon distribution from the Boltzmann equation in favor of the single-particle electron distribution. In the approximation of no collision damping, the result is an electron-electron collision term screened in the dynamic RPA, containing the effects of electron-plasmon scattering. The important effect of dynamic screening on the electron-electron interaction in nonequilibrium situations has been demonstrated in previous work.[16] For direct-gap doped semiconductors where umklapp processes are negligible, the collision term conserves total electron momentum and cannot by itself degrade an electrical current if energy surfaces are spherical. However, by rearranging the electron momentum distribution, electron-plasmon and electron-electron scattering can have a significant indirect effect on the outcomes of other scattering processes.

The low-energy hybrid mode arising from the plasmon-phonon coupling in doped polar semiconductors gives increased low-energy electron-phonon scattering strength compared to the uncoupled case. Numerical calculations including the plasmon-phonon coupling have given shortened inelastic lifetimes[6,11] and enhanced hot-electron energy relaxation,[17,18] especially at low temperatures and low doping. A simple way to treat the coupled modes is to use the plasmon-pole approximation[19,20] on the phonon self-energy. This procedure is used here to include scattering against the hybrid modes in the electron-phonon collision term so that mode coupling can be treated with the Boltzmann equation in a computationally efficient manner.

This paper is organized as follows. In Sec. II, W^{inel} is derived within the Born approximation in terms of the total nonequilibrium dielectric function for the coupled electron-phonon system. The RPA is invoked to separate W^{inel} into electron-electron and electron-phonon components. Section III deals with the electron Boltzmann equation by eliminating the nonequilibrium plasmon distribution from the electron-electron collision term. The electron-phonon collision term is simplified by applying the plasmon-pole approximation to the phonon self-energy.

II. INELASTIC DIFFERENTIAL SCATTERING RATE

A. Electron-phonon gas model

Consider a probe electron scattering from an interacting gas of electrons and polar optical phonons. Interactions with impurities and acoustic phonons can be added by hand later. The probe electron is treated as a quasiparticle with states $|\mathbf{k}\rangle$, effective mass m^*, and dispersion relation $E_k = \hbar^2 k^2 / 2m^*$. The Boltzmann equation relies on the validity of the quasiparticle description by assuming that the energy-momentum relation remains well defined when collisions are included. Interactions with the electron-phonon gas produce transitions between the quasiparticle states, but do not broaden them significantly.

For direct-gap polar semiconductors, local field effects are unimportant so that electrons couple only to the macroscopic electric field set up by the LO phonons and do not interact with the transverse-optical (TO) phonons. The Hamiltonian for the electron–LO-phonon gas is[10]

$$\tilde{H}_g = \sum_{\mathbf{k},\sigma} \mathcal{E}_k c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \sum_{\mathbf{q}} \hbar\omega_{\text{TO}}(a_{\mathbf{q}}^\dagger a_{\mathbf{q}} + \tfrac{1}{2})$$
$$+ \tfrac{1}{2} \sum_{\mathbf{q} \neq 0} v_q^\infty \left[\rho_T^\dagger(\mathbf{q}) \rho_T(\mathbf{q}) - N \right], \qquad (1)$$

where

$$v_q^\infty = \frac{v_q}{\epsilon_\infty} = \frac{4\pi e^2}{q^2 \epsilon_\infty}, \qquad (2)$$

the electron- and the LO-phonon annihilation operators are denoted by $c_\mathbf{k}$ and $a_\mathbf{q}$, respectively, σ labels the electron spin, and ω_{TO} is the TO-phonon frequency. The relevant phonon frequency in $\tilde{H}_g$ is the bare one ω_{TO}. The ion-ion Coulomb interactions explicitly included in $\tilde{H}_g$ shift ω_{TO} to the longitudinal optical frequency ω_{LO}, so that only ω_{LO} appears in expressions for observables.[10] The first and the second sums in $\tilde{H}_g$ describe the noninteracting systems of electrons and phonons, respectively. The last sum includes electron-electron, electron-phonon, and ion-ion Coulomb interactions. The total density operator ρ_T is the summation of the density operators of the electrons and LO phonons

$$\rho_T(\mathbf{q}) = \Omega^{-1/2}\rho(\mathbf{q}) + Zq \left(\frac{n\hbar}{2M\omega_{\text{TO}}} \right)^{1/2} A(\mathbf{q}), \qquad (3)$$

where $A(\mathbf{q}) = a_\mathbf{q} + a_{-\mathbf{q}}^\dagger$, M is the reduced mass of the basis ions, Ze is the effective ionic charge, n is the electron density, Ω is the system volume, and the Fourier components of the electron density operator are

$$\rho(\mathbf{q}) = \sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i} = \sum_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma}^\dagger c_{\mathbf{k},\sigma}. \qquad (4)$$

The electron self-interaction has been removed from $\tilde{H}_g$ by subtracting the term with N, the number of electrons

in the system. The influence of interband electronic transitions is taken into account by screening the Coulomb interaction v_q with the high-frequency dielectric constant ϵ_∞.

