Quantum kinetic-equation approach to semiconductor hot-carrier screening

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The Kadanoff-Baym formulation of quantum transport is used to derive a formulation for nonequilibrium carrier screening. The approach extends the Boltzmann-equation approach for calculating carrier-screening phenomena to include quantum effects due to the spatial nonlocality of the electron. To simplify calculations, the quantum relaxation-time approximation for the collisions used by Mermin is adapted for use in this quantum transport equation. As an example, we use this formulation and the quantum relaxation-time approximation to study the linear screening of a parabolic-band semiconductor in a high electric field, and we compare the results for this formulation with the classical Boltzmann-equation formulation of nonequilibrium screening. We find that the Boltzmann-equation method gives reliable results for the susceptibility $\chi(\mathbf{q},\omega)$ when q is much smaller than the average electron wave vector, but is unreliable for q much larger than the average electron wave vector. For $q\rightarrow\infty$, χ approaches a Lindhard-like formula for the susceptibility, but with the equilibrium distribution functions replaced by the nonequilibrium ones.

I. INTRODUCTION

Current trends in semiconductor physics emphasize the need to understand semiconductors in highly nonequilibrium situations.[1] For example, the very small scale on which semiconductor devices are currently fabricated leads to very high operating electric fields within these devices. Furthermore, advances in femtosecond spectroscopy permit the study of optically excited carriers that have not been thermalized by collisions and hence are very much out of equilibrium. In these highly nonequilibrium situations, many of the physical properties of the systems differ markedly from their values at equilibrium. In particular, the screening due to free carriers is substantially altered. The change in free-carrier screening then manifests itself in the alteration of the carrier-impurity, carrier-phonon, and carrier-carrier interactions, and therefore is of great importance in the study of high-field transport, and of carrier relaxation in photoexcited carriers.

Previous attempts to study screening in nonequilibrium situations have mainly dealt with screening due to carriers in a high electric field. Barker[2] and Lowe[3] studied the formal aspects of high-field screening by examining the nonequilibrium correlation functions. Lugli and Ferry[4] have performed a coupled molecular-dynamics–Monte Carlo simulation of electrons in silicon in a high electric field to obtain the nonequilibrium carrier-carrier correlation functions. Neither of these methods, however, is particularly suitable for calculating physically measurable quantities at high electric fields. Therefore, the drifted-Maxwellian approximation has often been used in performing these calculations,[5–7] despite the fact that this approximation is somewhat suspect at high electric fields.[8]

Recently, two of us[9] utilized the Boltzmann equation to calculate screening in nonequilibrium situations. The method consisted of solving the Boltzmann equation for the nonequilibrium situation being studied, and then superimposing a spatially and temporally varying potential on the system. The screening is then obtained by calculating the density response of the carriers to the applied potential. As an example, the linear susceptibility $\chi(\mathbf{q},\omega)$ was calculated for a nondegenerate semiconductor in a high static electric field within the relaxation-time approximation. In the course of the analysis of the results, two important length scales emerge from the calculations. These are $l_{\rm th}$, the thermal mean free path, and l_d, the drift mean free path, of the carriers. However, since the Boltzmann equation treats carriers as classical point particles, it ignores a third important length scale, which arises from the quantum-mechanical spatial broadening of carriers. When the scale of the spatial variation of the external potential is long compared to the scale of the typical electron wavelength, the quantum-mechanical nature of the carriers is unimportant, and the Boltzmann-equation picture suffices. However, when the scale of the spatial variation of the external potential is short compared to the scale of the typical electron wavelength, the quantum-mechanical nature of the carriers must be taken into account. Therefore, the results for the susceptibility $\chi(\mathbf{q},\omega)$ calculated from the Boltzmann equation cannot

be trusted in the regime where the wavelength $1/q$ is smaller than the typical electron wavelength.

In equilibrium, the quantum nature of the carriers can be included in determining the linear susceptibility by calculating the evolution of the one-particle density matrix in the presence of a slowly growing sinusoidal potential. This yields the Lindhard[10] or the random-phase-approximation expression for $\chi(\mathbf{q},\omega)$, and is valid for all q.[11] When we attempt to extend this method to include nonequilibrium situations, however, a problem immediately arises. It stems from the fact that in the calculation of the Lindhard susceptibility, the electrons are assumed not to interact with any scattering mechanisms (aside from the implicit assumption that the electrons couple to a heat bath, a role that is normally played by the lattice). However, scattering mechanisms are an extremely important and integral consideration when looking at any aspect of a nonequilibrium problem. For example, when carriers are placed in a high electric field, scattering mechanisms *must* be present in order for the system to achieve a steady state. Another example is the photoexcitation of electrons, where the scattering mechanisms are solely responsible for determining the evolution of the distribution of the electrons with time. Therefore, a method of incorporating scattering mechanisms into the problem must be found before results in the nonequilibrium regime can be achieved. In fact, in equilibrium, an extension of the Lindhard approach, which includes a quantum relaxation-time scattering term, has been expounded by Mermin.[12] This sets the stage for extending the formulation of equilibrium quantum screening to the nonequilibrium formulation of the problem.

In this paper, we show that this extension can be accomplished by utilizing the quantum theory of transport of Kadanoff and Baym.[13,14] The Kadanoff-Baym formulation has several advantageous features: (i) it is suited for the study of highly nonequilibrium situations; (ii) it reduces to the Boltzmann-equation formulation of Ref. 9 in the limit of slow spatial variations; and (iii) at equilibrium, it reproduces the Lindhard result for the susceptibility of a collisionless system. Furthermore, at equilibrium, when the quantum relaxation-time scattering term used by Mermin is inserted into the Kadanoff-Baym transport equation, the Mermin result for the susceptibility is reproduced. The obvious advantage of the Kadanoff-Baym approach is that, when scattering mechanisms are taken into account, it can readily be generalized to nonequilibrium situations. This generalization, which was impossible in the absence of a collision term in the transport equation (for reasons cited above), can now be achieved with the help of the quantum relaxation-time scattering term. This approach to quantum nonequilibrium screening is the main focus of this paper.

