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Dynamic dielectric response to electron-hole and electron-electron interactions

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The interaction potential between two charged particles in a dielectric medium is shown to have the form $U(\vec{q},\vec{v}_{\text{c.m.}})=V(\vec{q})/\epsilon(q,\omega=\vec{q}\cdot\vec{v}_{\text{c.m.}})$, where $V(\vec{q})$ is the bare Coulomb potential, $\vec{v}_{\text{c.m.}}$ is the center-of-mass velocity, and $\epsilon(q,\omega)$ is the dielectric constant of the medium. An analysis of the dielectric screening is performed, incorporating core electron, lattice ion, and free-carrier contributions. The random-phase-approximation dielectric constant for arbitrary degeneracy is employed in calculating the free-carrier component of $\epsilon(q,\omega)$. It is found that although screening of the bare potential by lattice ions may sometimes be evaluated in the static or high-frequency limits, it is virtually always a poor approximation to treat the free-carrier screening in either of these limits. Dynamic screening processes have been incorporated into a calculation of relaxation times for electron-hole scattering in semiconductors for which $m_h \gg m_e$. Sample calculations for GaAs at a wide variety of temperatures and photoexcited carrier densities show that dynamic screening has a significant effect on the relaxation time in most regimes. It is equally important to treat the screening of electron-electron interactions dynamically when calculating transport properties which are sensitive to electron-electron scattering.

I. INTRODUCTION

Carrier-carrier collisions have an important effect on a wide variety of transport processes in semiconductors and metals. For example, electron-electron scattering significantly influences the energy relaxation of hot carriers[1] and the low-temperature electron mobility[2] in semiconductors, as well as the low-temperature electron thermal conductivity in semiconductors[3] and metals.[4] Electron-hole scattering can affect the electron mobility in narrow-gap semiconductors at high temperatures.[5] Moreover, since the advent of the laser there has been considerable interest in the properties of optically generated free-carrier plasmas in semiconductors. In such plasmas, electron-hole scattering can become the dominant mechanism limiting the free-carrier mobility at high excitation levels. This effect has been observed experimentally in several materials.[6–9]

In each of the above cases, the free carriers interact via a screened Coulomb potential, where the dielectric screening may include contributions from core electrons, lattice ions, free electrons and holes, etc. In this respect, carrier-carrier scattering resembles the scattering of a free carrier by a charged impurity. The main difference between the two processes is that while the center of mass of the carrier-ion system may be considered stationary, that of the carrier-carrier system moves through the screening medium with a finite velocity. This difference can profoundly affect the dielectric screening of the interaction potential. Consequently, the transport properties of carriers scattered by mobile charges are expected to differ appreciably from those of carriers scattered by stationary ions. In spite of the importance of carrier-carrier interactions in transport processes in solids, no comprehensive theoretical treatment of the dielectric screening of these interactions has previously been reported. It has been recognized for some time that the more slowly responding screening processes, such as the contributions from lattice ions[5] and free holes,[10] may not always be able to respond rapidly enough to effectively screen a carrier-carrier interaction. However, the approach that some investigators have adopted for dealing with this phenomenon has been to simply ignore the screening by these mechanisms,[5,10–12] i.e., the dielectric response is evaluated in the high-frequency limit. At the opposite extreme, several investigations of free-carrier transport properties in semiconductors and metals have ignored the distinction between the screening of carrier-carrier interactions and carrier-ion interactions.[4,8,13] This is equivalent to evaluating the dielectric response due to all screening mechanisms in the low-frequency limit. In this work, we derive a general dynamically screened interaction potential which results when the center-of-mass motion of the two-particle system is fully taken into account.

Section II presents the two-particle Schrödinger equation, which has been separated into reduced-mass and center-of-mass components. The dynamically screened carrier-carrier scattering potential is then derived in Sec. III. Section IV presents an explicit formulation of the dynamic dielectric response, which includes the random-phase-approximation dielectric constant for screening by free electrons and holes of arbitrary degeneracy and damping. In Sec. V the electron-hole relaxation time is calculated using the Born approximation for semiconductors in which $m_h \gg m_e$. Screening by a system of core electrons, lattice ions, and free carriers is incorporated into the calculation. In Sec. VI, detailed sample calculations are performed for the case of photoexcited GaAs at a variety of temperatures and electron-hole densities, and comparison is made to results obtained in the static and high-frequency limits. The significance of the dynamic effects in treating electron-electron scattering is also discussed.

II. TWO-PARTICLE SCHRÖDINGER EQUATION

Consider a spatially infinite dielectric "medium" characterized by a wave-vector- and frequency-dependent dielectric constant $\epsilon(q,\omega)$. Into this medium we place two particles, which may or may not be identical, of masses m_1 and m_2 and charges q_1e and q_2e. The time-dependent Schrödinger equation for the two-particle system may be written

$$\left[\frac{i\hbar\partial}{\partial t} + \frac{\hbar^2}{2m_1}\nabla_1^2 + \frac{\hbar^2}{2m_2}\nabla_2^2 - U(\vec{r}_1 - \vec{r}_2)\right] \times\Psi(\vec{r}_1, \vec{r}_2, t) = 0, \quad (2.1)$$

where U is the interaction potential. We define the coordinate of the center of mass $\vec{R}$ and the relative coordinate $\vec{r}$ as follows:

$$\vec{R} \equiv \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}, \qquad \vec{r} \equiv \vec{r}_1 - \vec{r}_2, \quad (2.2)$$

where the total and reduced masses are given by $M \equiv m_1 + m_2$ and $\mu \equiv m_1 m_2/M$, respectively. In terms of these new coordinates the Schrödinger equation can be rewritten[14]

$$\left[\frac{i\hbar\partial}{\partial t} + \frac{\hbar^2}{2M}\nabla_R^2 + \frac{\hbar^2}{2\mu}\nabla_r^2 - U(\vec{r})\right] \times\Psi(\vec{R}, \vec{r}, t) = 0. \quad (2.3)$$

This equation is separable in that the solution has the form

$$\Psi(\vec{R}, \vec{r}, t) = \Psi_{\text{c.m.}}(\vec{R}, t)\Psi_{\text{RM}}(\vec{r}, t). \quad (2.4)$$

One obtains the equations[14]

$$\left[\frac{i\hbar\partial}{\partial t} + \frac{\hbar^2}{2M}\nabla_R^2\right]\Psi_{\text{c.m.}}(\vec{R}, t) = 0 \quad (2.5a)$$

and

$$\left[\frac{i\hbar\partial}{\partial t} + \frac{\hbar^2}{2\mu}\nabla_r^2 - U(\vec{r})\right]\Psi_{\text{RM}}(\vec{r}, t) = 0. \quad (2.5b)$$

We are primarily interested in the reduced-mass equation (2.5b), which is further separable if one assumes a solution of the form

$$\Psi_{\text{RM}}(\vec{r}, t) = \psi_{\text{RM}}(\vec{r})e^{-iE_{\text{RM}}t/\hbar}, \quad (2.6)$$

where E_{RM} is the internal energy of the two-particle system. Equation (2.5b) then becomes

$$\left[E_{\text{RM}} + \frac{\hbar^2}{2\mu}\nabla_r^2 - U(\vec{r})\right]\psi_{\text{RM}}(\vec{r}) = 0. \quad (2.7)$$

This is the familiar time-independent Schrödinger equation.