The effects of screening by conduction electrons and LO phonons are contained in the interaction term in $\tilde{H}_g$ and will appear explicitly in the total dielectric function below. The RPA or mean-field approximation for the interaction term is made by working with eigenstates $|n\rangle$ of the Hamiltonian H_g, which neglects the terms in $\tilde{H}_g$ that are quadratic in density fluctuations $\rho_T - \langle \rho_T \rangle$[9],

$$H_g|n\rangle = E_n|n\rangle, \tag{5}$$

$$H_g = \tilde{H}_g - \frac{1}{2}\sum_{\mathbf{q}} v_q^\infty [\rho_T^\dagger(\mathbf{q}) - \langle\rho_T^\dagger(\mathbf{q})\rangle][\rho_T(\mathbf{q}) - \langle\rho_T(\mathbf{q})\rangle] . \tag{6}$$

H_g includes Coulomb interactions at the Hartree level. Excitations of the electron-phonon gas described by H_g include both electron-hole pair and collective excitations.

Define $P(n, \mathbf{k} \to m, \mathbf{k} - \mathbf{q})$ as the probability per unit time for the probe electron to make a transition from $|\mathbf{k}\rangle$ to $|\mathbf{k} - \mathbf{q}\rangle$ while the electron-phonon gas makes a transition from $|n\rangle$ to $|m\rangle$, assuming that initially $|\mathbf{k}\rangle$ is occupied and $|\mathbf{k} - \mathbf{q}\rangle$ is unoccupied. The interactions included in H_g produce charge density correlations, resulting in an interaction potential between gas excitations and the probe electron, which is screened and assumed to be weak. Using Fermi's golden rule (or the Born approximation) with the probe particle plane wave states $|\mathbf{k}\rangle$, the transition probability is

$$P(n, \mathbf{k} \to m, \mathbf{k} - \mathbf{q})$$

$$= \frac{2\pi}{\hbar} \left(\frac{v_q^\infty}{\Omega}\right)^2 |\langle m \mid \rho_T^\dagger(\mathbf{q}) \mid n\rangle|^2 \, \delta(E_n - E_m + \hbar\omega_{k,k-q}) \tag{7}$$

$$= \left(\frac{v_q^\infty}{\Omega\hbar}\right)^2 \int_{-\infty}^{\infty} dt \, e^{i\omega_{k,k-q}t}\langle n \mid \rho_T(\mathbf{q}, t) \mid m\rangle$$

$$\times \langle m \mid \rho_T^\dagger(\mathbf{q}, 0) \mid n\rangle \tag{8}$$

$$\rho_T(\mathbf{q}, t) = e^{iH_g t/\hbar}\rho_T(\mathbf{q})e^{-iH_g t/\hbar} , \tag{9}$$

where $\omega_{k,k-q} = \hbar[k^2 - (\mathbf{k} - \mathbf{q})^2]/2m^*$.

The inelastic differential scattering rate $W^{\text{inel}}(\mathbf{k}, \mathbf{k} - \mathbf{q})$ is the probability per unit time for an electronic transition from the occupied state $|\mathbf{k}\rangle$ to the unoccupied state $|\mathbf{k} - \mathbf{q}\rangle$ due to scattering from the electron-phonon gas. It is found by summing $P(n, \mathbf{k} \to m, \mathbf{k} - \mathbf{q})$ over all possible final states $|m\rangle$ of the gas and averaging over its initial states $|n\rangle$. For the mobility problem, the average must be taken over the *nonequilibrium* gas ensemble.

B. Nonequilibrium ensemble averages

Consider that an electric potential $U(\mathbf{r}, t)$ is applied to the system of probe electron plus electron-phonon gas.

This influence is included by adding the term

$$H_{\text{ext}}(t) = e \int d^3r \, U(\mathbf{r}, t)\rho_T(\mathbf{r}, t) \tag{10}$$

to the Hamiltonian of the system. H_{ext} is independent of time in steady state, but it is useful to require the potential to be switched on at a time in the distant past when the gas was in thermal equilibrium. This requirement makes it possible to use the Kadanoff-Baym method[21] for evaluating a nonequilibrium expectation value. This method uses the equilibrium density matrix to evaluate an ensemble average at a time after U has been switched on by using the interaction picture to include the dependence on H_{ext} *explicitly*. The nonequilibrium expectation value of an operator $\mathcal{O}(\mathbf{r}, t)$ is[21]

$$\langle \mathcal{O}(\mathbf{r}, t)\rangle_{\text{noneq}} = \langle \mathcal{O}_U(\mathbf{r}, t)\rangle = \mathcal{Z}^{-1}\text{Tr}\left\{e^{-\beta H_g}\mathcal{O}_U(\mathbf{r}, t)\right\}, \tag{11}$$

$$\mathcal{O}_U(\mathbf{r}, t) = \mathcal{V}^{-1}(t)\,\mathcal{O}(\mathbf{r}, t)\,\mathcal{V}(t), \tag{12}$$

$$\mathcal{V}(t) = \mathcal{T}\exp\left[\frac{-i}{\hbar}\int_{-\infty}^{t} dt' H_{\text{ext}}(t')\right], \tag{13}$$

where $\langle\ \rangle$ denotes an average over the *equilibrium* population of the electron-phonon gas, $\beta = 1/k_BT$, $\mathcal{Z} = \text{Tr}\{e^{-\beta H_g}\}$ is the partition function for the equilibrium gas, and $\mathcal{T}$ denotes the time ordering operator, which orders operators with earliest times to the right.