Section II outlines the formalism for the calculation of nonequilibrium screening. Section III introduces the quantum-mechanical relaxation-time approximation for the collision term of the quantum-transport equation. We then utilize this approximation to calculate the linear screening for nondegenerate carriers in a high electric field. Section IV summarizes the result.

II. QUANTUM TRANSPORT FORMALISM

In this section, we briefly review the Kadanoff-Baym formalism of quantum transport. We also quickly discuss the difficulties encountered in the formalism, and the need for simplifying approximations.

The Kadanoff-Baym formalism of quantum transport is based on the equations of motion for the two-time correlation functions

$$g^{<}(\mathbf{x}_1,t_1,\mathbf{x}_2,t_2)=i\langle\psi^{\dagger}(\mathbf{x}_2,t_2)\psi(\mathbf{x}_1,t_1)\rangle\ , \tag{1a}$$

$$g^{>}(\mathbf{x}_1,t_1,\mathbf{x}_2,t_2)=-i\langle\psi(\mathbf{x}_1,t_1)\psi^{\dagger}(\mathbf{x}_2,t_2)\rangle\ , \tag{1b}$$

where $\psi^{\dagger}(\mathbf{x},t)$ and $\psi(\mathbf{x},t)$ are the Heisenberg electron creation and destruction operators, and the angular brackets denote the thermal average. Written in terms of Wigner coordinates (i.e., sum and difference coordinates)

$$\mathbf{r}=\mathbf{x}_1-\mathbf{x}_2,\quad t=t_1-t_2\ ,$$

$$\mathbf{R}=\tfrac{1}{2}(\mathbf{x}_1+\mathbf{x}_2),\quad T=\tfrac{1}{2}(t_1+t_2)\ , \tag{2}$$

the equation of motion of $g^{<}(\mathbf{r},t;\mathbf{R},t)=i\langle\psi^{\dagger}(\mathbf{R}-\frac{1}{2}\mathbf{r},T-\frac{1}{2}t)\psi(\mathbf{R}+\frac{1}{2}\mathbf{r},T+\frac{1}{2}t)\rangle$ in a parabolic band is[15]

$$\left[i\frac{\partial}{\partial T}+\frac{\hbar\nabla_{\mathbf{R}}\cdot\nabla_{\mathbf{r}}}{m}\frac{-U_{\text{eff}}}{\hbar}(\mathbf{R}+\tfrac{1}{2}\mathbf{r},T+\tfrac{1}{2}t)\frac{+U_{\text{eff}}}{\hbar}(\mathbf{R}-\tfrac{1}{2}\mathbf{r},T-\tfrac{1}{2}t)\right]g^{<}(\mathbf{r},t;\mathbf{R},T)=I[g^{<},g^{>},\Sigma^{<},\Sigma^{>}]\ , \tag{3}$$

where U_{eff} is the sum of the external potential and the Coulomb potential of the carriers, $I[g^{<},g^{>},\Sigma^{<},\Sigma^{>}]$ is the quantum collision term, and $\Sigma^{<},\Sigma^{>}$ are the self-energies.

To transform Eq. (3) into an equation which looks somewhat like the Boltzmann equation, one introduces the Wigner distribution function, which is defined by

$$f(\mathbf{p},\mathbf{R},T)=-i\int d\mathbf{r}\exp\left[-i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}\right]g^{<}(\mathbf{r},t=0;\mathbf{R},T)\ . \tag{4}$$

By virtue of this definition, $f(\mathbf{p},\mathbf{R},T)$ has many similarities to a classical distribution function. For example, the density at $\mathbf{R},T$ is given by the integral over all momenta

$$n(\mathbf{R},T)=2\langle\psi^{\dagger}(\mathbf{R},T)\psi(\mathbf{R},T)\rangle=\int\frac{d\mathbf{p}}{4\pi^3\hbar^3}f(\mathbf{p},\mathbf{R},T)\ . \tag{5}$$

(The factor of 2 comes from the sum over spins.) Using the Wigner distribution function, Eq. (3) can be rewritten as

$$\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{R}}}{m}\right]f(\mathbf{p},\mathbf{R},T)+i\int\int d\mathbf{r}\frac{d\mathbf{p}'}{(2\pi\hbar)^3}e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar}\left[\frac{U_{\text{eff}}}{\hbar}(\mathbf{R}+\tfrac{1}{2}\mathbf{r},T)-\frac{U_{\text{eff}}}{\hbar}(\mathbf{R}-\tfrac{1}{2}\mathbf{r},T)\right]f(\mathbf{p}',\mathbf{R},T)$$
$$=I[g^{<},g^{>},\Sigma^{<},\Sigma^{>}]\ . \quad (6)$$

Note that by expanding the potential U_{eff} in powers of $\mathbf{r}$, and keeping only the lowest-order term, the collisionless evolution terms of the Boltzmann equation are recovered on the left-hand side of Eq. (6).

Equation (6) embodies much of the physics of a nonequilibrium system. If it could be solved for any applied external field, we would have complete knowledge of the density response to the potential, or the screening, of the system. Unfortunately, Eq. (6) is very complicated equation. First, the equation is nonlinear in $f(\mathbf{p},\mathbf{R},T)$ because of the dependence of U_{eff} on f. Second, the quantum collision term I is nonlocal in time and space, and $\Sigma^{<}$ and $\Sigma^{>}$ are functionals of the correlation functions $g^{<}$ and $g^{>}$. Therefore, progress can be made only in straightforward situations under many simplifying approximations.

