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NONEQUILIBRIUM GREEN'S FUNCTIONS FOR HIGH-FIELD QUANTUM TRANSPORT THEORY

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A formulation of the Kadanoff-Baym-Keldysh theory of nonequilibrium quantum statistical mechanics is developed in order to describe nonperturbatively the effects of the electric field on electron-phonon scattering in nondegenerate semiconductors. We derive an analytic, gauge-invariant model for the spectral density of energy states that accounts for both intracollisional field effect and collisional broadening simultaneously. A kinetic equation for the quantum distribution function is derived and solved numerically. The nonlinear drift velocity versus applied field characteristics is also evaluated numerically. Many features of our nonlinear theory bear formal resemblance to linear-response theory.

1. Introduction

Quantum effects play an important role on the dynamics of charge transport in electronic devices whose sizes decrease and reach the nanometer scale.

The semiclassical description of charge transport phenomena in semiconductors, whether based on the Boltzmann equation[1] or on Monte Carlo techniques,[2] relies on the Fermi Golden Rule for the calculation of the transition rates. The sharp δ-function appearing in these quantities implies that both energy and momentum are well-defined observables of the system such that when a particle suffers a collision with one of the crystal modes, its energy and momentum can only change by an amount equal to the energy and momentum of the phonon involved in the scattering event.

As the size of the sample decreases, however, quantum interference effects may come into play[3] since now the charges may maintain their phase coherence over distances comparable with the characteristic length (e.g., the gate length or a depletion length) of the device. The uncertainty relations might therefore play an important role and the broadening of the electron momentum should be considered. Also the mean collision duration and the mean-free time may not be negligible compared with the transit time through the device and the long-time limit required to establish the conservation of energy if the Fermi Golden Rule will break down. This

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phenomenon is called "collisional broadening" (CB).[4] Furthermore, in submicron devices, ordinary applied voltages lead to very high electric fields, and since collisions cannot be treated as instantaneous, the presence of an electric field further contributes in modifying the energy difference between the initial and final states. This is the "intra-collisional field effect" (ICFE).[5]

It has been a long-standing problem in the physics of nonequilibrium phenomena, to construct a first-principles theory of transport which is capable of overcoming the limitations of the semiclassical approach and of treating arbitrarily strong accelerating field. Of the many candidate theories, the nonequilibrium Green's function formalism, as developed by Kadanoff and Baym,[6] and by Keldysh,[7] has received considerable attention in the recent past.

The central objects in this theory are the four quantities

$$\begin{aligned} G^{<}(1,2) &= \pm\frac{i}{\hbar}\langle\hat{\Psi}^{\dagger}(2)\hat{\Psi}(1)\rangle\ , \quad G^{r}(1,2) = -\frac{i}{\hbar}\langle[\hat{\Psi}(1),\ \hat{\Psi}^{\dagger}(2)]_{\pm}\rangle\vartheta(t_1-t_2) \\ G^{>}(1,2) &= -\frac{i}{\hbar}\langle\hat{\Psi}(1)\hat{\Psi}^{\dagger}(2)\rangle\ , \quad G^{a}(1,2) = \frac{i}{\hbar}\langle[\hat{\Psi}(1),\ \hat{\Psi}^{\dagger}(2)]_{\pm}\rangle\vartheta(t_2-t_1) \end{aligned} \tag{1.1}$$

expressing the correlation between the field operator $\hat{\Psi}(1)$ of the particle at the space-time point $1 \equiv (\mathbf{r}_1, t_1)$ and the conjugate field operator $\hat{\Psi}^{\dagger}(2)$ at another point $2 \equiv (\mathbf{r}_2, t_2)$. Here $\vartheta(x)$ is the unit step function and the $+(-)$ sign refers to fermions and anticommutation (boson and commutation). The angular bracket $\langle\ldots\rangle$ indicates a thermodynamic average for systems in equilibrium, and an average over the available states for nonequilibrium distributions. The interactions of the particles with the crystal are represented by the equivalent self-energy functions[8,9]

$$\begin{aligned} \Sigma^{<,>}(1,2) &= G^{<,>}(1,2)D^{<,>}(1,2) \\ \Sigma^{r,a}(1,2) &= G^{r,a}(1,2)D^{>}(1,2) + G^{<}(1,2)D^{r,a}(1,2) \end{aligned} \tag{1.2}$$

in the Born approximation, for weakly coupled systems, with D indicating the phonon propagator including the electron-phonon interaction matrix element.

