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Hot-carrier screening in semiconductors: A Boltzmann-equation approach

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Linear screening in strongly nonequilibrium semiconductors is studied by a Boltzmann-equation approach. In determining the nonequilibrium susceptibility $\chi(\mathbf{q},\omega)$, the correct distribution function is used, and the effects of scattering are included. As an application, we find that the ionized-impurity–scattering rate in a bulk semiconductor is significantly enhanced by a uniform, static electric field producing a drift velocity equal to the thermal velocity. A small-q limit of $\chi(\mathbf{q},\omega)$ is related to the longitudinal noise temperature $T_{n,\parallel}$ by a Debye-Hückel–type relation $\chi=-n/k_B T_{n,\parallel}$.

The trend towards smaller and smaller semiconductor devices has resulted in an increase in the operating fields within the devices, which has spurred the need to understand the physics of hot carriers. The nonequilibrium distribution of carriers produces many unique phenomena (e.g., the Gunn effect), and has interesting effects on the properties of semiconductors (e.g., the diffusion constant and the differential conductivity). In particular, screening due to the free carriers should be substantially altered. Screening in semiconductors is an important quantity primarily because it affects the carrier-scattering rates, modifying the mobilities and the distribution functions of the carriers. Previous applications of screening in nonequilibrium situations have generally assumed the static equilibrium Debye-Hückel form.[1] Recently, attempts have been made to characterize screening in the case of high static electric fields, but all these efforts either have been at a formal level,[2] or have relied on extensive computer simulations,[3] or have depended on the drifted Maxwellian approximation,[4] which may not be reliable for high electric fields.[5]

This paper describes a method for calculating nonequilibrium linear screening due to carriers, using the Boltzmann equation. This method is applicable to a wide range of nonequilibrium situations, such as optically excited semiconductor plasmas, hot carriers in superlattices, and ballistic carriers in tunneling transistors. Unlike previous analytic approaches, this method, in principle, does not make any assumptions about the carrier distribution function or the scattering processes.[6] However, we do assume linear response, which has widely been used in describing screening, mainly because calculating the full nonlinear screening is too complex a task. In a model study of the screening of carriers in a uniform, static electric field, we show that screening in the large- and small-wavelength limits can be understood from the drift-diffusion equation and the kinetics of a collisionless plasma, respectively. We show that the Debye-Hückel result for the static susceptibility $\chi(\mathbf{q},\,\omega=0)=-n/k_B T$, can be generalized in situations with a uniform static electric field. The effect of nonequilibrium screening is illustrated with the ionized-impurity–scattering rate.

Linear screening is a consequence of the linear carrier-density response $\delta n=n_1 e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$ to a potential $\delta U=U_1 e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$. The quantity that describes the screening is $\chi(\mathbf{q},\omega)=n_1/U_1$, and our procedure for the calculation of $\chi(\mathbf{q},\omega)$ is as follows. (i) Set up and solve the Boltzmann equation for the nonequilibrium situation being investigated. (ii) Linearly perturb the Boltzmann equation with an additional small sinusoidal force $iqU_1 e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$ to produce a distribution function response $f_1(\mathbf{p})e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$, and solve for $f_1(\mathbf{p})$. (iii) Integrate $f_1(\mathbf{p})$ with respect to $\mathbf{p}$ to obtain n_1. The ratio n_1/U_1 gives $\chi(\mathbf{q},\omega)$, and the dielectric constant $\epsilon(\mathbf{q},\omega)=1-4\pi e^2\chi(\mathbf{q},\omega)/q^2$. While this method has been used to determine χ in equilibrium[7,8] and for the study of ballistic transport through a heterostructure,[9] this is the first application to the calculation of the nonequilibrium susceptibility.