One straightforward situation in which the transport equation is studied is that of the application of a uniform external electric field, $U_{\text{eff}}(\mathbf{R},T)=-\mathbf{R}\cdot\mathbf{F}$. Then, the problem reduces to solving

$$\mathbf{F}\cdot\nabla_{\mathbf{p}}f(\mathbf{p})=I[g^{<},g^{>},\Sigma^{<},\Sigma^{>}]\ . \quad (7)$$

Under certain circumstances, approximations can be made with $I[g^{<},g^{>},\Sigma^{<},\Sigma^{>}]$ to make it look like the Boltzmann collision term, with field-dependent scattering probabilities.[16,17] As in Ref. 9, we will use the case of carriers in a static uniform electric field as a paradigm for the study of nonequilibrium screening using the Kadanoff-Baym approach, although we note that this approach is not confined to this situation.

III. LINEAR SCREENING

Since complete nonlinear screening is far too complex to solve analytically (even in equilibrium situations), we shall confine our attention to linear screening. As in Ref. 9, linear screening will be obtained by superimposing a sinusoidally varying potential and calculating the linear response of the distribution function to the perturbation.

In order to make the problem tractable, a simple yet realistic collision model must be chosen. In Ref. 9, the particle-conserving classical relaxation-time approximation was used. The natural extension of this relatively simple collision model is the particle-conserving quantum relaxation-time approximation that was given by Mermin,[12] and this model will be used here. While these relaxation-time approximations are admittedly only rough descriptions of real scattering processes, they still retain many of the important features of scattering. Furthermore, they are extremely useful because of their relative simplicity.

In this section, we review the particle-conserving quantum relaxation-time approximation. With it, we calculate linear screening for a nondegenerate semiconductor in a high, uniform, static electric field. This calculation will differ from Ref. 9 in that quantum mechanical effects will now be included.

A. Quantum relaxation-time approximation

We begin by reviewing the classical Boltzmann-equation relaxation-time approximation, and then we proceed to discuss the quantum relaxation-time approximation. In each case, we discuss how the calculation is simplified if situations where only small spatial changes in the overall density are considered.

In the classical Boltzmann-equation case, a simple and widely used collision model is the particle-conserving relaxation-time approximation, where the collision term is

$$I_{\text{cl}}=-\frac{f_{\text{cl}}(\mathbf{p},\mathbf{R})-f_{\text{eq}}(\mathbf{p},\mu+\delta\mu(\mathbf{R}))}{\tau}\ , \quad (8a)$$

$$f_{\text{eq}}(\mathbf{p},\mu+\delta\mu(\mathbf{R}))=\frac{1}{\exp\{\beta[\varepsilon(\mathbf{p})-\mu-\delta\mu(\mathbf{R})]\}+1}\ . \quad (8b)$$

The subscripts "cl" will henceforth be used to denote classical quantities. In Eqs. (8), $\beta=1/k_{\text{B}}T$, $\varepsilon(\mathbf{p})$ is the carrier kinetic energy, μ is the global chemical potential, and $\delta\mu(\mathbf{R})$ is the change in the local chemical potential. $\delta\mu(\mathbf{R})$ is determined by local particle conservation

$$n_{\text{cl}}(\mathbf{R})=n_{\text{eq}}(\mu+\delta\mu(\mathbf{R}))\ , \quad (9)$$

where

$$n_{\text{cl}}(\mathbf{R})=\int\frac{d\mathbf{p}}{4\pi^3\hbar^3}f_{\text{cl}}(\mathbf{p},\mathbf{R})\ , \quad (10a)$$

$$n_{\text{eq}}(\mu+\delta\mu(\mathbf{R}))=\int\frac{d\mathbf{p}}{4\pi^3\hbar^3}f_{\text{eq}}(\mathbf{p},\mu+\delta\mu(\mathbf{R}))\ . \quad (10b)$$

Therefore, with this collision model, the Boltzmann equation must be solved self-consistently, since $f_{\text{cl}}(\mathbf{p},\mathbf{R})$ depends on the collision term I_{cl}, which is dependent on $\delta\mu(\mathbf{R})$, which in turn depends on $f_{\text{cl}}(\mathbf{p},\mathbf{R})$ through Eq. (9).

The quantum formulation of the particle-conserving relaxation-time approximation is further complicated by the noncommutivity of $\mathbf{p}$ and $\mathbf{R}$, and writing down the collision term is itself a nontrivial problem. As a guide to obtaining the quantum relaxation-time collision term, we utilize the approach given by Mermin.[12] Mermin modeled the collisions by a constant-rate relaxation of the nonequilibrium density matrix $\hat{\rho}$ to the local equilibrium density matrix $\hat{\rho}_{l.\text{eq}}$, where

$$\hat{\rho}_{l.\text{eq}}=\frac{1}{\exp[\beta(\hat{\varepsilon}-\mu-\delta\hat{\mu})]+1}\ . \quad (11)$$

Here, μ is the global chemical potential, $\hat{\varepsilon}$ is the kinetic energy operator, which is diagonal in the momentum representation, and $\delta\hat{\mu}$ is the *operator* for the change in the chemical potential, which is local and hence diagonal in the coordinate representation.

Since particles must be conserved locally, the condition

$$\langle \mathbf{R}|\hat{\rho}|\mathbf{R}\rangle = \langle \mathbf{R}|\hat{\rho}_{l.\mathrm{eq}}|\mathbf{R}\rangle \tag{12}$$

must be satisfied for all $\mathbf{R}$. The momentum-space representation of Eq. (12) is

$$\int \langle \mathbf{k}-\tfrac{1}{2}\mathbf{q}|\hat{\rho}|\mathbf{k}+\tfrac{1}{2}\mathbf{q}\rangle d\mathbf{k} = \int \langle \mathbf{k}-\tfrac{1}{2}\mathbf{q}|\hat{\rho}_{l.\mathrm{eq}}|\mathbf{k}+\tfrac{1}{2}\mathbf{q}\rangle d\mathbf{k} \ , \tag{13}$$

which must be satisfied for all $\mathbf{q}$. The matrix elements $\delta\mu(\mathbf{q}) = \langle \mathbf{k}-\frac{1}{2}\mathbf{q}|\delta\hat{\mu}|\mathbf{k}+\frac{1}{2}\mathbf{q}\rangle$ must be obtained self-consistently in finding the solution of the nonequilibrium density matrix $\hat{\rho}$, so that both Eq. (13) and the equation for the evolution of $\hat{\rho}$ are simultaneously satisfied. [Note that $\delta\mu(\mathbf{q}) = \langle \mathbf{k}-\frac{1}{2}\mathbf{q}|\delta\hat{\mu}|\mathbf{k}+\frac{1}{2}\mathbf{q}\rangle$ does not depend on $\mathbf{k}$, because $\delta\hat{\mu}$ is a local operator, i.e., $\langle \mathbf{r}|\delta\hat{\mu}|\mathbf{r}'\rangle = \delta\mu\,\delta(\mathbf{r}-\mathbf{r}')$.]