From its definition, $G^{<}$ is proportional to the density of particles, and therefore has the character of a distribution function. Indeed, the average value $\langle Q\rangle$ of any operator Q that is the sum of one-body terms can be expressed immediately in terms of $G^{<}$,[10]

$$\langle Q(t)\rangle = \int d\mathbf{r}\langle\hat{\Psi}^{\dagger}(\mathbf{r},t)Q(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\rangle = \pm i\hbar\int d\mathbf{r}\lim_{\mathbf{r}\to\mathbf{r}'} Q(\mathbf{r},t)G^{<}(\mathbf{r},t;\mathbf{r}',t')\ , \tag{1.3}$$

by virtue of the commutation properties of the field operators.

Another important function is the special density defined as[11]

$$A(1,2) = \frac{1}{\hbar}\langle[\hat{\Psi}(1),\ \hat{\Psi}^{\dagger}(2)]_{+}\rangle\ . \tag{1.4}$$

When $t_1 = t_2$, this becomes

$$A(\mathbf{r}_1, \mathbf{r}_2, t) = \delta(\mathbf{r}_1 - \mathbf{r}_2) \ , \tag{1.5}$$

as a consequence of the equal-time commutation of the field operators. For homogeneous systems A is a function only of the difference of its arguments and Eq. (1.5) can be Fourier transformed leading to the sum-rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(\mathbf{k}, \omega) = 1 \ . \tag{1.6}$$

It is also easily seen that the summation over all momentum states provides the density of states

$$\rho(\omega) = \int_{-\infty}^{\infty} \frac{d\mathbf{k}}{(2\pi)^3} A(\mathbf{k}, \omega) \ . \tag{1.7}$$

All of these properties make the spectral density an essential quantity to evaluate, since it can be clearly interpreted as a weighting function (of total weight unity) giving the conditional probability that a particle in state $\mathbf{k}$ will have energy $\hbar\omega$.[6,12] In other words, the electron energy $\hbar\omega$ and its momentum $\hbar\mathbf{k}$ are treated as independent quantities, related to each other according to a spectral density function $A(\mathbf{k}, \omega)$ of finite width, rather than through the sharp δ-function of the Fermi Golden Rule. In the semiclassical theory, where the electrons are in plane-wave states, the spectral density function reduces to

$$A(\mathbf{k}, \omega) = 2\pi\delta(\hbar\omega - \varepsilon(\mathbf{k})) \ ,$$

expressing the fact that there is just one possible energy for each momentum $\hbar\mathbf{k}$.

The definition (1.4) is equivalent to[6]

$$A = i(G^{>} - G^{<}) = i(G^{r} - G^{a}) = -2\,\mathrm{Im}\,G^{r} \ , \tag{1.8}$$

so that A can be determined from the knowledge of the retarded Green's function G^r. The evaluation of $G^<$ and G^r therefore, allows, a least in principle, to completely characterize the transport properties of a quantum system.

The equations of motion for the various Green's function follow directly, and exactly (provided a self-energy can be defined), from the Schrödinger equation for the field operators $\hat{\Psi}$ and $\hat{\Psi}^{\dagger}$. They can be expressed, by using the matrix notation[13]

$$\overleftrightarrow{\mathbf{G}} = \begin{pmatrix} G_t & -G^{<} \\ G^{>} & -G_{\bar{t}} \end{pmatrix} \ , \quad \overleftrightarrow{\Sigma} = \begin{pmatrix} \Sigma_t & -\Sigma^{<} \\ \Sigma^{>} & -\Sigma_{\bar{t}} \end{pmatrix}$$

($G_t = G^< + G^r$, $G_{\bar{t}} = G^< - G^a$, and analogously for $\Sigma_{t,\bar{t}}$) as

$$\left[G_0^{-1}(1) - U(1)\right] \overleftrightarrow{\mathbf{G}}(1, 2) = \delta^4(1-2)\overleftrightarrow{\mathbf{I}} + \int d3\overleftrightarrow{\Sigma}(1, 3)\overleftrightarrow{\mathbf{G}}(3, 2) \tag{1.9a}$$

$$\left[G_0^{-1}(2) - U(2)\right] \overleftrightarrow{\mathbf{G}}(1, 2) = \delta^4(1-2)\overleftrightarrow{\mathbf{I}} + \int d3\overleftrightarrow{\mathbf{G}}(1, 3)\overleftrightarrow{\Sigma}(3, 2) \ , \tag{1.9b}$$