In the presence of $U(\mathbf{r}, t)$, the transition rate $P(n, \mathbf{k} \to m, \mathbf{k} - \mathbf{q})$ in the Born approximation is unchanged from its equilibrium form (7), except that the influence of H_{ext} must be included in the time dependence of the matrix element. Using Eqs. (11)–(13) to determine $W^{\text{inel}}(\mathbf{k}, \mathbf{k} - \mathbf{q})$ from $P(n, \mathbf{k} \to m, \mathbf{k} - \mathbf{q})$ for the nonequilibrium case yields

$$W^{\text{inel}}(\mathbf{k}, \mathbf{k} - \mathbf{q}) = \left(\frac{v_q^\infty}{\Omega\hbar}\right)^2 N S_{TU}(\mathbf{q}, \omega_{k,k-q}), \tag{14}$$

$$S_{TU}(\mathbf{q}, \omega) = \frac{1}{N}\int_{-\infty}^{\infty} dt \, e^{i\omega t}\langle \rho_{TU}(\mathbf{q}, t)\,\rho_{TU}(-\mathbf{q}, 0)\rangle, \tag{15}$$

$$\rho_{TU}(\mathbf{q}, t) = \mathcal{V}^{-1}(t)\, e^{iH_g t/\hbar}\, \rho_T \, e^{-iH_g t/\hbar}\, \mathcal{V}(t), \tag{16}$$

where $S_{TU}(\mathbf{q}, \omega)$ is the nonequilibrium total dynamic structure factor or spectral function for ρ_{TU}, describing the density fluctuation excitations of the nonequilibrium electron-phonon gas. Similarly, the time-reversed rate is

$$W^{\text{inel}}(\mathbf{k} - \mathbf{q}, \mathbf{k}) = \left(\frac{v_q^\infty}{\Omega\hbar}\right)^2 N S_{TU}(-\mathbf{q}, -\omega_{k,k-q}). \tag{17}$$

When the gas excitations are not too highly damped so that they may usefully be regarded as elementary excitations and when the deviations from equilibrium are slowly varying in space and time on a scale determined by

the frequencies and decay rates of the elementary excitations, it is possible to define nonequilibrium distribution functions and response functions.[1,3] The imaginary (dissipative) part of the response function for the nonequilibrium coupled electron-phonon system is

$$\text{Im}[\chi_{TU}(\mathbf{q}, \omega)]$$

$$= \frac{-1}{2\hbar\Omega} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle [\rho_{TU}(\mathbf{q}, t), \rho_{TU}(-\mathbf{q}, 0)] \rangle \qquad (18)$$

$$= \frac{-n}{2\hbar} [S_{TU}(\mathbf{q}, \omega) - S_{TU}(-\mathbf{q}, -\omega)], \qquad (19)$$

where $[\rho, \rho']$ is the commutator $\rho\rho' - \rho'\rho$.

In general, there is no simple relation between a nonequilibrium spectral function and corresponding response function such as the fluctuation-dissipation theorem (FDT) for the equilibrium case:

$$S_T(\mathbf{q}, \omega) = \frac{-2\hbar}{n} [N^0(\omega) + 1] \text{Im}[\chi_T(\mathbf{q}, \omega)], \qquad (20)$$

where $N^0(\omega) = (e^{\beta\hbar\omega} - 1)^{-1}$ is the equilibrium Bose-Einstein distribution function, while S_T and $\text{Im}\chi_T$ are the *equilibrium* forms of (15) and (18). In particular, since the relation between the time-reversed nonequilibrium spectral functions $S_{TU}(\mathbf{q}, \omega)$ and $S_{TU}(-\mathbf{q}, -\omega)$ is not known, $\text{Im}[\chi_{TU}(\mathbf{q}, \omega)]$ is not determined by $S_{TU}(\mathbf{q}, \omega)$ alone. It is possible, of course, to define unknown dimensionless functions $N^>(\mathbf{q}, \omega)$ and $N^<(\mathbf{q}, \omega)$ such that

$$S_{TU}(\mathbf{q}, \omega) = \frac{-2\hbar}{n} N^>(\mathbf{q}, \omega) \text{Im}[\chi_{TU}(\mathbf{q}, \omega)], \qquad (21)$$

$$S_{TU}(-\mathbf{q}, -\omega) = \frac{-2\hbar}{n} N^<(\mathbf{q}, \omega) \text{Im}[\chi_{TU}(\mathbf{q}, \omega)]. \qquad (22)$$

Equations (19), (21), and (22) then imply

$$N^>(\mathbf{q}, \omega) - N^<(\mathbf{q}, \omega) = 1. \qquad (23)$$

Adopting the notation $N^<(\mathbf{q}, \omega) = N(\mathbf{q}, \omega)$, we have, from (14), (21), and (23),

$$W^{\text{inel}}(\mathbf{k}, \mathbf{k} - \mathbf{q}) = \frac{-2(v_q^\infty)^2}{\Omega\hbar} [N(\mathbf{q}, \omega_{k,k-q}) + 1]$$
$$\times \text{Im}[\chi_{TU}(\mathbf{q}, \omega_{k,k-q})]. \qquad (24)$$

Equivalently, the Born aproximation for W^{inel} can be expressed in terms of the imaginary part of the total screened Coulomb interaction v_q/ϵ_{TU} between the probe particle and the electron-phonon gas

$$W^{\text{inel}}(\mathbf{k}, \mathbf{k} - \mathbf{q}) = \frac{-2v_q}{\Omega\hbar} [N(\mathbf{q}, \omega_{k,k-q}) + 1]$$
$$\times \text{Im}\left[\epsilon_{TU}^{-1}(\mathbf{q}, \omega_{k,k-q})\right]. \qquad (25)$$