Assuming an interaction where the initial wave vectors of the two particles are $\vec{k}_1$ and $\vec{k}_2$ while the final wave vectors are $\vec{k}'_1$ and $\vec{k}'_2$, we define the "direct" wave-vector transfer $\vec{q}_D \equiv \vec{k}'_1 - \vec{k}_1$ and the "exchange" wave-vector transfer $\vec{q}_E \equiv \vec{k}'_2 - \vec{k}_1$. From Eq. (2.7), the elastic scattering amplitude $f(\vec{q})$ can be obtained for scattering of the reduced-mass particle by the potential U. The differential elastic scattering cross section for distinguishable particles is then

$$\sigma(\vec{k}_1 \to \vec{k}'_1, \vec{k}_2 \to \vec{k}'_2) = |f(\vec{q}_D)|^2, \quad (2.8)$$

whereas that for identical fermions of spin $\frac{1}{2}$ is

$$\sigma(\vec{k}_1, \vec{k}_2 \to \vec{k}'_1, \vec{k}'_2) = \tfrac{1}{4}|f(\vec{q}_D) + f(\vec{q}_E)|^2 + \tfrac{3}{4}|f(\vec{q}_D) - f(\vec{q}_E)|^2. \quad (2.9)$$

While a number of approaches can be used to obtain the scattering cross sections, probably the simplest is the Born approximation, which gives the scattering amplitude[15]

$$f(\vec{q}) = -\frac{\mu}{2\pi\hbar^2}U(\vec{q}), \quad (2.10)$$

where $U(\vec{q})$ is the Fourier transform of $U(\vec{r})$. Because the scattering potential obtained below in Secs. III and IV is complex, there are also inelastic transitions.[16] These can occur when energy is exchanged with the screening medium. Such exchanges in the form of plasmon and phonon emission and absorption have been discussed by several investigators.[17] However, the inelastic cross sections are expected to be small since the imaginary part of the potential is usually much smaller than the real part.

III. DERIVATION OF THE SCATTERING POTENTIAL

In order to obtain cross sections for carrier-carrier scattering one must first specify the interaction potential $U(\vec{r})$. We consider the case of a reduced mass particle scattered by a central potential[18] which moves through the dielectric medium with the center-of-mass velocity $\vec{v}_{\text{c.m.}} = \partial \langle \vec{R} \rangle / \partial t$. Here the brackets represent an expectation value and $\vec{v}_{\text{c.m.}}$ is a conserved quantity since there are no external forces to alter the total momentum $M\vec{v}_{\text{c.m.}}$. The bare interaction is an unscreened Coulomb potential

$$V(\vec{r}) = \frac{q_1 q_2 e^2}{|\vec{r}|}. \tag{3.1}$$

This potential will be altered by the resulting dielectric polarization. In this section we derive expressions which characterize the screening with the interaction by a medium with dielectric constant $\epsilon(q, \omega)$.

We first point out that the calculation of the dielectric response must be performed in the rest frame of the screening medium rather than in the center-of-mass frame. This distinction leads to important differences between the screening of a carrier-carrier interaction and that of a stationary potential. Since the center of mass moves with velocity $\vec{v}_{\text{c.m.}}$ relative to the medium's rest frame, the position of the reduced-mass "particle" and the center of mass in that frame are given by $\vec{r}' = \vec{r} + \vec{v}_{\text{c.m.}}t$ and $\vec{R} = \vec{v}_{\text{c.m.}}t$, respectively, where we have defined the origin to be the location of the center of mass at $t = 0$. The bare potential in the coordinate system of the rest frame is then

$$V'(\vec{r}', t) = \frac{q_1 q_2 e^2}{|\vec{r}' - \vec{v}_{\text{c.m.}}t|}. \tag{3.2}$$

A Fourier-transform to momentum space gives

$$V'(\vec{q}, t) = \int d^3r' \, e^{i\vec{q}\cdot\vec{r}'} \left[\frac{q_1 q_2 e^2}{|\vec{r}' - \vec{v}_{\text{c.m.}}t|} \right] \tag{3.3}$$

$$= \frac{4\pi q_1 q_2 e^2}{q^2} e^{i\vec{q}\cdot\vec{v}_{\text{c.m.}}t} \tag{3.4}$$

and a second transform to frequency space yields

$$V'(\vec{q}, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \, e^{-i\omega t} V'(\vec{q}, t) = \frac{4\pi q_1 q_2 e^2}{q^2} \delta(\omega - \vec{q}\cdot\vec{v}_{\text{c.m.}}). \tag{3.5}$$

In free space the interaction potential would have its bare form $V'(\vec{q}, \omega)$. In the dielectric medium it is[19]

$$U'(\vec{q}, \omega) = \frac{V'(\vec{q}, \omega)}{\epsilon(q, \omega)}. \tag{3.6}$$

We now transform back to t space

$$U'(\vec{q}, t) = \int_{-\infty}^{\infty} d\omega \, e^{i\omega t} U'(\vec{q}, \omega) = \frac{4\pi q_1 q_2 e^2 \, e^{i\vec{q}\cdot\vec{v}_{\text{c.m.}}t}}{q^2 \epsilon(q, \omega = \vec{q}\cdot\vec{v}_{\text{c.m.}})} \tag{3.7}$$

and to $\vec{r}'$ space

$$U'(\vec{r}', t) = 4\pi q_1 q_2 e^2 \left[\frac{1}{2\pi}\right]^3 \times \int \frac{d^3q \, e^{-i\vec{q}\cdot(\vec{r}' - \vec{v}_{\text{c.m.}}t)}}{q^2 \epsilon(\vec{q}, \omega = \vec{q}\cdot\vec{v}_{\text{c.m.}})}. \tag{3.8}$$

We finally convert back to the center-of-mass frame, since the potential $U(\vec{r})$ which appears in Eq. (2.7) must be given in r coordinates:

$$U(\vec{r}) = 4\pi q_1 q_2 e^2 \left[\frac{1}{2\pi}\right]^3 \times \int \frac{d^3q \, e^{-i\vec{q}\cdot\vec{r}}}{q^2 \epsilon(q, \omega = \vec{q}\cdot\vec{v}_{\text{c.m.}})}. \tag{3.9}$$

Finally the potential in $\vec{q}$ space, expressed in the center-of-mass frame, can be obtained by a simple identification of $U(\vec{r})$ in Eq. (3.9) as the Fourier transform of

$$U(\vec{q}) = \frac{4\pi q_1 q_2 e^2}{q^2 \epsilon(q, \omega = \vec{q}\cdot\vec{v}_{\text{c.m.}})}. \tag{3.10}$$

The scattering problem can now be treated either in general using Eq. (2.7) or in the Born approximation using Eqs. (2.8)–(2.10).

In Eq. (3.10) we have obtained the strikingly simple result that the screened potential in $\vec{q}$ space due to a charge moving at a constant velocity $\vec{v}_{\text{c.m.}}$ is the same as that due to a stationary charge except that the dielectric constant of the medium $\epsilon(q, \omega)$ is evaluated at the frequency $\omega = \vec{q}\cdot\vec{v}_{\text{c.m.}}$ instead of at $\omega = 0$. The physical meaning of this result is easily interpreted as follows.[20] Consider the time

$\tau \equiv r_0/v_{\rm c.m.}$ required for the center of mass to traverse a typical interaction distance r_0. This can be thought of as the time scale for the charge disturbance in the medium set up by the moving potential. One can show from the properties of the Fourier transform that interactions with the potential at distances on the order of r_0 are dominated by wave-vector transfers on the order of $q_0 \approx r_0^{-1}$. If one defines a frequency $\omega \approx \tau^{-1}$ for the charge disturbance then $\omega \approx q_0 v_{\rm c.m.}$, which is roughly comparable to the frequency $\omega = \vec{q}_0 \cdot \vec{v}_{\rm c.m.}$ which appears when $U(\vec{q}_0)$ is evaluated using Eq. (3.10). For an interaction with a stationary center of mass, such as that between an electron and an ionized impurity in a solid, this frequency vanishes and the dielectric response of the medium has its static form, i.e., $\epsilon(q,\omega=0)$. However, for an interaction with a rapidly moving center of mass, the frequency $\omega = \vec{q} \cdot \vec{v}_{\rm c.m.}$ can be quite high and the dynamic nature of the medium's dielectric response must be properly accounted for. It will be seen below that for cases involving electron-hole and electron-electron scattering in solids, these considerations are almost always important.