$\overleftrightarrow{\mathbf{I}}$ is the identity matrix, U the external potential and G_0^{-1} the operator $G_0^{-1} = i\hbar\frac{\partial}{\partial t} - H_0$, with H_0 the unperturbed Hamiltonian. Equivalently, we can calculate $\overleftrightarrow{\mathbf{G}}$ by solving Dyson's equation

$$\overleftrightarrow{\mathbf{G}}(1, 2) = \overleftrightarrow{\mathbf{G}}_0(1, 2) + \int d3\overleftrightarrow{\mathbf{G}}_0(1, 3)U(3)\overleftrightarrow{\mathbf{G}}(3, 2) + \int d3d4\overleftrightarrow{\mathbf{G}}_0(1, 3)\overleftrightarrow{\Sigma}(3, 4)\overleftrightarrow{\mathbf{G}}(4, 2) \ , \tag{1.10}$$

with $\overleftrightarrow{\mathbf{G}}_0$ as the free-particle propagator.

These equations are easily solved for homogeneous systems in equilibrium, where the arguments of the Green's functions depend only upon the difference of their arguments: $(1, 2) = (1-2)$. In these cases, the Fourier transforms of these quantities will be diagonal in both $\mathbf{k}$ and ω. Equations (1.9) are then just algebraic equations,[12] each leading to the same result[14]

$$\begin{aligned} G^r(\mathbf{k}, \omega) &= \left[G_0^{-1}(\mathbf{k}, \omega) - \Sigma^r(\mathbf{k}, \omega)\right]^{-1} \ , \\ G^<(\mathbf{k}, \omega) &= G^r(\mathbf{k}, \omega)\Sigma^<(\mathbf{k}, \omega)G^a(\mathbf{k}, \omega) \ , \end{aligned} \tag{1.11}$$

or, equivalently[6]

$$G^<(\mathbf{k}, \omega) = A(\mathbf{k}, \omega)f(\mathbf{k}, \omega) \ , \tag{1.12a}$$

$$f(\mathbf{k}, \omega) = -\frac{\Sigma^<(\mathbf{k}, \omega)}{2\,\mathrm{Im}\,\Sigma^r(\mathbf{k}, \omega)} \ , \tag{1.12b}$$

directly connecting (through A) G^r to $G^<$.

This is also true in linear response theory, where the low external fields are treated as a perturbation of the homogeneous system and the quantities involved in the calculation of the conductivity, turn out to be just equilibrium quantities.[15,16]

In highly nonequilibrium conditions, we have to consider functions of their separate arguments, no relation of the type (1.12) holds, and a separate equation of motion for $G^<$ is required.[17] Equations (1.9) and (1.10) then, become quite difficult to solve. First of all, the complicated intertwining of temporal and space coordinates, that appears when the interactions are modified by the external fields, make the multiple integrations prohibitively involved. Secondly, the various Green's functions (1.1) are now linked to each other in a complicated manner and one must solve two coupled equations self-consistently. For instance, the equation of motion

for $G^<$ (the Kadanoff-Baym-Keldysh (KBK) equation) requires, as input, the retarded function G^r. The equation for G^r (Dyson's equation (DE)) demands, in its turn, the knowledge of the self-energy Σ^r which involves $G^<$ itself. All this results in extreme complications whose full consequences have not been analyzed yet in the literature.

Consequently, many groups[17] have studied the equation of motion for the Wigner function f^{W}, which is related to the correlation function $G^<$ via

$$f^{\mathrm{W}}(\mathbf{k}) \equiv \int \frac{d\omega}{2\pi i} G^<(\mathbf{k}, \omega) \ , \tag{1.13}$$

with the hope that a more manageable result emerges. This line of attack is not without problems, however. First, there is no universal agreement about the sequence of approximations reducing the full KBK equation to an equation for the Wigner function (in fact, it is not clear if this can be done, even in principle), and second, the final equations are so complicated that additional approximations are needed before numerical work becomes feasible. Not surprisingly, a variety of different, and partially contradicting results have been published.[18–22] In this review, our intention is not to take part in this discussion, but rather to present a new scheme which was recently proposed[14,23–26] by the author and her collaborators and which, we believe, is free from the above mentioned difficulties.