We now use this to construct the equivalent relaxation-time approximation for the Wigner distribution function which will be used in the collision term in Eq. (6). This is achieved by simply replacing $\hat{\rho}$ and $\hat{\rho}_{l.\mathrm{eq}}$ by their Wigner-function representations, $f(\mathbf{p},\mathbf{R})$ and $f_{l.\mathrm{eq}}(\mathbf{p},\mathbf{R})$, respectively. Then, in this approximation, the collision term in the quantum transport equation, Eq. (6), is

$$I = -\frac{f(\mathbf{p},\mathbf{R}) - f_{l.\mathrm{eq}}(\mathbf{p},\mathbf{R})}{\tau} \ , \tag{14}$$

where $f_{l.\mathrm{eq}}(\mathbf{p},\mathbf{R})$ is given by

$$f_{l.\mathrm{eq}}(\mathbf{p},\mathbf{R}) = \int \frac{d\mathbf{q}}{(2\pi)^3} \langle \hbar^{-1}\mathbf{p}-\tfrac{1}{2}\mathbf{q}|\hat{\rho}_{l.\mathrm{eq}}|\hbar^{-1}\mathbf{p}+\tfrac{1}{2}\mathbf{q}\rangle e^{i\mathbf{q}\cdot\mathbf{R}} \ . \tag{15}$$

As described above, the matrix elements $\delta\mu(\mathbf{q})$ must be obtained self-consistently so that the particle-conserving condition

$$\int \frac{d\mathbf{p}}{4\pi^3\hbar^3} f(\mathbf{p},\mathbf{R}) = \int \frac{d\mathbf{p}}{4\pi^3\hbar^3} f_{l.\mathrm{eq}}(\mathbf{p},\mathbf{R}) \tag{16}$$

and Eq. (6) are simultaneously satisfied.

In either the classical or the quantum-mechanical relaxation-time models, solving the equations self-consistently with arbitrary spatial density variations is an extremely formidable task. In one case, the classical model has been used in a highly spatially inhomogeneous system to study transport of carriers through a microstructure,[18] but extensive numerical calculations had to be performed to obtain the full solution. Any attempt to do the quantum case would be considerably more difficult. However, when only small spatial variations in the density are considered, the calculations simplify considerably, as we will now show.

In the classical case, if the density $n_{\mathrm{cl}}(\mathbf{R})$ has small spatial variations, then $\delta\mu(\mathbf{R})$ will be small, and hence $f_{\mathrm{eq}}(\mathbf{R},\mu+\delta\mu(\mathbf{R}))$ can be expanded in powers of $\delta\mu(\mathbf{R})$:

$$f_{\mathrm{eq}}(\mathbf{p},\mu+\delta\mu(\mathbf{R})) = f_{\mathrm{eq}}(\mathbf{p},\mu) + \frac{\partial f_{\mathrm{eq}}}{\partial\mu}(\mathbf{p},\mu)\delta\mu(\mathbf{R}) + O(\delta\mu^2) \ . \tag{17}$$

Therefore, when the spatial variations in density are small, $\delta\mu(\mathbf{R})$ is proportional to the change in the density. When Eq. (17) is substituted into the I_{cl} in Eq. (8a) and terms second order and higher in $\delta\mu$ are neglected, we see that the term due to the inhomogeneity in density is linear in the change in density. This often simplifies matters considerably.

As in the classical case, in the quantum-mechanical relaxation-time approximation, simplifications also occur when only small spatial variations in density are considered. The matrix elements of $\langle \mathbf{k}+\frac{1}{2}\mathbf{q}|\hat{\rho}_{l.\mathrm{eq}}|\mathbf{k}+\frac{1}{2}\mathbf{q}\rangle$ can be written in a series expansion in powers of $\delta\mu(\mathbf{q})$, viz.,[12]

$$\langle \mathbf{k}-\tfrac{1}{2}\mathbf{q}|\hat{\rho}_{l.\mathrm{eq}}|\mathbf{k}+\tfrac{1}{2}\mathbf{q}\rangle = f_{\mathrm{eq}}(\hbar\mathbf{k})\delta_{\mathbf{q},0} - \frac{f_{\mathrm{eq}}(\hbar\mathbf{k}-\frac{1}{2}\hbar\mathbf{q}) - f_{\mathrm{eq}}(\hbar\mathbf{k}+\frac{1}{2}\hbar\mathbf{q})}{\varepsilon(\hbar\mathbf{k}-\frac{1}{2}\hbar\mathbf{q}) - \varepsilon(\hbar\mathbf{k}+\frac{1}{2}\hbar\mathbf{q})}\delta\mu(\mathbf{q}) + O((\delta\mu)^2) \ . \tag{18}$$

(For convenience, we will suppress the μ dependence of f_{eq}.) For small spatial variations in the density, the second-order terms in $\delta\mu$ are negligible, and therefore, the Fourier components of the spatial density are simply linearly dependent on $\delta\mu(\mathbf{q})$.