IV. DIELECTRIC CONSTANT FOR A SEMICONDUCTOR WITH ARBITRARY DEGENERACY

In order to further investigate the consequences of the results obtained in the previous sections, we consider below a semiconductor having a total dielectric constant $\epsilon(q,\omega)$ of the form:

$$\epsilon(q,\omega) = \epsilon_\infty + \epsilon_{\rm lat}(\omega) + \epsilon_e(q,\omega) + \epsilon_h(q,\omega), \quad (4.1)$$

where $\epsilon_\infty - 1$ is the core electron contribution, $\epsilon_i(q,\omega)$ is the contribution due to free carriers of type i (see below), and the lattice ion contribution $\epsilon_{\rm lat}$ is taken to have the form

$$\epsilon_{\rm lat}(\omega) = \frac{(\epsilon_0 - \epsilon_\infty)\omega_t^2}{\omega_t^2 - \omega^2 + i\omega\Gamma_t}. \quad (4.2)$$

For simplicity, we have assumed a single TO phonon mode of frequency ω_t and damping Γ_t. Note that the static limit can be used only for frequencies much less than ω_t. In the remainder of this section we discuss the random phase approximation[21] (RPA) for the free-carrier components ϵ_e and ϵ_h. Although $\epsilon_{\rm RPA}(q,\omega)$ has been used extensively in treating the dielectric properties of degenerate electron populations, particularly in metals, it has rarely been employed in cases involving nondegenerate statistics.[8,22,23] Because we wish to treat carrier-carrier scattering in semiconductors, we will discuss the most general form of the RPA result for arbitrary degeneracy.

For carriers of type i one obtains the expression[19]

$$\epsilon_i(q,\omega) = \frac{4\pi e^2}{q^2} \sum_{\vec{k}} \frac{f_{0i}(\vec{k}) - f_{0i}(\vec{k}+\vec{q})}{E_i(\vec{k}+\vec{q}) - E_i(\vec{k}) - \hbar\omega - \frac{1}{2} i\hbar\Gamma_i}, \quad (4.3)$$

where f_0 is the Fermi distribution function and Γ_i may be interpreted as a damping constant. In order to be consistent with previous work[24,25] in the limit of large ω and small but finite damping, we define $\Gamma_i = e/m_i\mu$. That is, Γ_i is the inverse of the average momentum relaxation time, which has been set to a positive infinitesimal in most previous applications to screening.[19] For simplicity, nonparabolicity effects, wave-function admixture, and coupling between the various electron and hole bands have been ignored in Eq. (4.3). These effects usually give corrections of second order, and are outside the scope of the present work.

The dielectric constant given by Eq. (4.3) may be divided into real and imaginary parts: $\epsilon_i(q,\omega) \equiv \epsilon_{iR}(q,\omega) + i\epsilon_{iI}(q,\omega)$. Each part can be evaluated analytically in the case of extreme degeneracy,[26] but can be reduced only to a onefold integral which must be evaluated numerically for arbitrary degeneracy. One obtains

$$\epsilon_{iR}(q,\omega) = \frac{x_{pi}^2}{8\pi^{1/2} x_i^{3/2} \mathscr{F}_{1/2}(\eta_i)} \int_0^\infty dz\, f_0(z) \ln\left[\left[\frac{(2z^{1/2}x_i^{1/2} + x_i + y)^2 + \frac{1}{4}\gamma_i^2}{(2z^{1/2}x_i^{1/2} - x_i - y)^2 + \frac{1}{4}\gamma_i^2}\right] \times \left[\frac{(2z^{1/2}x_i^{1/2} + x_i - y)^2 + \frac{1}{4}\gamma_i^2}{(2z^{1/2}x_i^{1/2} - x_i + y)^2 + \frac{1}{4}\gamma_i^2}\right]\right], \quad (4.4a)$$

$$\epsilon_{iI}(q,\omega) = \frac{x_{pi}^2}{4\pi^{1/2}x_i^{3/2}\mathcal{F}_{1/2}(\eta_i)} \int_0^\infty dz\, f_0(z) \left[\tan^{-1}\left[\frac{2z^{1/2}x_i^{1/2}+x_i+y}{\frac{1}{2}\gamma_i}\right] + \tan^{-1}\left[\frac{2z^{1/2}x_i^{1/2}-x_i-y}{\frac{1}{2}\gamma_i}\right] + \tan^{-1}\left[\frac{-2z^{1/2}x_i^{1/2}-x_i+y}{\frac{1}{2}\gamma_i}\right] + \tan^{-1}\left[\frac{-2z^{1/2}x_i^{1/2}+x_i-y}{\frac{1}{2}\gamma_i}\right] \right], \tag{4.4b}$$

where we have introduced the dimensionless variables: $y \equiv \hbar\omega/k_BT$, $\gamma_i \equiv \hbar\Gamma_i/k_BT$, $z_i \equiv E_i/k_BT$, $\eta_i \equiv E_{Fi}/k_BT$, $x_i \equiv \hbar^2q^2/2m_ik_BT$, and $x_{pi} = \hbar\omega_{pi}/k_BT$. The plasma frequency is given by $\omega_{pi}^2 = 4\pi n_i e^2/m_i$ and $\mathcal{F}_j(m)$ is a Fermi integral of order j.[27] Equations (4.4a) and (4.4b) can be simplified considerably in the limit of low damping (i.e., $\gamma_i \to 0+$). The imaginary part of $\epsilon_i(q,\omega)$ can be evaluated analytically to give

$$\epsilon_{iI}(q,\omega) \xrightarrow[\gamma_i\to 0+]{} \frac{\pi^{1/2}x_{pi}^2}{4x_i^{3/2}\mathcal{F}_{1/2}} \ln\left|\frac{\exp[-(x_i+y)^2/4x_i+\eta_i]+1}{\exp[y-(x_i+y)^2/4x_i+\eta_i]+1}\right|. \tag{4.5}$$

It is easily seen from Eq. (4.5) that ϵ_{iI} vanishes in both the low-frequency ($y \to 0$) and high-frequency ($y \to \infty$) limits. In the low-frequency limit, the real part can be expanded as

$$\epsilon_{iR}(q,\omega\to 0) \xrightarrow[\gamma_i\to 0+]{} \frac{\epsilon_0 q_{si}^2}{q^2}\left[1 - \frac{1}{6}x_i\frac{\mathcal{F}_{-3/2}}{\mathcal{F}_{-1/2}} + \frac{1}{60}x_i^2\frac{\mathcal{F}_{-5/2}}{\mathcal{F}_{-1/2}} - \cdots\right], \tag{4.6}$$

where

$$q_{si}^2 = \frac{4\pi n_i e^2}{\epsilon_0 k_BT}\frac{\mathcal{F}_{-1/2}}{\mathcal{F}_{1/2}}. \tag{4.7}$$