This follows from the relations between the total susceptibility $\chi_{TU}(\mathbf{q}, \omega)$, polarization $P_{TU}(\mathbf{q}, \omega)$, and dielectric function $\epsilon_{TU}(\mathbf{q}, \omega)$ for the nonequilibrium coupled system

$$\chi_{TU}(\mathbf{q}, \omega) = \frac{P_{TU}(\mathbf{q}, \omega)}{1 - v_q^\infty P_{TU}(\mathbf{q}, \omega)}, \qquad (26)$$

$$\epsilon_{TU}(\mathbf{q}, \omega) = \epsilon_\infty \left[1 - v_q^\infty P_{TU}(\mathbf{q}, \omega)\right]. \qquad (27)$$

The relation $(v_q^\infty)^2 \text{Im}\chi_{TU}(\mathbf{q}, \omega) = v_q \text{Im}\epsilon_{TU}^{-1}$ follows from (26) and (27) and yields (25) from (24).

The weight factor $N(\mathbf{q}, \omega)$ in (25) plays the role of the distribution function for the nonequilibrium excitations of the coupled electron-phonon system. Just as for the equilibrium case in Eq. (20), the structure factor has been written as a product of a function $(\text{Im}[\epsilon_T^{-1}])$ describing the strength of interactions with the electron phonon gas and a function giving the occupation probabilities for the gas excitations. However, it should be emphasized that the FDT has not been used to derive (25) and $N(\mathbf{q}, \omega)$ is an *unknown* function.

C. Separation of the total interaction

The total nonequilibrium structure factor S_{TU} defined by (15) is exactly separable into a purely electronic part S_U^e plus the remainder S_U^{ph}, which includes electron-phonon and ion-ion Coulomb interactions. Using the nonequilibrium version of the total density operator (3),

$$S_{TU}(\mathbf{q}, \omega) = S_U^e(\mathbf{q}, \omega) + S_U^{\text{ph}}(\mathbf{q}, \omega), \qquad (28)$$

$$S_U^e(\mathbf{q}, \omega) = \frac{1}{\Omega N} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle \rho_U(\mathbf{q}, t)\rho_U(-\mathbf{q}, 0) \rangle, \qquad (29)$$

$$S_U^{\text{ph}}(\mathbf{q}, \omega) = \frac{1}{N} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \left\{ Zq \left(\frac{n\hbar}{2M\omega_{\text{TO}}\Omega}\right)^{1/2} \left[\langle \rho_U(\mathbf{q}, t)A_U(-\mathbf{q}, 0)\rangle + \langle A_U(\mathbf{q}, t)\rho_U(-\mathbf{q}, 0)\rangle\right] \right.$$
$$\left. + (Zq)^2 \frac{n\hbar}{2M\omega_{\text{TO}}} \langle A_U(\mathbf{q}, t)A_U(-\mathbf{q}, 0)\rangle \right\}. \qquad (30)$$

This section relates S^e and S^{ph} to corresponding electron and phonon parts of the response function, just as (21) relates the total structure factor to the total response function. To do so, Eq. (25) must be split into electron-electron and electron-phonon parts. Im-

posing the RPA for the dielectric function is a crucial step towards this goal. The response of the coupled system in the RPA is the sum of the electron and ion response taken separately.[9,22] In this approximation, the total screened interaction v_q/ϵ_{TU} is the sum of a purely

electron-electron part and an electron-phonon interaction that includes a phonon self-energy due to the polarization of the conduction electrons,[23]

$$\frac{v_q}{\epsilon_{TU}} = \frac{v_q^\infty}{\epsilon_U} + \frac{M_q^2}{\mid \epsilon_U \mid^2} D_U(\mathbf{q}, \omega) \,. \tag{31}$$

The electron-electron part of the total interaction is v_q^∞/ϵ_U, where ϵ_U is the nonequilibrium RPA dielectric function determined by electron-electron interactions only. The polarization for the noninteracting electron gas $P^{(1)}$ has the same Lindhard form as the equilibrium case, except that the nonequilibrium electron distribution function f is used instead of the Fermi-Dirac function,[3]

$$\epsilon_U(\mathbf{q}, \omega) = 1 - v_q^\infty P^{(1)}(\mathbf{q}, \omega), \tag{32}$$

$$P^{(1)}(\mathbf{q}, \omega) = \frac{1}{\Omega} \sum_{p,\sigma} \frac{f(\mathbf{p}) - f(\mathbf{p} + \mathbf{q})}{\hbar\omega_{p,p+q} - \hbar\omega - i\delta} \,. \tag{33}$$

The remaining part of the total interaction is a product of the screened electron-phonon matrix element $M_q^2 \mid \epsilon_U \mid^{-2}$ and the nonequilibrium phonon Green's function $D_U(\mathbf{q}, \omega)$ containing the self-energy correction

$M_q^2 \chi_U$ to the noninteracting Green's function $D_U^{(0)}$,

$$M_q^2 = v_q \frac{\hbar\omega_{\rm LO}^2}{2\omega_{\rm TO}} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right), \tag{34}$$

$$D_U(\mathbf{q}, \omega) = \frac{D_U^{(0)}}{1 - M_q^2 D_U^{(0)} \chi_U(\mathbf{q}, \omega)} \,. \tag{35}$$