The expansion (18) can be used to simplify the relaxation-time collision term in the quantum transport equation. We assume there is a small spatial sinusoidal variation in the density; small arbitrary variations in the density can be treated as linear superpositions of these sinusoidal variations. Then, the Wigner distribution function is[19]

$$f(\mathbf{p},\mathbf{R},T) = f_0(\mathbf{p}) + f_1(\mathbf{p})e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)} \ , \tag{19}$$

with $n_0 \gg |n_1|$, where

$$n_0 = \int \frac{d\mathbf{p}}{4\pi^3\hbar^3} f_0(\mathbf{p}) \ , \tag{20a}$$

$$n_1 = \int \frac{d\mathbf{p}}{4\pi^3\hbar^3} f_1(\mathbf{p}) \ . \tag{20b}$$

Using Eqs. (15), (16), (18), and (19), we obtain

$$\delta\mu(\mathbf{q}) = -\frac{n_1}{\chi_L(\mathbf{q},0)} , \tag{21}$$

where

$$\chi_L(\mathbf{q},\omega) = \int \frac{d\mathbf{p}}{4\pi^3\hbar^3} \frac{f_{eq}(\mathbf{p}+\frac{1}{2}\hbar\mathbf{q}) - f_{eq}(\mathbf{p}-\frac{1}{2}\hbar\mathbf{q})}{\varepsilon(\mathbf{p}+\frac{1}{2}\hbar\mathbf{q}) - \varepsilon(\mathbf{p}-\frac{1}{2}\hbar\mathbf{q}) - \hbar\omega} \tag{22}$$

will be recognized as the Lindhard expression for the susceptibility.[20] The relaxation-time collision term for the Wigner distribution function, in the limit of small sinusoidal density variations, is obtained by substituting Eqs. (15) and (19) into Eq. (14) and using Eq. (18), yielding

$$I = -\frac{f_0(\mathbf{p}) + f_1(\mathbf{p}) e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)} - [f_{eq}(\mathbf{p}) + \delta f(\mathbf{p},\mathbf{q}) n_1 e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)}]}{\tau} , \tag{23}$$

where

$$\delta f(\mathbf{p},\mathbf{q}) = \frac{1}{\chi_L(\mathbf{q},0)} \frac{f_{eq}(\mathbf{p}+\frac{1}{2}\hbar\mathbf{q}) - f_{eq}(\mathbf{p}-\frac{1}{2}\hbar\mathbf{q})}{\varepsilon(\mathbf{p}+\frac{1}{2}\hbar\mathbf{q}) - \varepsilon(\mathbf{p}-\frac{1}{2}\hbar\mathbf{q})} . \tag{24}$$

In the limit that $q \to 0$, $\delta f(\mathbf{p},\mathbf{q})$ approaches

$$\delta f(\mathbf{p}, q\to 0) = \frac{\partial f_{eq}(\mathbf{p})}{\partial\mu} \frac{\partial\mu}{\partial n_{eq}} . \tag{25}$$

This is the expression for the classical relaxation-time approximation, obtained by substituting Eq. (17) into Eq. (8a). As expected, as the q approaches zero, the Bohr correspondence principle ensures that we regain the classical result from the quantum formulation. As q increases, $\delta f(\mathbf{p},\mathbf{q})$ broadens in momentum space, as expected from the Heisenberg uncertainly principle. In Fig. 1, $\delta f(\mathbf{p},\mathbf{q})$ is shown as a function of p for various values of q.

B. Linear screening in high electric fields

Linear screening is due to the linear carrier-density response $n_1 e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)}$ to a potential $U_1 e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)}$. The procedure for calculating linear screening with the quantum transport equation, Eq. (6), is essentially identical to the procedure used with the Boltzmann equation, as described in Ref. 9. The procedure is as follows. (i) For the nonequilibrium situation being investigated, set up and solve the quantum transport equation to obtain the "unperturbed" Wigner distribution function $f_0(\mathbf{R},\mathbf{p},T)$. (ii) Linearly perturb the transport equation with an additional small sinusoidal potential $U_{eff}(\mathbf{R},T) = U_1 e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)}$ to produce a response $f_1(\mathbf{p}) e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)}$ in the Wigner function, 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 $\epsilon(\mathbf{q},\omega) = 1 - 4\pi e^2 \chi(\mathbf{q},\omega)/q^2$. Kadanoff and Baym used a similar technique to calculate screening in a collisionless plasma at equilibrium, and they obtained the Lindhard result.[21]

As in Ref. 9, we study the linear screening of carriers in a uniform, static electric field as an example of this technique. The collisions are approximated by the quantum particle-conserving relaxation-time model described in Sec. III A, and to keep the calculation as simple as possible, the carriers are chosen to be in parabolic-band semiconductor. Then, the "unperturbed" quantum transport equation is identical to the Boltzmann equation with the relaxation-time approximation model