If the expansion in Eq. (4.6) is terminated after the first term (i.e., the small-q limit), one obtains the usual Dingle-Mansfield result[28] for the static screening of a point change by a free-carrier plasma. When the contributions due to the different types of carriers are summed, the screening length is given by

$$\lambda_s = q_s^{-1} = \left[\sum_{i=e,h} q_{si}^2\right]^{-1/2}. \tag{4.8}$$

In the opposite limit of high frequencies, it is easy to show[29] that Eq. (4.3) gives

$$\epsilon_{iR} \xrightarrow[\gamma_i\to 0+]{} -\omega_{pi}^2/\omega^2.$$

For the small-damping limit ($\gamma \to 0+$), Fig. 1 illustrates the behavior of ϵ_{iR} as a function of frequency (y) for several values of the wave vector (x_i). The result, obtained for nondegenerate statistics, is normalized to the Dingle-Mansfield value $\epsilon_{DM} = (x_p^2/2x_i)\mathcal{F}_{-1/2}/\mathcal{F}_{1/2}$. Also shown as the dashed curves are results calculated in the high-frequency limit using $\epsilon_{iR}/\epsilon_{DM} \to -(2x_i/y^2)\mathcal{F}_{1/2}/\mathcal{F}_{-1/2}$. The figure shows that while Dingle-Mansfield

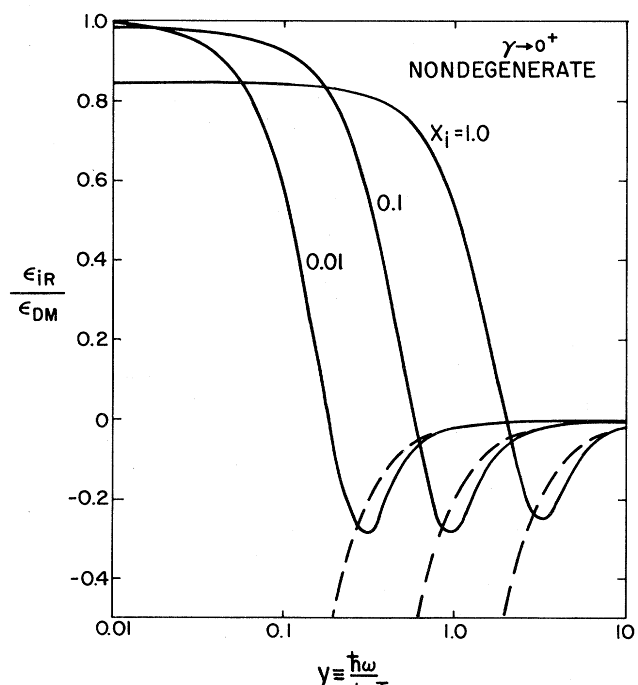

FIG. 1. RPA dielectric constant normalized to the Dingle-Mansfield (static) result. The dashed curves represent the high-frequency form: $\epsilon_{RPA} \to -\omega_p^2/\omega^2 = -x_p^2/y^2$.

screening is usually a fairly good approximation at $y=0$, it begins to break down above some frequency which depends on x_i. From Eq. (4.3) we see that the frequency dependence becomes important when the $\hbar\omega$ in the denominator becomes comparable to or larger than $\hbar^2 k_i q/2m_i$, where k_i is a typical wave vector for the particles of type i. After substituting $\omega = \vec{q} \cdot \vec{v}_{\text{c.m.}}$ one finds that the frequency dependence is important when $v_{\text{c.m.}} \gtrsim v_i$, where $v_i = \hbar k_i/m_i$. This result is quite reasonable in that if $v_i \gg v_{\text{c.m.}}$, the scattering center appears to be nearly stationary and can be screened as if it were a static potential. On the other hand, if $v_i \lesssim v_{\text{c.m.}}$ the free carriers cannot screen as effectively because they are unable to keep up with the "moving" potential. In any interaction between two particles of types i and j where $m_j \leq m_i$, one has $v_{\text{c.m.}} \approx v_i$. That is, the assumption of static screening is virtually always poor for at least one of the two types of carriers. Figure 1 illustrates that the RPA static limit can be used up to higher frequencies when x_i is large (i.e., large q).

Figure 2 shows both real and imaginary parts of ϵ_{RPA} for both low and high damping cases at $x_p = 1$ and $x_0 = 0.1$. While ϵ tends to be mostly real at low and high frequencies, $|\epsilon_I|$ is often larger than $|\epsilon_R|$ at intermediate frequencies. This is significant in that it prevents the quantity $(\epsilon_R^2 + \epsilon_I^2)^{-1}$ which appears below in Eq. (5.5) from diverging in the region where ϵ_R crosses zero.

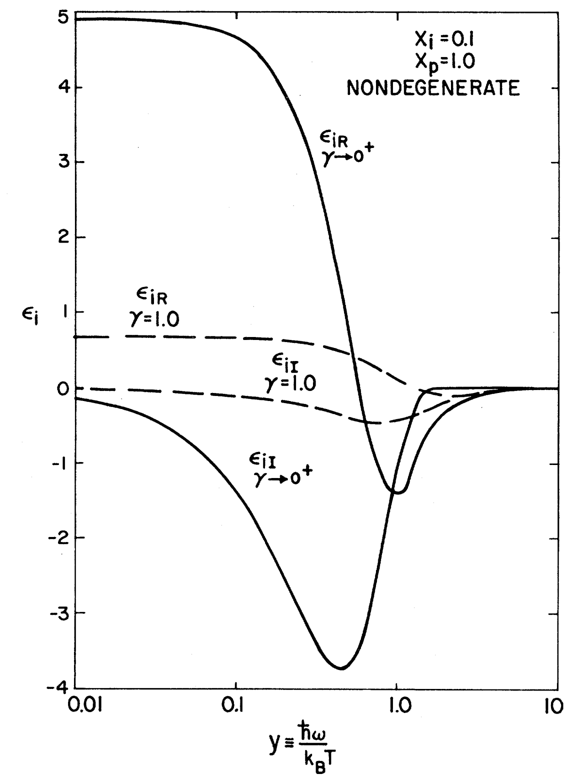

FIG. 2. Real and imaginary parts of the RPA dielectric constant for cases of high ($\gamma = 1$) and low ($\gamma = 0$) damping at fixed values of x_p ($=1.0$) and x_0 ($=0.1$).

V. ELECTRON-HOLE SCATTERING RELAXATION TIME

Electron-hole scattering can be most generally incorporated into a free carrier transport theory using Kohler's variational method.[30] Such calculations have been performed by McLean and Paige,[31] who assumed a bare Coulomb interaction with a finite cut-off radius, by Appel,[13] who employed a screened Coulomb interaction, and by Meyer and Glicksman,[8] who used a static RPA potential. However, unless a particularly simple scattering potential is employed or other simplifying assumptions are made, the variational formalism yields expressions containing fivefold integrals which cannot be performed analytically. Unfortunately, no such simplifications are possible if one employs the rather complicated potential represented by Eqs. (3.10) and (4.1).