Now define unknown dimensionless functions $N_e^{\gtrless}$ and $N_{\rm ph}^{\gtrless}$ to relate the electron and the phonon components of $S_{TU}(\mathbf{q}, \omega)$ in (28) to the respective components of the imaginary part of $v_q \epsilon_{TU}^{-1}$ in (31),

$$(v_q^\infty)^2 S_U^e(\pm\mathbf{q}, \pm\omega) = \frac{-2\hbar}{n} v_q^\infty N_e^{\gtrless}(\mathbf{q}, \omega) {\rm Im}[\epsilon_U^{-1}(\mathbf{q}, \omega)], \tag{36}$$

$$(v_q^\infty)^2 S_U^{\rm ph}(\pm\mathbf{q}, \pm\omega)$$

$$= \frac{-2\hbar}{n} \frac{M_q^2}{\mid \epsilon_U \mid^2} N_{\rm ph}^{\gtrless}(\mathbf{q}, \omega) {\rm Im}[D_U(\mathbf{q}, \omega)] \,. \tag{37}$$

Finally, using (14), (28), (36), and (37),

$$W^{\rm inel}(\mathbf{k}, \mathbf{k} - \mathbf{q}) = \frac{-2}{\Omega\hbar} \Bigg\{ v_q^\infty [N_e(\mathbf{q}, \omega_{k,k-q}) + 1] \, {\rm Im} \left[\epsilon_U^{-1}(\mathbf{q}, \omega_{k,k-q}) \right]$$

$$+ \frac{M_q^2}{\mid \epsilon_U(q, \omega_{k,k-q}) \mid^2} [N_{\rm ph}(\mathbf{q}, \omega_{k,k-q}) + 1] \, {\rm Im} \left[D_U(\mathbf{q}, \omega_{k,k-q}) \right] \Bigg\} \,. \tag{38}$$

Within the RPA, the expressions (25) and (38) for $W^{\rm inel}$ are equivalent. The last expression contains *two* unknown functions N_e and $N_{\rm ph}$ playing the roles of the nonequilibrium occupation functions for the excitations of the electronic and lattice components of the coupled system. Notice that N_e must describe a distribution with boson properties. This is because the density fluctuation $\rho_q^\dagger$ produces excitations of the electron gas that conserve the total number of electrons, such as electron-hole pairs and plasmons, which have boson properties.

III. ELECTRON BOLTZMANN EQUATION

The time rate of change of the nonequilibrium electron distribution $f(\mathbf{k})$ due to collisions is determined by the differential scattering rate $W(\mathbf{k}, \mathbf{k} - \mathbf{q})$, i.e., the probability per unit time for the transition $|\mathbf{k}\rangle \rightarrow |\mathbf{k} - \mathbf{q}\rangle$. The depletion rate of $f(\mathbf{k})$ is just $W(\mathbf{k}, \mathbf{k} - \mathbf{q})$ weighted by the probabilities that $|\mathbf{k}\rangle$ is occupied and $|\mathbf{k} - \mathbf{q}\rangle$ is unoccupied, summed over all possible final states. The collision term $-\{\dot{f}(\mathbf{k})\}_{\rm coll}$, in the Boltzmann equation is this depletion rate minus the replenishment rate determined similarly. The electric field in the sample is $\mathbf{F}(\mathbf{r}, t) = -\nabla[U(\mathbf{r}, t) + \langle U_{\rm ind}(\mathbf{r}, t) \rangle]$, where $\langle U_{\rm ind} \rangle$ is the average induced potential resulting from the system's re-

sponse to the applied potential U. Thus, for a homogeneous system under the influence of a static electric field $\mathbf{F}$,

$$\frac{-e\mathbf{F}}{\hbar} \cdot \frac{\partial f(\mathbf{k})}{\partial \mathbf{k}} = -\left\{ \dot{f}(\mathbf{k}) \right\}_{\rm coll}$$

$$= \frac{1}{\Omega} \sum_{\mathbf{q}} \{ W(\mathbf{k}, \mathbf{k} - \mathbf{q}) f(\mathbf{k})[1 - f(\mathbf{k} - \mathbf{q})]$$

$$- W(\mathbf{k} - \mathbf{q}, \mathbf{k}) f(\mathbf{k} - \mathbf{q})[1 - f(\mathbf{k})]\} \,. \tag{39}$$

$W(\mathbf{k}, \mathbf{k} - \mathbf{q})$ is a sum of rates for elastic and inelastic processes $W = W^{\rm el} + W^{\rm inel}$. Using the separation of the inelastic rate $W_{\rm inel}$ in (38), the inelastic contribution to the collision term separates into electron-electron and electron-phonon collision terms,

$$\{\dot{f}\}_{\rm coll}^{\rm inel} = \{\dot{f}\}_{\rm coll}^{e-e} + \{\dot{f}\}_{\rm coll}^{e-{\rm ph}} \,. \tag{40}$$

A. Electron-electron collision term

The purely electronic component of $W^{\rm inel}$ in (38) gives the collision term

$$-\{\dot{f}(\mathbf{k})\}_{\text{coll}}^{e-e} = -\frac{2}{\hbar\Omega^2}\sum_{\mathbf{q}} v_q^\infty \{[N_e(\mathbf{q},\omega_{k,k-q})+1]\text{Im}[\epsilon_U^{-1}(\mathbf{q},\omega_{k,k-q})]f(\mathbf{k})[1-f(\mathbf{k}-\mathbf{q})]$$

$$-N_e(\mathbf{q},\omega_{k,k-q})\text{Im}[\epsilon_U^{-1}(\mathbf{q},\omega_{k,k-q})]f(\mathbf{k}-\mathbf{q})[1-f(\mathbf{k})]\}. \tag{41}$$