As an example of this procedure, we study the case of a parabolic-band, nondegenerate semiconductor in a uniform, static electric field exerting a force $\mathbf{F}$ on the carriers in the z direction, with the collisions approximated by a particle-conserving relaxation-time model[10] giving the Boltzmann equation[11]

$$F\frac{\partial f}{\partial p_z}=-\frac{f(\mathbf{p},\mathbf{x})-f_{1.\text{eq}}(p,\mathbf{x})}{\tau}\ . \tag{1}$$

This collision model, while being only a rough description of a real system, nonetheless is useful as a heuristic tool because of its simplicity. The solution for the distribution function $f(\mathbf{p})$ for Eq. (1) [step (i) above] is straightforward.[12,13] Insertion of $U_1 e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$ and $f_1(\mathbf{p})e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}$ into the Boltzmann equation gives a differential equation for $f_1(\mathbf{p})$, which, when solved [step (ii) above], yields

$$f_1(\mathbf{p})=\int_{-\infty}^{p_z}dp_z'\left[\frac{iqU_1}{F}\frac{\partial f}{\partial p_z'}+n_1\frac{f_{\text{eq}}(\mathbf{p}')}{nF\tau}\right]\exp\left\{\frac{p_z'-p_z}{F\tau}\left[1+i\left[\frac{p_xq_x+p_yq_y}{m}-\omega\right]\tau\right]+i\frac{[(p_z')^2-p_z^2]q_z}{2mF}\right\}\ . \tag{2}$$

This equation can be interpreted by the Chambers path-integral formulation of the Boltzmann equation.[14] The first term in the bold parentheses in Eq. (2) is due to the carriers which get swept by the small added potential into the path leading to **p** and are not scattered while on the path. The second term is due to carriers which are scattered *into* the path leading to **p** and are not scattered again while on the path.

After integrating $f_1(\mathbf{p})$ over momenta to find n_1 [step (iii) above], we obtain the nonequilibrium field-dependent susceptibility

$$\chi_F(\mathbf{q},\omega)=i\int_{-\infty}^{0} dt\,\exp\left[-\frac{it^2\mathbf{v}_d\cdot\mathbf{q}}{\tau}+\frac{t}{\tau}\right]\int d\mathbf{p}\,\mathbf{q}\cdot\nabla f(\mathbf{p})\exp[i(\mathbf{v}\cdot\mathbf{q}-\omega)t]$$
$$\times\left[1-\int_0^{\infty}dx\,\exp[-i\tau\mathbf{v}_d\cdot\mathbf{q}x^2/2-x(1-i\omega\tau)-(ql_{\rm th})^2x^2/4]\right]^{-1}, \quad (3)$$

where $l_{\rm th}=v_{\rm th}\tau=[(2k_BT/m)]^{1/2}\tau$, $\mathbf{v}=\mathbf{p}/m$, and $\mathbf{v}_d=\mathbf{F}\tau/m$. Figure 1 displays $\chi_F(\mathbf{q},\omega)$ for $\mathbf{v}_d\cdot\hat{\mathbf{q}}=2v_{\rm th}$. Below, we examine the large- and small-**q** limits of $\chi_F(\mathbf{q},\omega)$.

Large-q limit of χ_F. In this limit, the Eq. (3) approaches

$$\chi_F(\mathbf{q},\omega)\approx\int d\mathbf{p}\frac{\mathbf{q}\cdot\nabla f(\mathbf{p})}{\mathbf{q}\cdot\mathbf{v}-\omega-i0^+}\ . \quad (4)$$

This is the result for χ of a *collisionless* plasma with *no* external fields,[7] with carrier distribution $f(\mathbf{p})$. This expression is valid only for wavelengths small enough so that (a) there is no significant scattering in the time that a carrier takes to traverse the distance of a wavelength, allowing us to ignore the effects of collisions, and (b) the energy gained from the static field by a carrier in traversing a wavelength is not significant compared to the kinetic energy it already possesses, allowing us to ignore the effect of the uniform electric field. While Eq. (4) was derived from a relaxation-time model, it should describe χ_F for any collision model so long as the above conditions are met *and* quantum effects such as the finite spatial extent of the carrier wave function can be ignored. For the relaxation-time model used above, these constraints on the wavelength are quantified by (a) $q\gg 1/l_{\rm th}$ and (b) $q\gg F/k_BT$.