Accurate transport results for electron-hole scattering can be obtained from a much simpler relaxation-time calculation in cases where the effective mass of the heavy holes is much larger than that of the electrons. We perform such a calculation below, ignoring the relatively infrequent collisions of electrons with light holes. Consider a free-carrier plasma consisting of n_e electrons and n_h holes with isotropic effective masses m_e and m_h, respectively. When $m_h \gg m_e$ and the electron degeneracy is not too great,[32] the collisions involve little transfer of energy between the electron and hole and the relaxation time approximation may be employed. Since the electron mobility in such a semiconductor is usually much larger than the hole mobility, the electrical conductivity is governed by the electron relaxation time, τ. For a system in which all of the scattering centers are equivalent, one obtains

$$\tau^{-1}(k_e) = N_s v_e \sigma_T(k_e), \tag{5.1}$$

where N_s is the density of scattering centers, $v_e = \hbar k_e/m_e$ is the electron velocity, and σ_T is the momentum-transfer scattering cross section

$$\sigma_T(k_e) = \int_0^{2\pi} d\phi \int_0^{\pi} \sigma(\vec{k}_e \to \vec{k}_e')(1 - \cos\theta)\sin\theta \, d\theta. \tag{5.2}$$

In Eq. (5.2), θ and ϕ are the polar and azimuthal angles between the initial state $\vec{k}_e$ and the final state $\vec{k}'_e$, where $|\vec{k}_e| = |\vec{k}'_e|$ for elastic interactions.

To obtain the differential scattering cross section σ, we will employ the Born approximation.[33] From Eqs. (2.8), (2.10), and (3.10) one obtains

$$\sigma(\vec{k}_e \to \vec{k}'_e,\ \vec{k}_h \to \vec{k}'_h) = \left[\frac{\mu}{2\pi\hbar^2}\right]^2 \left[\frac{4\pi e^2}{q^2}\right]^2 \left[\frac{1}{\epsilon_R^2(q,\omega) + \epsilon_I^2(q,\omega)}\right], \tag{5.3}$$

where $\vec{q} = \vec{k}_e - \vec{k}'_e = \vec{k}'_h - \vec{k}_h$, $\omega = \vec{q} \cdot \vec{v}_{\text{c.m.}}$, and $\mu \to m_e$. Since the center of mass of a system consisting of a hole and a much lighter electron may be taken to travel with the hole, we set $\vec{v}_{\text{c.m.}}$ equal to $\vec{v}_h$.

In order to obtain the relaxation time for electron-hole scattering in a real semiconductor with a Fermi distribution of hole scattering centers, Eq. (5.1) must be integrated over hole velocities. One obtains

$$\tau_{eh}^{-1}(k_e) = v_e \left[2 \left[\frac{m_h}{2\pi\hbar}\right]^3 \int d^3v_h f_0(v_h)[1 - f_0(v'_h)] \times \int_0^{2\pi} d\phi \int_0^{\pi} \sigma(\vec{k}_e \to \vec{k}'_e,\ \vec{k}_h \to \vec{k}'_h)(1 - \cos\theta)\sin\theta\, d\theta \right]. \tag{5.4}$$

The factor $f_0(v_h)[1 - f_0(v'_h)]$ comes from the requirement that the initial hole state be occupied and the final hole state be unoccupied, where for elastic interactions: $v'_h = v_h$. Were the differential cross section in Eq. (5.4) independent of the velocity of the scattering center v_h, the electron relaxation time would reduce to the form of Eqs. (5.1)—(5.2) with the effective density of scattering centers N_s given by $n'_h \equiv n_h \mathcal{F}_{-1/2}(\eta_h)/\mathcal{F}_{1/2}(\eta_h)$. For a nondegenerate hole population n'_h is simply the hole density n_h, whereas for degenerate holes n'_h is much less than n_h because of the unavailability of final states. Since the electron-hole scattering cross section does depend on v_h, we must in practice employ the more general result Eq. (5.4).

Three of the five integrals in Eq. (5.4) can be performed analytically to yield

$$\tau_{eh}^{-1}(k_e) = \frac{8e^4 m_e m_h^2 k_B T k_e}{\pi\hbar^6} \int_0^{\pi} \frac{(1 - \cos\theta)}{q^5} \sin\theta d\theta \int_0^{\infty} \frac{d\omega}{[\epsilon_R^2(q,\omega) + \epsilon_I^2(q,\omega)](e^{m_h\omega^2/2q^2k_BT - \eta_h} + 1)}, \tag{5.5}$$

where $q^2 = 2k_e^2(1 - \cos\theta)$. If the lattice contribution to the dielectric constant is evaluated in the low-frequency limit and the screening is taken to have the Dingle-Mansfield form given by Eq. (4.4) [i.e., $\epsilon(q,\omega) \to \epsilon_0(1 + q_s^2/q^2)$], Eq. (5.5) reduces to the familiar static result[28]

$$(\tau_{eh}^s)^{-1} = \frac{2\pi n'_h e^4 m_e}{\hbar^3 k_e^3 \epsilon_0^2} g(b), \tag{5.6}$$

where $b \equiv 4k_e^2\lambda_s^2$ and $g(b) = \ln(b + 1) - b/(b + 1)$. It will be shown in the following section that it is rarely a good approximation to evaluate the dielectric constant which appears in the general result Eq. (5.5) in either the low- or high-frequency limits.

VI. SAMPLE CALCULATIONS

A. Electron-hole scattering

Electron-hole scattering can be important whenever significant densities of electrons and holes are present. For example, this situation exists in semiconductors at high temperatures where the intrinsic carrier density is large. However, the effects of electron-hole scattering on the semiconductor transport properties are generally greater at low temperatures when nonequilibrium carriers are generated in the material through either electrical or optical injection. In order to illustrate the consequences of the results obtained in the previous section, we consider in this section the example of electron-hole scattering in photoexcited, high-purity GaAs. The most general form of the theory is employed to fully treat dynamic dielectric screening of the electron-hole interactions. Inverse relaxation times are obtained from Eq. (5.5) as a function of carrier density for a wide range of temperatures and hole damping coefficients. While the material parameters employed are appropriate for GaAs (see Table I), it can be shown that the main qualitative features are quite similar if the calculations are performed for any of the other common direct-gap semiconductors.

Of the three frequency-dependent components in

TABLE I. GaAs material parameters.

m_e	0.068	a
m_h	0.45	a
κ_0	12.53	a
κ_∞	10.9	a
$\hbar\omega_t$	0.0324 eV	a
$\hbar\Gamma_1$	$\hbar\omega_t/100$	Estimated

[a]M. Neuberger, *Handbook of Electronic Materials* (IFI/Plenum, New York, 1970), Vol. 2.

the total dielectric constant given by Eq. (4.1), the ω dependence of the free-electron contribution is relatively unimportant. On the other hand, the slower response by the lattice ions and free holes has a significant effect on the relaxation time for electron-hole scattering. Before we discuss the most general form of the calculation, it is useful to isolate the effects observed when the frequency dependences of these two components are considered separately.

The term "dielectric constant" is often used to designate the quantity $\epsilon'(\omega) \equiv \epsilon_\infty + \epsilon_{\text{lat}}(\omega)$, which reduces to ϵ_0 in the static limit and ϵ_∞ in the high-frequency limit. We now define ϵ'_{eff} to be the single, frequency-independent real value of ϵ' which yields the same relaxation time as one obtains by integrating over $d\omega$ in the more general expression Eq. (5.5). One may approximate

$$\epsilon'_{\text{eff}} \approx \epsilon_0 \, [\tau_{eh}/\tau_{eh}\,(\omega_t \rightarrow \infty)]^{1/2},$$

since τ_{eh}^{-1} in Eq. (5.5) goes as ϵ_0^{-2} if $\epsilon_{\text{lat}}(\omega)$ is evaluated in its static limit and (i.e., if $\omega_t \rightarrow \infty$) as ϵ_∞^{-2} if $\epsilon_{\text{lat}}(\omega)$ is evaluated in its high-frequency limit ($\omega_t \rightarrow 0$). (This expression for ϵ'_{eff} is not exact because the removal of the factor ϵ'^{-2} from the relaxation time does not account for the dependence of the free-carrier screening on ϵ'.) For high-purity photoexcited GaAs, Fig. 3 shows ϵ'_{eff} as a function of carrier density and temperature in the limit of large electron and hole mobilities ($\gamma_{e,h} \rightarrow 0+$). We have evaluated $\tau_{eh}(k_e)$ in Eq. (5.5) at the "typical" wave vector k_T, where $\hbar^2 k_T^2/2m_e \equiv E_T \equiv \frac{3}{2} k_B T \times \mathscr{F}_{1/2}(\eta_e)/\mathscr{F}_{-1/2}(\eta_e)$. That is, $E_T = E_F$ for degenerate statistics, while for nondegenerate statistics $E_T = \frac{3}{2} k_B T$.