The next step towards putting the collision term into a useful form is to eliminate the unknown function N_e, which gives the occupation probabilities of the density fluctuation excitations of the electron system. In the RPA, the response function contains only single-particle–hole pair and plasmon contributions to the excitation spectrum; multipair excitations are excluded.[24] We proceed by making an association between N_e and the nonequilibrum plasmon distribution, denoted here by N_p. In steady state, there exists a local detailed balance (LDB) between the plasmons and the electron-hole pairs that can be used to eliminate N_e in favor of f in the electron-electron collision term.[3,25] The LDB condition is equivalent to the FDT for the nonequilibrium ensemble,[26] which applies when χ determines the response not to external forces, but to internal fluctuation forces. It holds when the Landau damping rate $\gamma = 2\text{Im}P^{(1)}$ is large compared to the time variation of f, so that the plasmons come into equilibrium with the electrons *before* f changes appreciably. For the mobility problem, f is stationary and the condition holds exactly, except at small q values (where γ vanishes), which do not contribute to the electron collision integral because of energy and momentum conservation restrictions.

If LDB is used in combination with the "collisionless damping" approximation,[3] Eq. (41) is equivalent to the standard single-particle electron-electron collision term, but screened with the dynamic RPA dielectric function. This may be shown easily for the case of weak damping, in which the plasmons are well-defined excitations, by considering the Boltzmann equation for the nonequilibrium plasmon distribution $N_p(q) = N_p(\mathbf{q},\omega_q)$ with $\omega_q = \omega_p(q)$.[25,27] Plasmons are represented by the peaks in the spectral function $\text{Im}\epsilon_U^{-1}$. In the RPA, this function contains no corrections for collision broadening, so

that the relaxation of $N_p(q)$ is completely described by coherent absorption and emission of electron-hole pairs,

$$\dot{N}_p(q) = \frac{\pi v_q \omega_q}{\Omega^2}\sum_{\mathbf{k}}\{[N_p(q)+1]f(\mathbf{k}+\mathbf{q})[1-f(\mathbf{k})]$$

$$-N_p(q)f(\mathbf{k})[1-f(\mathbf{k}+\mathbf{q})]\}$$

$$\times\delta(\hbar\omega_{k,k+q}-\hbar\omega_q). \tag{42}$$

In steady state, $\dot{N}_p = 0$. Therefore, the relation between the distributions N_p and f is necessarily

$$N_p(q)\text{Im}[P_U^{(1)}(\mathbf{q},\omega_q)] = \frac{n}{2\hbar}S_U^{(1)}(\mathbf{q},\omega_q), \tag{43}$$

$$\text{Im}[P_U^{(1)}(\mathbf{q},\omega)] = \frac{2\pi}{\Omega}\sum_{\mathbf{p}}[f(\mathbf{p})-f(\mathbf{p}+\mathbf{q})]$$

$$\times\delta(\hbar\omega_{p,p+q}-\hbar\omega), \tag{44}$$

$$S_U^{(1)}(\mathbf{q},\omega) = \frac{4\pi\hbar}{N}\sum_{\mathbf{p}}f(\mathbf{p}+\mathbf{q})[1-f(\mathbf{p})]$$

$$\times\delta(\hbar\omega_{p,p+q}-\hbar\omega), \tag{45}$$

relating the response function $\text{Im}[P_U^{(1)}]$ and structure factor $S_U^{(1)}$ for the noninteracting nonequilibrium electron gas.

The detailed balance relation (43) between plasmons and electron-hole pairs simplifies the electron-electron collision term (41), if we assume that N_e corresponds to the distribution N_p for well-defined plasmons. Using the RPA interaction $\text{Im}[\epsilon_U^{-1}] = v_q^\infty|\epsilon_U|^{-2}\text{Im}[P_U^{(1)}]$ and (43)–(45) gives

$$-\{\dot{f}(\mathbf{k}_1)\}_{\text{coll}}^{e-e} = \frac{4\pi}{\hbar\Omega^3}\sum_{2,3,4}\frac{(v_q^\infty)^2}{|\epsilon_U(q,\frac{E_1-E_3}{\hbar})|^2}\delta(E_1+E_2-E_3-E_4)\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)$$

$$\times\{f(\mathbf{k}_1)f(\mathbf{k}_2)[1-f(\mathbf{k}_3)][1-f(\mathbf{k}_4)] - [1-f(\mathbf{k}_1)][1-f(\mathbf{k}_2)]f(\mathbf{k}_3)f(\mathbf{k}_4)\}, \tag{46}$$

when the notational changes $\mathbf{k}\to\mathbf{k}_1$ and $\mathbf{p}\to\mathbf{k}_2$ are made, the summation variable $\mathbf{q}$ is changed to $\mathbf{k}_3 = \mathbf{k}_1-\mathbf{q}$, and a summation over a δ function for momentum conservation is included. Notice that the *nonequilibrium* inverse dielectric function was needed to obtain the collision term with nonequilibrium distributions for all four (incoming and outgoing) electrons. The remaining factor of $|\epsilon_U|^2$ in Eq. (46) appears only in its equilibrium form $|\epsilon|^2$ if the Boltzmann equation is linearized with respect to the field strength $\mathbf{F}$, since the other factors vanish in equilibrium. Also notice that ϵ_∞ rather than ϵ_0 appears in the electronic dielectric function $\epsilon_U(q,\omega)$ [see Eq. (32)],

which screens the interaction in the electron-electron collision term (46), unlike some previous calculations using ϵ_0 for electron-electron scattering in GaAs.[13,15]