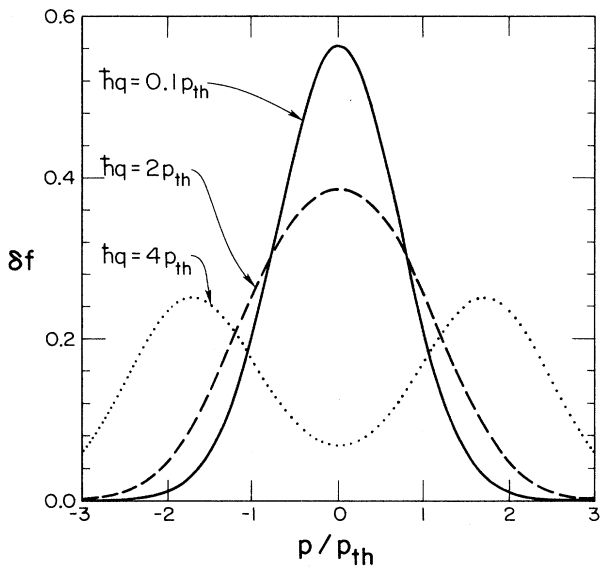

FIG. 1. The function $\delta f(\mathbf{p},\mathbf{q})$ to which a small sinusoidal density perturbation $f_1(\mathbf{p}) e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)}$ relaxes, in the quantum relaxation-time approximation of the collision term. $\delta f(p)$ is plotted as a function of p for various values of q (the component of $\mathbf{q}$ parallel to $\mathbf{p}$), and $\delta f(p)$ is normalized so that the area under each curve is 1. That is for a nondegenerate system, where $f_{eq}(p)$ is the Maxwell-Boltzmann distribution function. The three curves correspond to $\hbar q = 0.1 p_{th}$, $\hbar q = 2 p_{th}$, and $\hbar q = 4 p_{th}$. In the limit $\hbar q \to 0$, $\delta f(p)$ approaches the Maxwell-Boltzmann distribution function. For $\hbar q = 0.1 p_{th}$, $\delta f(p)$ is still very similar to the Maxwell-Boltzmann distribution. As $\hbar q$ increases, $\delta f(p)$ broadens in momentum space (see the $\hbar q = 2 p_{th}$ curve), as expected from the uncertainty relation between p and q. For even larger values of q, the maximum of $\delta f(p)$ moves away from $p = 0$, as shown in the $\hbar q = 4 p_{th}$ curve.

$$F\frac{\partial f_0}{\partial p_z}(\mathbf{p})=-\frac{f_0(\mathbf{p})-f_{\rm eq}(\mathbf{p})}{\tau}\ . \tag{26}$$

The perturbation $U_{\rm eff}(\mathbf{R},T)=U_1 e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)}$ is then added to the quantum transport equation, Eq. (6), and the Wigner distribution function is assumed to respond linearly with the field, i.e.,

$$f(\mathbf{p},\mathbf{R},T)=f_0(\mathbf{p})+f_1(\mathbf{p})e^{i(\mathbf{q}\cdot\mathbf{R}-\omega T)}\ , \tag{27}$$

with $f_1\propto U_1$. This sinusoidal density variation modifies the quantum relaxation-time collision approximation, as is shown in Eq. (23). When the "unperturbed" solution is subtracted away from the "perturbed" transport equation, and keeping only first-order terms in U_1 and f_1 from the resulting equation, we have

$$F\frac{\partial f_1}{\partial p_z}+i\left[\frac{\mathbf{p}\cdot\mathbf{q}}{m}-\omega\right]f_1(\mathbf{p})-\frac{iU_1}{\hbar}(f_0(\mathbf{p}+\tfrac{1}{2}\hbar\mathbf{q})-f_0(\mathbf{p}-\tfrac{1}{2}\hbar\mathbf{q}))$$
$$=-\frac{1}{\tau}\left[f_1(\mathbf{p})-\frac{n_1}{\chi_L(q,0)}\frac{f_{\rm eq}(\mathbf{p}+\frac{1}{2}\hbar\mathbf{q})-f_{\rm eq}(\mathbf{p}-\frac{1}{2}\hbar\mathbf{q})}{\varepsilon(\mathbf{p}+\frac{1}{2}\hbar\mathbf{q})-\varepsilon(\mathbf{p}-\frac{1}{2}\hbar\mathbf{q})}\right]\ . \tag{28}$$

This is a simple first-order inhomogeneous differential equation, and can be solved to yield

$$f_1(\mathbf{p})=\int_{-\infty}^{p_z}dp_z'\left[\frac{iU_1}{\hbar F}[f_0(\mathbf{p}'+\tfrac{1}{2}\hbar\mathbf{q})-f_0(\mathbf{p}'-\tfrac{1}{2}\hbar\mathbf{q})]+\frac{n_1}{F\tau\chi_L(q,0)}\left[\frac{f_{\rm eq}(\mathbf{p}'+\frac{1}{2}\hbar\mathbf{q})-f_{\rm eq}(\mathbf{p}'-\frac{1}{2}\hbar\mathbf{q})}{\hbar\mathbf{p}'\cdot\mathbf{q}/m}\right]\right]$$
$$\times\exp\left\{\frac{(p_z'-p_z)}{F\tau}\left[1+i\left[\frac{p_xq_x+p_yq_y}{m}-\omega\right]\tau\right]+i\frac{[(p_z')^2-p_z^2]q_z}{2mF}\right\}\ . \tag{29}$$

To obtain an equation relating n_1 to U_1, Eq. (29) is integrated with respect to $\mathbf{p}$, yielding

$$n_1\left[1-\frac{1}{\chi_L(q,0)}\int_0^\infty\frac{dt}{\tau}\exp\left[-\frac{i\mathbf{F}\cdot\mathbf{q}t^2}{2m}+i\omega t-\frac{t}{\tau}\right]\int\frac{d\mathbf{p}}{4\pi^3\hbar^3}\exp\left[-i\frac{t}{m}\mathbf{p}\cdot\mathbf{q}\right]\left[\frac{f_{\rm eq}(\mathbf{p}+\frac{1}{2}\hbar\mathbf{q})-f_{\rm eq}(\mathbf{p}-\frac{1}{2}\hbar\mathbf{q})}{\hbar\mathbf{q}\cdot\mathbf{p}/m}\right]\right]$$
$$=\frac{iU_1}{\hbar}\int_0^\infty dt\exp\left[-\frac{i\mathbf{F}\cdot\mathbf{q}t^2}{2m}+i\omega t-\frac{t}{\tau}\right]\int\frac{d\mathbf{p}}{4\pi^3\hbar^3}\exp\left[-i\frac{t}{m}\mathbf{p}\cdot\mathbf{q}\right][f_0(\mathbf{p}+\tfrac{1}{2}\hbar\mathbf{q})-f_0(\mathbf{p}-\tfrac{1}{2}\hbar\mathbf{q})]\ . \tag{30}$$

As a check, on setting $\mathbf{F}=0$ and $f_0=f_{\rm eq}$, we regain the result obtained by Mermin[12] for an equilibrium system.