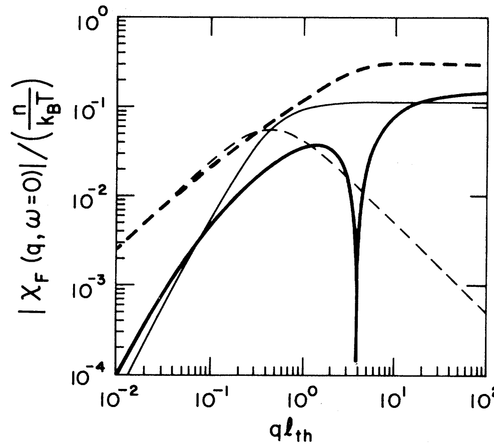

FIG. 1. The imaginary (dashed lines) and magnitude of real (solid lines) parts of the nonequilibrium static susceptibility $\chi_F(\mathbf{q},\omega=0)/(n/k_BT)$ for $\mathbf{v}_d\cdot\hat{\mathbf{q}}=2v_{\rm th}$. The bold lines are for χ_F obtained from the Boltzmann equation [Eq. (3)]. The thin lines are $\chi_{F,DD}$, an approximation obtained from the drift-diffusion equation [Eq. (5)]. The real parts are negative, except for the bold curve for $ql_{\rm th}<4$. For $q\to 0$, $\chi_{F,DD}$ approximates the imaginary part of χ_F accurately, but there is a discrepancy in sign for the real part. This discrepancy can be removed by the inclusion on a field-gradient term in the drift-diffusion equation (see Ref. 17). For $q\to\infty$, χ_F approaches the form for a collisionless plasma with distribution function $f(\mathbf{p})$, because the carriers are not significantly scattered or accelerated by the static field over the distance of a wavelength. In this limit, $\chi_{F,DD}$ is a poor approximation.

Small-q and -ω limit of χ_F. In the slow spatial-temporal variation limit $ql_{\rm th}$ and $\omega\tau\ll 1$, Eq. (3) can be approximated by making asymptotic expansions of the numerator and denominator. To understand $\chi_F(\mathbf{q},\omega)$ in this limit, we employ the drift-diffusion equation ($\mathbf{j}=n\mathbf{v}_d(\mathbf{F})-\sum_{i,j=1}^{3}D_{ij}(\mathbf{F})(\partial n/\partial x_j)\hat{\mathbf{x}}_i$ [where $D_{ij}(\mathbf{F})$ is the field-dependent diffusion tensor]) which is valid in this slow q,ω variation limit.[15] This equation, together with the continuity equation $\nabla\cdot\mathbf{j}+\partial n/\partial t=0$, yields the susceptibility

$$\chi_{F,DD}(\mathbf{q},\omega)=-\frac{n\sum_{i,j=1}^{3}q_iq_j\frac{\partial v_{d,i}}{\partial F_j}}{i(\mathbf{v}_d\cdot\mathbf{q}-\omega)+\sum_{i,j=1}^{3}D_{ij}(\mathbf{F})q_iq_j}\ . \quad (5)$$

The diffusion tensor can be obtained from the current-noise power spectrum,[16] which, in turn, can be calculated using a Green-function technique;[13] for the relaxation-time model $D_{zz}=k_BT(1+2v_d^2/v_{\rm th}^2)\tau/m$, $D_{xx}=D_{yy}=k_BT\tau/m$, and $D_{ij}=0$ for $i\neq j$. These results, together with $\partial v_{d,i}/\partial F_j=\delta_{ij}\tau/m$ (δ_{ij} is the Kronecker delta), when substituted into Eq. (5), yields an expression for $\chi_{F,DD}(\mathbf{q},\omega)$ that agrees with the small q,ω asymptotic expansion of Eq. (3) to lowest order in ω and q, even when the first-order terms cancel in the denominator (i.e., when $\omega=\mathbf{v}_d\cdot\mathbf{q}$).[17]

Equation (5) approximates Eq. (3) only if $\omega\tau\ll 1$ and $1/q\gg\max(v_d,v_{\rm th})\tau$, i.e., when quasi-steady-state conditions are achieved, and carriers are not ballistic over the distance of a wavelength. When these conditions are not met, Eq. (5) does not accurately represent Eq. (3), as exemplified by Fig. 1. However, when these conditions are satisfied, Eq. (5) is valid even in real systems, and not just for the relaxation-time model used here. Equation (5) can then be used to generalize the Debye-Hückel result $\chi_F(\mathbf{q}, \omega=0)=-n/k_B T$ to systems in a static electric field, where T is replaced by the longitudinal noise temperature $T_{n,\parallel}$.