It should be emphasized that (46) includes the effect of electron-plasmon scattering through the resonance in $\epsilon(q,\omega)$ at $\omega = \omega_q$. For dc transport, the two-step process

electron-hole pair $\to$ plasmon $\to$ electron-hole pair

is equivalent to a dynamically screened electron-electron scattering event because of the detailed balance between plasmons and electrons.[28] Since (46) conserves total elec-

tron momentum (in the absence of umklapp processes), its effect on the electrical current in materials with spherical energy surfaces is nonvanishing only because it rearranges the momentum distribution, which influences other scattering processes. The most important difference between using (46) and a previous treatment[30] of the effects of electron-plasmon scattering on mobility is that the earlier work assumed an *equilibrium* (Bose-Einstein) distribution function for the plasmons. In the latter case, there is a net momentum loss from the nonequilibrium electron system.

B. Electron-phonon collision term

If the phonons interacted only with electrons by non-umklapp processes, they would reach a local detailed balance with the electrons just as the plasmons do. But, in

fact, the phonons interact with other phonons through anharmonic lattice forces. The excess momentum given to the LO phonons by the nonequilibrium electron system is dissipated primarily through interactions with acoustic phonons, which can lose momentum to the environment through umklapp processes. Traditionally, mobility calculations employed the "Bloch assumption" that the phonon system may be treated as if it were in thermal equilibrium,[31] valid when anharmonic processes are much faster than electron-phonon scattering. However, recent work[32] shows that correctly accounting for nonequilibrium LO phonons can significantly modify electronic transport in polar semiconductors. This section maintains the notation $N_{\rm ph}$ for the nonequilibrium phonon distribution, though the field dependence of the phonon Green's function is suppressed.

The electron-phonon component of $W^{\rm inel}$ in (38) gives the collision term

$$-\{\dot{f}(\mathbf{k})\}_{\rm coll}^{\rm e\text{-}ph} = -\frac{2}{\hbar\Omega^2}\sum_{\mathbf{q}}\frac{M_q^2}{|\,\epsilon_U(q,\omega_{k,k-q})\,|^2}\{[N_{\rm ph}(\mathbf{q},\omega_{k,k-q})+1]\,{\rm Im}D(q,\omega_{k,k-q})f(\mathbf{k})\,[1-f(\mathbf{k}-\mathbf{q})]$$

$$-N_{\rm ph}(\mathbf{q},\omega_{k,k-q}){\rm Im}D(q,\omega_{k,k-q})f(\mathbf{k}-\mathbf{q})\,[1-f(\mathbf{k})]\}\,. \qquad (47)$$

The electron-phonon matrix element is screened by only the electronic part of the total dynamic dielectric function. The long-wavelength, static limit of the RPA $\epsilon(q,\omega)$ is the temperature-dependent Thomas-Fermi dielectric function with the *high-frequency* dielectric constant ϵ_∞. Therefore, Eq. (47) in this limit gives a somewhat different result than treatments of electron–LO-phonon scattering using Thomas-Fermi screening with the *static* dielectric constant ϵ_0.[14] For the nondegenerate case, the long-wavelength limit of (47) is in agreement with the original treatment of screening in polar semiconductors by Ehrenreich.[33]

The ion-ion Coulomb interactions included in $\tilde{H}_g$ [Eq. (1)] make a self-energy contribution to the phonon Green's function.[10] The real part of this contribution shifts the LO-phonon energy from $\hbar\omega_{\rm TO}$ to $\hbar\omega_{\rm LO}$ in the denominator of the noninteracting Green's function $D^{(0)} = -2\omega_{\rm TO}/\hbar(\omega_{\rm LO}^2 - \omega^2)$. Damping due to anharmonic interactions and disorder is neglected here.

The interacting phonon Green's function

$$D(q,\omega) = \frac{D^{(0)}}{1-M_q^2 D^{(0)}\chi(q,\omega)}$$

$$= \frac{2\omega_{\rm TO}/\hbar}{\omega^2-\omega_{\rm LO}^2-2\omega_{\rm TO}M_q^2\chi(q,\omega)/\hbar} \qquad (48)$$

contains the self-energy term $\Pi^{\rm e\text{-}ph} = M_q^2\chi$ due to the polarization of the electron gas. The real part of $\Pi^{\rm e\text{-}ph}$ renormalizes the LO-phonon frequency, giving rise to two hybrid modes of mixed electron-phonon character. The coupled modes have been treated previously[20] with the finite-temperature plasmon-pole approximation for χ.[19] In this approximation, the electronic excitation spectrum that couples to the phonons is represented by a single mode with energy varying between