As the carrier density is varied in Fig. 3, ϵ'_{eff} exhibits features which result from the frequency dependence of $\epsilon_{\text{lat}}(\omega)$ [see Eq. (4.2)]. This occurs because increasing the reduced hole Fermi level η_h serves to increase the frequencies emphasized in Eq. (5.5). The behavior shown in Fig. 3 is determined primarily by the real part of $\epsilon_{\text{lat}}(\omega)$, since the imaginary part is important only near $\omega \approx \omega_t$ where it prevents $(\epsilon_R^2 + \epsilon_I^2)^{-1}$ from diverging. Recall that for $\omega \ll \omega_t$, $\epsilon_{\text{lat}R} \rightarrow \epsilon_0 - \epsilon_\infty$ and that as ω increases, $\epsilon_{\text{lat}R}$ slowly increases before passing through a sharp peak near ω_t. It then becomes negative for $\omega \gtrsim \omega_t$, and approaches zero from the negative side in the limit of high frequencies. This frequency spectrum is roughly echoed in the 4-K curve of Fig. 3, with ϵ'_{eff} approaching ϵ_0 at low n and ϵ_∞ at high n.[34] Raising the temperature from 4 to 30 K has the effect of broadening the range of frequencies which contribute at any given η_h, thus leading to a smearing out of the features. For $T \gtrsim 150$ K, not only does one obtain broadening, but also the emphasized frequencies become comparable to ω_t. Consequently, even at low carrier densities the dominant frequencies correspond to those on the descending portion of the 4-K curve. It is evident that only under very limited circumstances may $\epsilon_{\text{lat}}(\omega)$ be evaluated in either the high- or low-frequency limit.

We now consider a similar analysis of the effectiveness of the screening by free holes. If the hole screening is treated statically, one obtains a contribution to the dielectric constant of the form $\epsilon_h \rightarrow \epsilon_0(q_{sh}/q)^2$. For carrier-ion interactions one would employ the Dingle-Mansfield screening $(q_{sh}^{\text{DM}})^2$ given by Eq. (4.7). For electron-hole scattering, one can obtain an "effective" static screening term $(q_{sh}^{\text{eff}})^2$ which yields the same relaxation time one would obtain rigorously using Eq. (5.5).

Figure 4 shows the ratio of the effective hole screening $(q_{sh}^{\text{eff}})^2$ to the full Dingle-Mansfield value

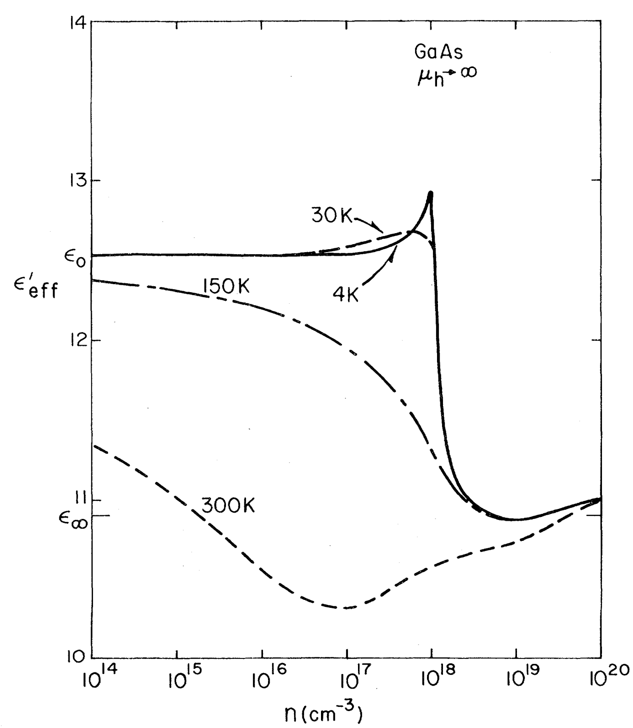

FIG. 3. "Effective" value of the dielectric constant due to core electron and lattice ions (see text for definition).

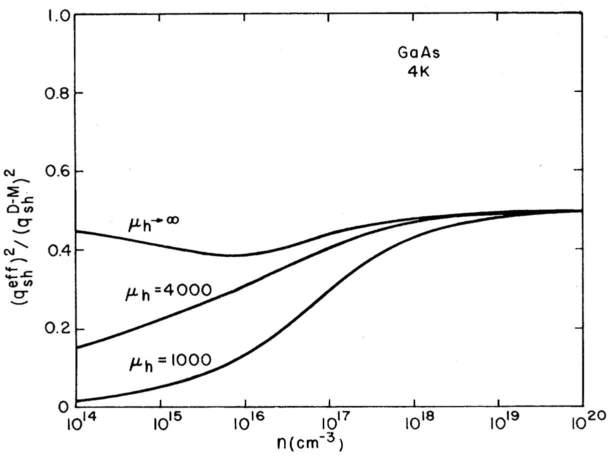

FIG. 4. Effectiveness of the screening by free holes compared to the static case (see text for definitions).

$(q_{sh}^{\rm DM})^2$ for various values of μ_h. The ratio is plotted as a function of carrier density at 4 K, with $k_e \approx k_T$. If the damping of the hole screening is negligible ($\mu_h \rightarrow \infty$) the screening effectiveness is approximately 50% of the static value over the entire range of n. This is because the average hole velocity is approximately the same as the average center-of-mass velocity. That is, the holes are always marginally able to screen the electron-hole interactions, but are never able to do so with complete effectiveness. For hole mobilities less than $\approx$4000 cm^2/V sec,[35] the effectiveness of the free hole screening can be greatly reduced by damping at low carrier densities [see Eq. (4.4)]. As is apparent from Fig. 4, the damping is much less important at high carrier densities where higher frequencies are emphasized.