The longitudinal noise temperature $T_{n,\parallel}$ is defined as the generalization of the Nyquist relation between the current-noise spectrum and the impedence of a system,[16,18] and it obeys a generalized Einstein relationship $k_B T_{n,\parallel}=eD_{zz}/\tilde{\mu}_{zz}$, where $\tilde{\mu}_{zz}=\partial v_{d,z}/\partial E_z$, for $\mathbf{v}_d$ parallel to z. On the other hand, for $\mathbf{q}$ parallel to $\mathbf{v}_d$ and $\omega=\mathbf{v}_d\cdot\mathbf{q}$, Eq. (5) gives $\chi(\mathbf{q}, \omega=\mathbf{v}_d\cdot\mathbf{q})=n\tilde{\mu}_{zz}/eD_{zz}$. Combining these results yields

$$\chi_F(\mathbf{q}=q\hat{\mathbf{v}}_d, \omega=\mathbf{v}_d\cdot\mathbf{q})=-\frac{n}{k_B T_{n,\parallel}} \quad (q\to 0) . \tag{6}$$

Hence, the longitudinal noise temperature is a measure of the long-wavelength susceptibility for a wave moving at the drift velocity of the carriers. Thus, a negative $T_{n,\parallel}$ (due to a negative differential conductivity) gives a positive susceptibility, which is indicative of the existence of a plasmon instability, and the concomitant Gunn effect.

Knowing $\chi_F(\mathbf{q},\omega)$ allows one to calculate the density of carriers around an external charge. Figure 2 shows the redistribution of carriers around an ionized impurity in the presence of an electric field. The shift in the centroid of the screening charge produces a dipole field at large distances from the impurity. In the relaxation-time model the long-wavelength limit, $\chi_F(\mathbf{q}, \omega=0)\to inq^2/\mathbf{F}\cdot\mathbf{q}$, implies a long-range effective potential

$$\phi_{\text{eff}}(\mathbf{r})=-\frac{Q_{\text{imp}}\mathbf{F}\cdot\mathbf{r}}{4\pi ne^2 r^3} \quad (r\to\infty) , \tag{7}$$

corresponding to an effective dipole formed at the impurity, $Q_{\text{imp}}\mathbf{F}/4\pi ne^2$ (where Q_{imp} is the charge on the impurity).

The range of $\phi_{\text{eff}}(\mathbf{r})$ in Eq. (7) is much longer than the Debye-Hückel screened Coulomb potential. This implies that hot carriers are not as effective in screening a static charge as carriers in equilibrium, and consequently, ionized-impurity–scattering rates are enhanced when carriers are hot. Figure 3 shows a rough estimate of the magnitude of this enhancement. The carrier-ionized-impurity–scattering rates were first calculated using the equilibrium (Debye-Hückel) dielectric function $\epsilon_{\text{eq}}(q)$, and then recalculated using the nonequilibrium dielectric function $\epsilon_{\text{noneq}}(\mathbf{q})$. The scattering rates are given by

$$\frac{1}{\tau_{(\text{non})\text{eq}}}=-\frac{1}{mv_d}\sum_{\mathbf{k},\mathbf{q}}\hbar q_z\frac{2\pi}{\hbar}\left|\frac{4\pi e^2}{q^2\epsilon_{(\text{non})\text{eq}}(\mathbf{q})}\right|^2 \times f(\hbar\mathbf{k})\delta(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}}) , \tag{8}$$

where the $f(\hbar\mathbf{k})$ used in both cases is the solution of Eq. (1).

Figure 3, displaying the ratio $\tau_{\text{eq}}/\tau_{\text{noneq}}$ as a function of v_d, shows that the effect of nonequilibrium screening increases with decreasing temperature. At equilibrium, the typical momentum transfer due to a collision of a carrier with an ionized impurity is $\sim q_{\text{dB}}=(2mk_B T)^{1/2}/\hbar$, the thermal de Broglie wave vector. Screening influences momentum transfers of magnitude zero up to $\sim q_{\text{sc}}=(4\pi ne^2/\epsilon_0 k_B T)^{1/2}$. Therefore, the larger the ratio $q_{\text{sc}}/q_{\text{dB}}$, the larger the fraction of collisions that are affected by screening, and hence the more sensitive the system is to changes in the behavior of the screening. Lowering the temperature increases $q_{\text{sc}}/q_{\text{dB}}$ and hence enhances the effect of nonequilibrium screening. Figure 3 shows that under favorable conditions the percentage in-