We specialize further to the case of a nondegenerate semiconductor, when $f_{\rm eq}(\mathbf{p})$ is the Maxwell-Boltzmann distribution function,

$$f_{\rm eq}(\mathbf{p})=n_0\frac{4\hbar^3(\pi^3)^{1/2}}{p_{\rm th}^3}\exp(-p^2/p_{\rm th}^2)\ , \tag{31}$$

where $p_{\rm th}=(2k_BmT)^{1/2}$ is the carrier thermal momentum. The Fourier transform of $f_0(\mathbf{p})$ is easily obtained from Eq. (26), and when used in Eq. (30), we obtain

$$n_1\left[1-\frac{n_0}{k_BT\chi_L(q,0)}\int_0^\infty dx\exp\left[-\frac{i\mathbf{s}\cdot\mathbf{k}_dx^2}{2}+i\omega\tau x-x\right]\exp\left[-\frac{x^2s^2}{4}\right]\left[\frac{\exp(-ixs\tilde{q}/2)Z(-ixs/2+\tilde{q}/2)+\text{c.c.}}{2\tilde{q}}\right]\right]$$
$$=-\frac{2U_1\tau n_0}{\hbar}\int_0^\infty dx\exp\left[-\frac{i\mathbf{s}\cdot\mathbf{k}_dx^2}{2}+i\omega\tau x-x\right]\sin\left[\frac{x\tilde{q}s}{2}\right]\frac{\exp(-x^2s^2/4)}{1+i\mathbf{k}_d\cdot\mathbf{s}x}\ . \tag{32}$$

Here, $\mathbf{k}_d=\mathbf{p}_d/p_{\rm th}$ ($\mathbf{p}_d=\mathbf{F}\tau$ is the average drift momentum of the carriers), $\tilde{q}=\hbar q/p_{\rm th}$, $\mathbf{s}=\mathbf{q}l_{\rm th}$ ($l_{\rm th}=p_{\rm th}\tau/m$), and $Z(\xi)$ is the plasma dispersion function.[22] The susceptibility $\chi(\mathbf{q},\omega)=n_1/U_1$ can be produced from Eq. (32).

C. Discussion

In the classical derivation of the susceptibility, the only two length scales that were important were the carrier thermal mean free path $l_{\rm th}=p_{\rm th}\tau/m$ and the carrier drift mean free path $l_d=p_d\tau/m$. In the regime $q\max(l_{\rm th},l_d)\ll 1$ and $\omega\tau\ll 1$, the carriers are not ballistic over the distance of a wavelength, and local equations apply; therefore the screening can be derived from the drift-diffusion and continuity equations.[9]

The quantum-mechanical nature of the carriers necessitates the introduction of a third length scale. For a nondegenerate semiconductor, this length is the thermal de Broglie wave vector, $q_{\rm dB}=p_{\rm th}/\hbar$, which is the inverse

of the average wavelength of a thermal electron. This sets the scale at which the quantum-mechanical screening differs from the classical screening.

In Fig. 2 we show the static susceptibility $\chi(\mathbf{q},\omega=0)$ obtained from (1) the Kadanoff-Baym quantum transport equation and (2) the Boltzmann equation, both using their respective relaxation-time approximations. For $q_{\rm dB} \ll q$, the two approaches yield virtually identical results. On the other hand, for $q > q_{\rm dB}$ the two approaches produce markedly different curves. For $q \to \infty$ the curve derived from the Boltzmann equation asymptotically approaches the susceptibility of a collisionless classical plasma.[9] The curve derived from the quantum kinetic equation, however, tends towards the Lindhard form, with the equilibrium distribution functions replaced by the nonequilibrium ones, i.e.,

$$\chi(\mathbf{q},\omega)=\int \frac{d\mathbf{p}}{4\pi^3\hbar^3} \times \frac{f_0(\mathbf{p}+\frac{1}{2}\hbar\mathbf{q})-f_0(\mathbf{p}-\frac{1}{2}\hbar\mathbf{q})}{\varepsilon(\mathbf{p}+\frac{1}{2}\hbar\mathbf{q})-\varepsilon(\mathbf{p}-\frac{1}{2}\hbar\mathbf{q})-\hbar\omega-i0^+} \quad \text{as } q \to \infty \ . \tag{33}$$

This result for $\chi(\mathbf{q},\omega)$ was obtained by Barker,[2] but with no apparent limits on the validity of the result as a function of q. This paper shows that Eq. (33) is valid only in the regime where the carriers are essentially ballistic over the wavelength $1/q$; that is, in the regime where the classical transport equation would have given a $\chi(\mathbf{q},\omega)$ of the form for a collisionless plasma[9,23]

$$\chi(\mathbf{q},\omega)=\int \frac{d\mathbf{p}}{4\pi^3\hbar^3} \frac{\mathbf{q}\cdot\nabla f_0(\mathbf{p})}{\mathbf{q}\cdot\mathbf{p}/m-\omega-i0^+} \ . \tag{34}$$

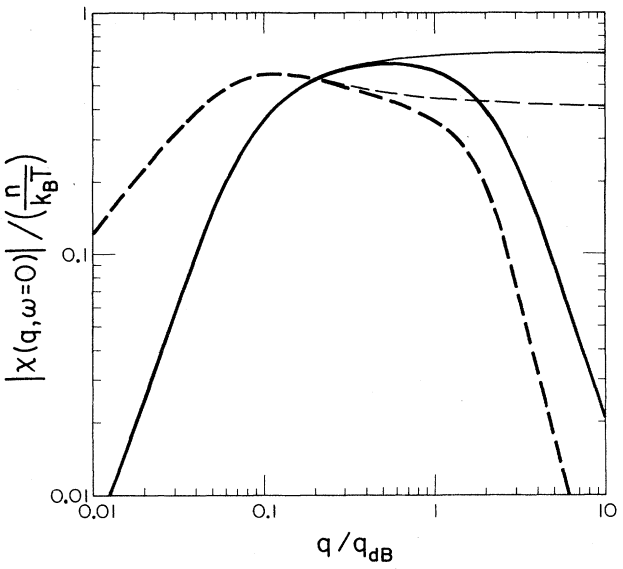

FIG. 2. The imaginary (dashed lines) and negative real (solid lines) parts of the normalized nonequilibrium static susceptibility $\chi(\mathbf{q},\omega=0)/(n/k_BT)$, for $\mathbf{p}_d\cdot\hat{\mathbf{q}}=0.4p_{\rm th}$ and $q_{\rm dB}l_{\rm th}=10$. The normalization is chosen so that, at equilibrium, $\chi(\mathbf{q}\to 0,\omega=0)/(n/k_BT)=-1$. The bold lines are obtained from the quantum kinetic equations, while, for comparison, the thin lines are obtained from the Boltzmann equation (see Ref. 9). For q smaller than $q_{\rm dB}$, the two approaches give similar results, but for $q > q_{\rm dB}$, they differ. In this $q \to \infty$ limit, the thin line tends to the susceptibility of a collisionless classical plasma, whereas the bold line tends to that of the Lindhard form with the equilibrium distribution functions replaced by the nonequilibrium ones.