The reduced effectiveness of the hole screening can have a significant effect on the calculated relaxation time. To illustrate this, we consider the case where the lattice-ion and free-electron contributions to the dielectric constant are treated statically. For GaAs at 4 K and μ_h = 1000 cm^2/V sec, Fig. 5 shows the inverse relaxation time $(\tau'_{eh})^{-1}$ for two cases: (1) the hole screening is treated dynamically (solid curve) and (2) the holes are assumed not to screen at all (dashed curve). In the figure, both quantities are normalized to the result $(\tau^s_{eh})^{-1}$ which is obtained when all screening is treated statically [see Eq. (5.6)]. The inverse relaxation time is found to be larger by a factor of between 1.4 and 5.2 when the hole screening is treated dynamically. One also finds that it is rarely a good approximation to ignore the hole screening, as some previous authors have suggested.[5,11] The peak near 10^{16} cm^{-3} corresponds to a minimum[36] in the parameter b, which is defined

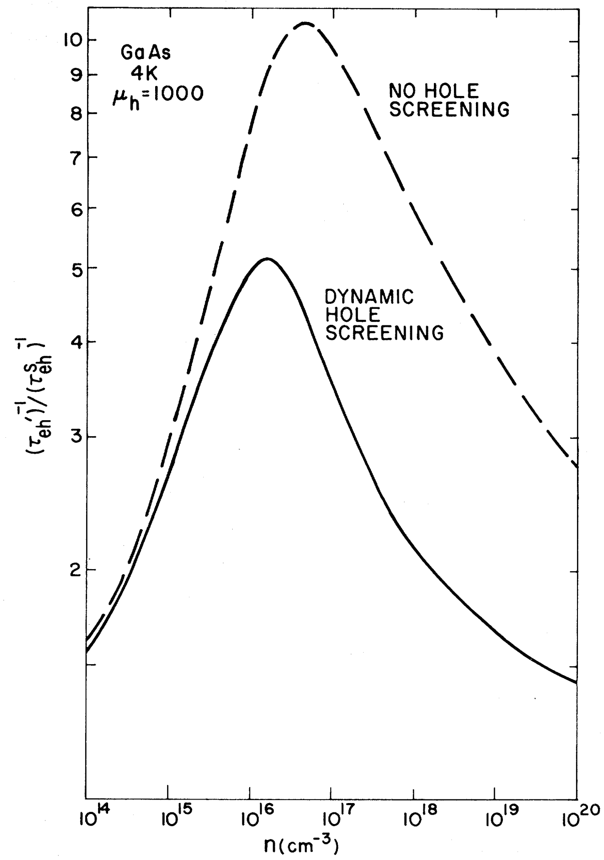

FIG. 5. τ^s_{eh}/τ_{eh} vs n for hole screening treated dynamically (solid curve) and hole screening ignored (dashed curve). Screening by lattice ions and electrons treated statically.

following Eq. (5.6). The reason is that the calculated relaxation time (5.5) is much more sensitive to changes in the screening length when b is small.

We have discussed above the effects introduced when the frequency dependences of the screening by lattice ions and free holes are taken into account separately. We now calculate the inverse relaxation time $(\tau_{eh})^{-1}$ for the more general case in which the contributions by lattice ions, free electrons, and free holes are all treated dynamically at the same time. Shown in Fig. 6 is a plot of the ratio $(\tau_{eh})^{-1}/(\tau^s_{eh})^{-1}$ as a function of n at 4 K for several values of μ_h, where $(\tau_{eh})^{-1}$ and $(\tau^s_{eh})^{-1}$ are given by Eqs. (5.5) and (5.6), respectively. As should be expected from a comparison with Fig. 4, $(\tau_{eh})^{-1}/(\tau^s_{eh})^{-1}$ depends much more strongly on μ_h at low carrier densities than at high densities. A broad peak is obtained as in Fig. 5, but superimposed on this is a smaller dip near $n \approx 10^{18}$ cm^{-3}.

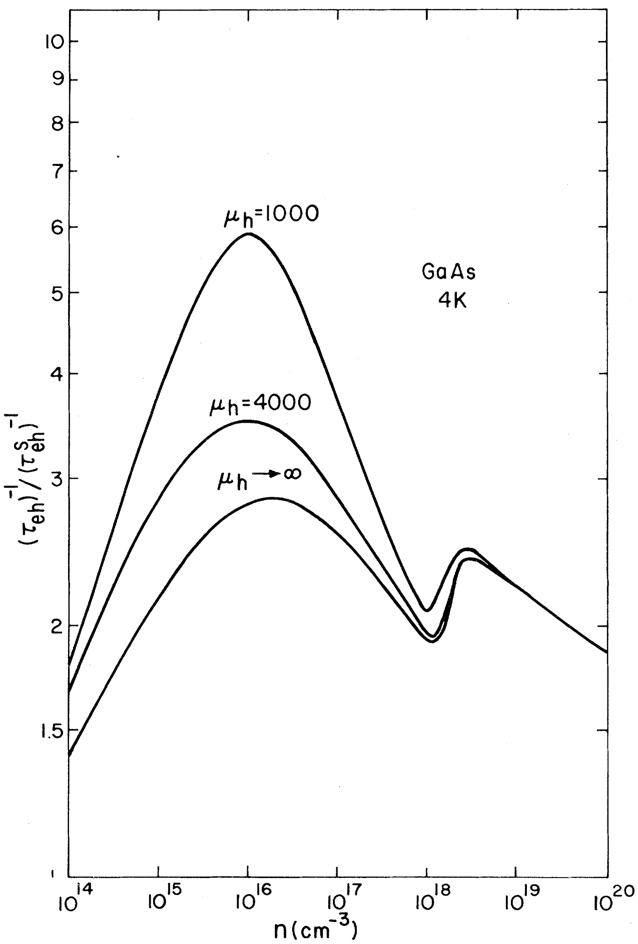

FIG. 6. τ_{eh}^s/τ_{eh} vs n for GaAs at 4 K with all screening treated dynamically.

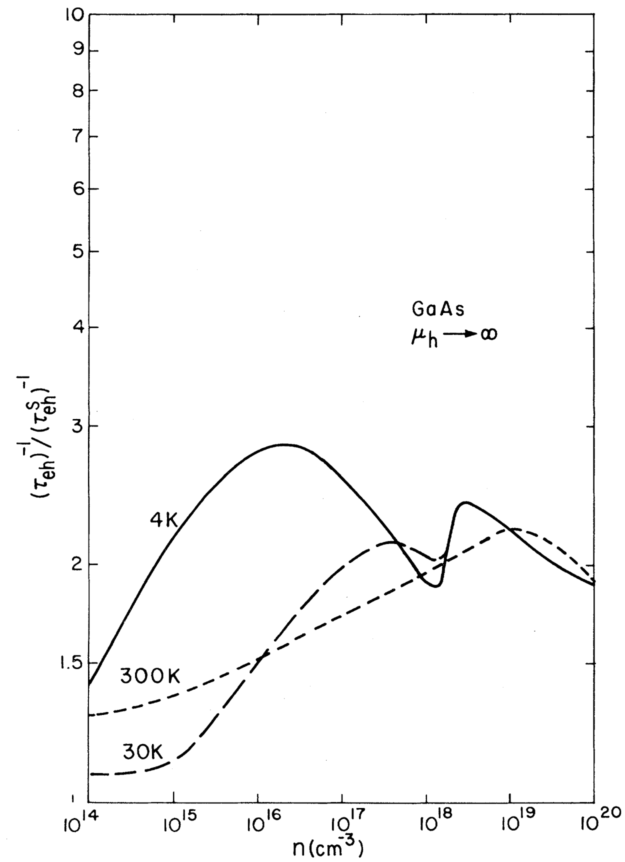

FIG. 7. τ_{eh}^s/τ_{eh} vs n at 4, 30, and 300 K, with all screening treated dynamically.

This is related to the frequency dependence of the lattice dielectric constant, and corresponds to the peak in ϵ'_{eff} observed in Fig. 3 near $n \approx 10^{18}$ cm^{-3}.