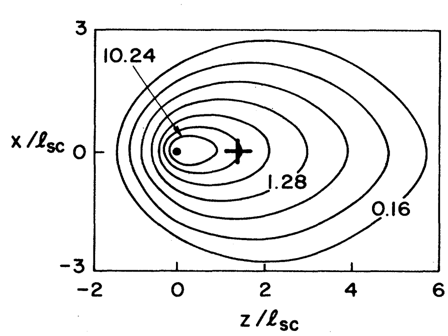

FIG. 2. Contours of the screening electron density (multiplied by 100) around a negatively charged impurity, for $v_d/v_{\text{th}}=1.0$, with $\omega_p\tau=1$ (ω_p is the plasma frequency). The densities of adjacent contours differ by a factor of 2. These parameters correspond to, e.g., GaAs with $n=10^{16}$ cm^{-3}, $\tau=2\times10^{-13}$ s, at 77 K and a field of 3.5×10^3 V/cm. The shift of the centroid of the screening cloud (denoted by +) from the position of the impurity (denoted by the dot) creates a long-range dipole field, which increases the ionized-impurity–scattering rate. For the above parameters, the screening length $l_{\text{sc}}=(\epsilon_0 k_B T/4\pi ne^2)^{1/2}$ is 40 Å and the dipole length is 60 Å.

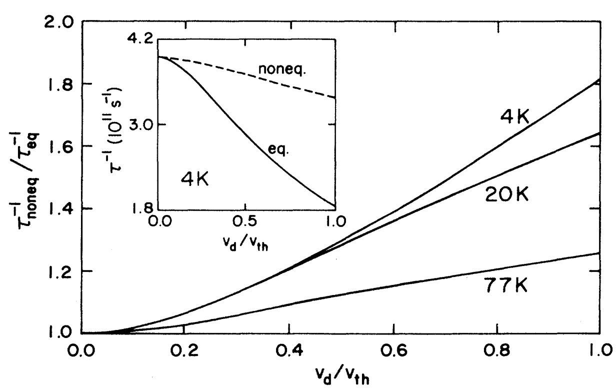

FIG. 3. Increase in the ionized-impurity–scattering rates due to nonequilibrium screening, for different temperatures. The densities are varied to keep the chemical potential μ_c a fixed ratio of $k_B T$. The effective mass used was that for GaAs. At $T=4$, 20, and 77 K, $n=10^{14}$, 1.14×10^{15}, and 8.5×10^{15} cm^{-3}, and $q_{\text{sc}}/q_{\text{th}}=0.67$, 0.45, and 0.32, respectively. When $q_{\text{sc}}/q_{\text{th}}$ increases, the fraction of carriers influenced by screening increases, enhancing the effect of nonequilibrium screening. In the inset the scattering rates with equilibrium (solid line) and nonequilibrium (dashed line) screening are shown for the case of $T=4$ K.

crease in the scattering rates can be fairly large, and so reanalyzing old data on high-field transport may prove interesting.[19]

Other scattering processes in nonequilibrium situations are similarly screened by $\epsilon_{\rm noneq}(\mathbf{q},\omega)$. In carrier-phonon scattering, unlike impurity scattering, screening is not critical in making the scattering rates finite (and often is ignored altogether) and so the effect of nonequilibrium screening is expected to be much smaller. Carrier-carrier scattering differs from impurity scattering in that carrier-carrier interactions are dynamically screened, which already reduces the effectiveness of screening.[20] Therefore, further reduction due to nonequilibrium screening is also expected to be smaller.

In conclusion, we have presented a method utilizing the Boltzmann equation for calculating the screening due to nonequilibrium carrier distributions. In applying the method to a system in a uniform, static electric field, we have (i) derived a nonequilibrium Debye-Hückel–type relationship, Eq. (6), and (ii) shown that for low T (but for a nondegenerate system) the increase in the ionized-impurity–scattering rate due to screening by hot carriers can be substantial.

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$$f_{\rm l.eq}(p,\mathbf{x})=n(\mathbf{x})\exp(-p^2/2mk_BT)/(2\pi mk_BT)^{3/2}\ ,$$

where n is the carrier density.

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