The ratio of lengths scales $q_{\rm dB}l_{\rm th}$ for Fig. 1 was chosen to be 10. Because $q_{\rm dB}l_{\rm th} \gg 1$, the "drift-diffusion" regime $q \ll 1/l_{\rm th}$ is separated from the Lindhard regime $q \gg q_{\rm dB}$. In the limit where $q_{\rm dB}l_{\rm th} < 1$, on the other hand, the results in this paper would be rather suspect. This is because the system would be in a regime where the scattering was so strong that the mean free path was less than the electron wavelength, leading to a "weak-localization"-type regime, where the concept of freely propagating quasiparticles is somewhat questionable.

Finally, we mention that in this paper we have ignored the effects of the high field on the scattering *per se* in the transport equation—what is known as the "intracollisional field effect." It has been estimated[17] that this effect, which broadens the energy-conserving δ functions in the scattering term, start to become noticeable at fields of the order of several MV m^{-1}. This effect might be important when precise scattering mechanisms are used, but since scattering is represented in this paper only at a simple and imprecise level, inclusion of this effect would only serve to make the approximation much more complicated, but no more precise.

IV. SUMMARY

We have applied the Kadanoff-Baym transport equation develop a method for calculating the screening of systems that are out of equilibrium. This method is an extension of the Boltzmann-equation method utilized by Hu and Wilkins.[9] In order to make calculations tractable, we have used a particle-conserving quantum relaxation-time approximation, introduced by Mermin, as the collision term for the transport equation. This collision term is again the quantum extension of the classical particle-conserving relaxation-time approximation used previously by Hu and Wilkins.

As an example, we have used this formulation and the quantum relaxation-time approximation to study the linear screening of a parabolic-band semiconductor in a high electric field, and we have compared the results for this formulation with the classical Boltzmann-equation formulation of nonequilibrium screening used earlier. We have found that the Boltzmann-equation method gave reliable results for $q \ll q_{\rm dB}$, but for $q > q_{\rm dB}$ quantum effects due to spatial nonlocality of the electrons start to dominate, and the susceptibility approaches a Lindhard-like formula, with the equilibrium distribution functions replaced by the nonequilibrium ones.

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*Present address.
[1]See, e.g., *Hot Carriers in Semiconductors,* edited by J. Shah and G. J. Iafrate (Pergamon, London, 1988).
[2]J. R. Barker, Solid State Commun. **32**, 1013 (1979).
[3]D. Lowe, Ph.D. thesis, University of Warwick, 1983.
[4]P. Lugli and D. K. Ferry, Phys. Rev. Lett. **56**, 1295 (1986).
[5]G. Berthold and P. Kocevar, J. Phys. C **17**, 4981 (1984).
[6]D. Lowe and J. R. Barker, J. Phys. C **18**, 2507 (1985).
[7]X. L. Lei and C. S. Ting, J. Phys. C **18**, 77 (1985); X. L. Lei and C. S. Ting, Phys. Rev. B **32**, 1112 (1985).
[8]N. S. Wingreen, C. J. Stanton, and J. W. Wilkins, Phys. Rev. Lett. **57**, 1084 (1986).
[9]B. Y.-K. Hu and J. W. Wilkins, this issue, Phys. Rev. B **39**, 8464 (1989).
[10]J. Lindhard, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. **28**, No. 8 (1954).
[11]Strictly speaking, this is known to be rigorously valid only in the high-density limit, but it has been used with success even in low-density situations.
[12]N. D. Mermin, Phys. Rev. B **1**, 2362 (1970).
[13]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, Reading, Mass., 1962).
[14]An equivalent but slightly different formulation was given independently by L. V. Keldysh, Zh. Eksp. Teor. Fiz. **47**, 1515 (1964) [Sov. Phys.—JETP **20**, 1018 (1965)]. A fusion of these two formalisms is given by D. C. Langreth, in *Linear and Non-Linear Electron Transport in Solids,* edited by J. T. Devreese and E. Van Boren (Plenum, New York, 1976).
[15]L. P. Kadanoff and G. Baym, in *Linear and Non-Linear Electron Transport in Solids,* Ref. 14, p. 103.
[16]J. R. Barker and D. K. Ferry, Phys. Rev. Lett. **42**, 1779 (1979).
[17]K. S. Khan, J. H. Davies, and J. W. Wilkins, Phys. Rev. B **36**, 2578 (1987).
[18]H. U. Baranger and J. W. Wilkins, Phys. Rev. B **30**, 7349 (1984).
[19]The Wigner distribution function is always real. Therefore, in Eq. (19), we implicity assume that the real part is taken.
[20]In the notation of Ref. 12, $\chi_L(\mathbf{q},\omega)=-B(\mathbf{q},\omega)$.
[21]L. P. Kadanoff and G. Baym, *Linear and Non-Linear Electron Transport in Solids,* Ref. 14, p. 70.
[22]B. D. Fried and S. D. Conte, *The Plasma Dispersion Function* (Academic, London, 1961).
[23]Note that the expression χ in Eq. (33) reduces to that of a collisionless plasma, Eq. (34), in the limit that $\hbar q \to 0$. Therefore, the collisionless-plasma result is simply the classical limit of Eq. (33).