$\hbar\omega_p = \sqrt{4\pi n e^2/m^*\epsilon_\infty}$ at small q and $\hbar^2q^2/2m^*$ at large q. The plasmon coupling strength and energy are determined by requiring fulfillment of the f-sum rule and zero-frequency Kramers-Kronig relation, so that the plasmon-pole approximation for χ is[19,20]

$$\chi^{pp}(q,\omega) = \frac{1}{v_q^\infty}\frac{\omega_p^2}{\omega^2-\tilde{\omega}_p^2}, \qquad (49)$$

$$\tilde{\omega}_p^2 = \omega_p^2[1-\epsilon^{-1}(q,0)]^{-1}\,. \qquad (50)$$

Using the plasmon-pole susceptibility χ^{pp} in the phonon self-energy $\Pi^{\rm e\text{-}ph}$ gives a phonon Green's function with poles at the two frequencies ω_+ and ω_-,

$$D(q,\omega) = \frac{2\omega_{\rm TO}(\omega^2-\tilde{\omega}_p^2)}{\hbar(\omega^2-\omega_+^2)(\omega^2-\omega_-^2)}, \qquad (51)$$

$$\omega_\pm^2 = \frac{1}{2}\left\{\omega_{\rm LO}^2+\tilde{\omega}_p^2 \pm \left[(\omega_{\rm LO}^2-\tilde{\omega}_p^2)^2 +4\omega_p^2(\omega_{\rm LO}^2-\omega_{\rm TO}^2)\right]^{1/2}\right\}\,. \qquad (52)$$

In the plasmon-pole model for the coupled modes, the phonon spectral function $-\pi{\rm Im}[D(q,\omega)]$ appearing in the electron-phonon collision term (47) has δ function peaks at ω_+ and ω_-,

$${\rm Im}[D(q,\omega)] = {\rm Im}[D^+(q,\omega)+D^-(q,\omega)], \qquad (53)$$

$${\rm Im}[D^\pm(q,\omega)] = \mp\frac{\pi\omega_{\rm TO}(\omega^2-\tilde{\omega}_p^2)}{\hbar\omega_\pm(\omega_+^2-\omega_-^2)}$$

$$\times[\delta(\omega+\omega_\pm)-\delta(\omega-\omega_\pm)]\,. \qquad (54)$$

At low densities, the low-energy hybrid mode has frequency ω_- close to the uncoupled plasmon frequency $\tilde{\omega}_p$, but has nonzero weight in the phonon spectral function determined by the factor $(\omega_-^2 - \tilde{\omega}_p^2)/(\omega_+^2 - \omega_-^2)$. Even though this factor is small at low densities, the low-energy mode has an exponentially larger thermal occupation $N_{ph}(\omega_-)$ at low temperatures than the high-energy hybrid mode or uncoupled phonon mode do. Therefore, for low densities and temperatures, the presence of N_{ph} in (47) suggests that the mobility calculated by including scattering from the coupled modes should be lower than the mobility calculated by using the uncoupled mode approximation. In addition, "antiscreening" effects due to the dynamic nature of the system response can generate screened potentials that are actually greater than in the unscreened case.[33] Reference 7 presents numerical results for n-type GaAs that show that including dynamic screening, mode coupling, and electron-electron scattering does significantly lower calculated mobilities in situations where ionized impurity scattering does not dominate, as in modulation-doped structures.

IV. CONCLUSION

The total dielectric function $\epsilon_T(q,\omega)$ lends itself to a simple and general method for deriving the inelastic collision term in the electron Boltzmann equation for scattering from a coupled electron-phonon system. When the Born approximation is valid, the inelastic differential scattering rate W^{inel} can be expressed in terms of the nonequilibrium total dielectric function ϵ_T, which includes screening by both electrons and phonons. In the RPA, W^{inel} separates into a purely electron-electron interaction plus an electron-phonon term describing interactions with the hybrid modes. These interactions are dynamically screened by only the electrons. Reference 7 investigates the effects of the phonon self-energy, dynamical screening, and electron-electron scattering on the mobility in n-type GaAs by means of a numerical solution of the linearized Boltzmann equation.

Because the total dielectric function approach to the Boltzmann equation treats the electrons and ions in a unified manner, it can be applied quite generally to a wide variety of coupled systems. More accurate and complete treatments[8,9] of the lattice part of ϵ_T^{-1} could be useful for more complex electron-phonon systems. Also, it would be very interesting to try to include electron-impurity scattering through the $\epsilon_T(q,\omega)$ for an imperfect crystal with local phonon modes. Another logical direction to pursue would start from a dielectric function that goes beyond the RPA to include electron exchange effects in order to derive the exchange scattering term in the Boltzmann equation. However, a systematic approach to improving on the RPA is required, since exchange corrections can be largely canceled by correlation terms.

ACKNOWLEDGMENTS

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[28] For readers who wonder how plasmon collision damping would affect this result, it could be added that a more general detailed balance relation between plasmons and electron-hole pairs is expected to hold even if collision damping is included. For example, consider the lowest-order collision damping process whereby a plasmon decays into an electron-hole pair and the electron scatters from an ionized impurity or another electron in the surrounding medium. This type of plasmon damping process dominates over Landau damping at long wavelengths (Ref. 29). If the process is included in the plasmon Boltzmann equation, a detailed balance relation such as Eq. (43) holds under steady-state conditions, but the response function and the structure factor are replaced by functions that include a multiparticle term as well as the one-pair Landau term. In this way, the plasmon distribution N_e can still be eliminated from Eq. (41) if multiparticle processes are included, but ϵ_U must be appropriately defined. The resulting electron-electron collision term will contain additional terms for multiparticle interactions, some of which do not conserve total electron momentum.

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