Figure 7 shows $(\tau_{eh})^{-1}/(\tau_{eh}^s)^{-1}$ vs n at 4, 30, and 300 K, for the case of undamped screening[37] (the 4-K curve is identical to the $\mu_h \to \infty$ curve in Fig. 6). At sufficiently high carrier densities the electrons and holes are degenerate at all of the temperatures shown. The relaxation times therefore have little dependence on T at high n, whereas they depend strongly on T for $n < 10^{18}$ cm^{-3}. For low carrier densities, i.e., $n < 10^{16}$ cm^{-3}, $(\tau_{eh})^{-1}/(\tau_{eh}^s)^{-1}$ does not vary monotonically with T because of competing processes. Figure 3 indicated that when only the screening by lattice ions is treated dynamically, the greatest reduction in the effective dielectric constant is obtained at high temperatures, i.e., the 300-K curve would be the highest in Fig. 7 if only $\epsilon_{\text{lat}}(\omega)$ is allowed to depend on frequency. However, it was pointed out in connection with Fig. 5 that due to dynamic hole screening $(\tau_{eh})^{-1}/(\tau_{eh}^s)^{-1}$ is greatest when $b(k_T)$ is smallest, which occurs at moderate carrier densities and lower temperatures. The differing temperature and carrier density dependences of these two effects are responsible for the crossover at low carrier densities of the 30- and 300-K curves in Fig. 7. As in Fig. 6, one finds that the structure due to the frequency dependence of ϵ_{lat} is superimposed on the broader features of the curve for $T \lesssim 30$ K.

It is apparent from Figs. 5—7 that in most regimes, accounting for the dynamic dielectric response has a significant effect on the calculated electron-hole scattering relaxation time. Both the static and high-frequency limits used in previous theories are usually inappropriate in the case of GaAs, and similar corrections are obtained if application is made to other direct-gap semiconductors for which $m_e \ll m_h$. Dynamic dielectric screening is expected to have a qualitatively similar effect on carrier transport when $m_e \approx m_h$, even though the relaxation time formulation used here is not applicable to that case.

Unfortunately data on GaAs are not available for comparison to the theoretical transport results shown in Figs. 5–7 which incorporate dynamic dielectric screening. However, the importance of the above effects has been verified experimentally in a recent study of low-temperature electron mobilities in photoexcited $Hg_{1-x}Cd_xTe$ ($x \approx 0.2$).[9] At high excitation levels where electron-hole scattering dominates, the calculated mobility is too high if the screening is treated statically and too low if the screening by photoexcited holes is ignored. However, theory and experiment are in good agreement when the more general dynamic screening formalism is employed.

B. Electron-electron interactions

It is well known that, although conservation of momentum implies conservation of current in any given electron-electron scattering event, *e-e* scattering can have a significant second-order effect on the mobility. This is because *e-e* scattering affects the energy distribution of the electron population.[2] Appel has solved the Boltzmann equation for nondegenerate electrons taking both ionized impurity scattering and *e-e* scattering into account.[2] If one assumes the densities of impurities and free electrons to be equal, the electron mobility is decreased by as much as a factor of 1.7 [depending on the parameter $b(k_T)$ discussed in the previous section]. Use of the more general dynamic potential will increase this factor. Since the typical center-of-mass velocity $v_{\mathrm{c.m.}}$ of the two-electron system is much higher than that of the electron-hole system considered above (i.e., for $m_h \gg m_e$), the free electron screening of the *e-e* interaction will now be much less effective than in the static case.[38]

Other transport properties, such as the electron thermal conductivity, depend on *e-e* scattering in first order. The neglect of dynamic screening effects may partly account for why *e-e* scattering thermal resistances calculated for simple metals using a statically screened Coulomb potential[4,39] are much lower than experimental values. Appel employed Kohler's variational method[30] to solve the Boltzmann equation including *e-e* scattering for the case of static screening.[2] The mobility and the thermal conductivity of the electrons obtained from this formalism can be easily generalized to incorporate the more general scattering potential represented by Eqs. (3.10) and (4.1). However, since this would involve rather complicated multifold integrals which must be evaluated numerically, we do not attempt such a calculation here.

VII. CONCLUSIONS

We have shown that the screening of an interaction between two charged particles moving in a dielectric medium may be treated in the static limit only if the center of mass of the two-particle system is at rest with respect to the medium. For a moving system the dielectric constant $\epsilon(q,\omega)$ must be evaluated at the frequency $\omega = \vec{q} \cdot \vec{v}_{\mathrm{c.m.}}$, where $\vec{v}_{\mathrm{c.m.}}$ is the center-of-mass velocity. We have considered a semiconductor system in which the total dielectric constant has core electron, lattice ion, and free-carrier contributions. The free-carrier screening is treated using the most general form of the RPA dielectric constant, which accounts for arbitrary degeneracy and damping. Dynamic screening has been incorporated into a detailed treatment of electron-hole scattering relaxation times in a semiconductor for which $m_h \gg m_e$. The importance of these effects has been demonstrated in electron-hole scattering calculations for photoexcited GaAs. The dynamic formulation often yields inverse relaxation times which are higher than the static values by a factor of 2 or more. In general, it is rarely appropriate to treat either the lattice ion contribution to the dielectric constant or the free carrier screening in either the static or high-frequency limits.

It should be emphasized that the dynamic screening effects discussed in this work should affect most semiconductor and metal transport properties which are sensitive to the dielectric screening of the carrier-carrier interactions. This holds quite generally because the screening by at least one of the two types of carriers involved in such interactions is always considerably less effective than it would be in the static limit. Except in the limit of high damping, it is also usually a poor approximation to ignore the screening due to either type of carrier.

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[16]This "inelasticity" should not be confused with the usage of the term to indicate a transfer of energy from one scattered particle to the other.

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[18]A more rigorous treatment would require a difficult many-body calculation rather than the two-body formulation considered here.

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[32]Appendix C of Ref. 9 discusses the conditions for which this type of inelasticity (see Ref. 16) may be neglected. In Figs. 3—7 of the present work, these conditions are not always strictly satisfied in some regions of low temperature and high carrier density.

[33]Although the Born approximation is not always strictly valid in the regions of interest [see J. R. Meyer and F. J. Bartoli, Phys. Rev. B 23, 5413 (1981)], more exact alternative methods are extremely laborious in the present case.

[34]Because the form we employ for ϵ'_{eff} is approximate, it does not quite reach ϵ_∞ at the carrier densities shown.

[35]Values in the range 1000—4000 cm^2/V sec for relatively impure material have been reported by O. V. Emel'yanenko, T. S. Lagunova, and D. N. Nasledov, Fiz. Tverd. Tela (Leningrad) 2, 192 (1960) [Sov. Phys. Solid State 2, 176 (1960)]; 3, 198 (1961) 3, 144 (1961)]. For purer samples, low-temperature mobilities up to 3×10^4 cm^2/V sec were observed by K.H. Zschauer, in *Proceedings of the Fourth International Symposium on GaAs and Related Compounds, Boulder, 1972* (Institute of Physics, London, 1973). At room temperature, phonon-scattering limits the mobility to ≈ 300 cm^2/V sec. The actual mobility under given circumstances will vary with temperature, doping, and level of photoexcitation.

[36]At $T = 4$ K and $n = 10^{14}\ \mathrm{cm}^{-3}$, $b(k_T) \equiv 4k_T^2\lambda_s^2$ originally decreases with increasing n due to the shorter screening length at higher carrier densities. However, as the electrons become degenerate b eventually increases with increasing n due to the larger Fermi wave vector. In this example, the minimum in b is near $n \approx 10^{16}\ \mathrm{cm}^{-3}$.

[37]Here the assumption of low damping is made because of its simplicity, not because the damping is expected to be unimportant. The actual hole mobility is expected to vary a great deal over the range of temperatures and carrier densities, in a manner which has not been determined experimentally.

[38]Using Fig. 4 as a guide, one might to a first approximation estimate that the electron screening becomes 50% as effective as in the static case.

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