The approach is based on the idea that, in order to include both CB and ICFE simultaneously, scattering events should not be considered as occurring between states described by the plane waves of a free electron, as was the case of previous formulations, but between the states of an electron in the external potential. In order to introduce the proper symmetries of the nonequilibrium system from the very beginning and maintain them consistently throughout the calculations, however, these states should be used as a transform basis. In other words, instead of the usual Fourier transform, one should be define the integral transform which is most appropriate for the system under consideration, according to the type and form of the external field.

Finally, one should assure the gauge invariance of the result obtained in this way because of the explicit gauge dependence that may be introduced by these transforms.

We have implemented this idea for an electron system under the influence of an external, uniform electric field theory of arbitrary strength represented through a scalar potential. In this case, the transform basis is made of Airy functions. Airy-function based descriptions of high-field transport have been discussed in the literature before,[27–29] but we believe that the present approach, through the systematic use of the Airy transform and of the gauge invariant formulation, is the first where the program has been carried out to completion.

In order to show how this works, in Sec. 2 we present the details of the formalism and explain with a simple example how an Airy-transformed function can be cast

into gauge-invariant form. In Sec. 3, we apply the method to derive a model self-energy for the coupled electron-phonon system at high fields.

In Sec. 4, we solve DE for the retarded Green's function and determine a spectral density function model which is consistent with the frequency sum-rule, and include collisional broadening and intracollisional field effect on equal footing. The density of states is also calculated in order to show how the concomitance of an external field and the scattering processes modify the electron energies. We solve the KBK equations and derive a closed equation for a generalized distribution which contains information about the nonequilibrium occupation of energy states in Sec. 5.

Finally, in Sec. 6, we relate the function determined in Sec. 5 to experimentally observable quantities, such as a number densities of nonlinear conductivities. The consistency of our results with the linearized Boltzmann equation are checked in the appropriate limit and the quantum distribution function as well as the nonlinear drift velocity versus applied field characteristics are evaluated numerically.

2. Formalism

2.1. *The Airy representation*

In order to study the properties of charge transport in a quantum system, we consider an ensemble of electrons in a semiconductor crystal, coupled to the phonon gas. We assume carriers do not interact with each other, so that the interaction of one carrier with the phonon will represent the behavior of the whole electron gas. The electron band structure is handled in the effective-mass approximation, with a simple spherical and parabolic band.

The system Hamiltonian is given by

$$H = H_{\mathrm{e}} + H_{\mathrm{p}} + H_{\mathrm{e-p}} + U(z)$$

where $H_{\mathrm{e}} = -\hbar^2\nabla^2/2m$ is the term corresponding to an electron in a perfect crystal with m as the effective mass. $\sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \hat{b}^{\dagger}_{\mathbf{q}} \hat{b}_{\mathbf{q}}$ describes the free-phonon system, with $\hat{b}^{\dagger}_{\mathbf{q}}$ and $\hat{b}_{\mathbf{q}}$ as the creation and annihilation operators of a phonon mode $\mathbf{q}$. The expression for the electron-phonon interaction Hamiltonian $H_{\mathrm{e-p}}$ depends on the particular scattering mechanism considered. Finally, $U(z)$ is the perturbing, one-dimensional potential applied along the z-direction of motion. For instance, $U(z)$ could represent an external field as well as the position-dependent conduction-band edge found in heterostructures.

In the absence of the scattering processes, the eigenfunctions $\psi(\mathbf{r})$ of the system can be factorized as

$$\psi_{\mathbf{k}_\perp, s}(\mathbf{r}) = \frac{1}{2\pi} e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} \varphi_s(z) \ , \tag{2.1}$$

with $\mathbf{r}_\perp$ and $\mathbf{k}_\perp$ being the position and wave vector of the electron in the plane normal to the field direction, and $\varphi_s(z)$ determined by

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + U(z) + \frac{\hbar^2\mathbf{k}_\perp^2}{2m}\right]\varphi_s(z) = \varepsilon_s(\mathbf{k}_\perp)(z) \ . \tag{2.2}$$

The index s labels the eigenvalues that can constitute either a discrete or a continuous spectrum.

In the Hilbert space of the eigenfunctions $\varphi_s(z)$, for any function or operator F, we can define the transformation

$$F(\mathbf{k}_\perp, z, z', \omega) = \sum_{s,s'} \varphi_s(z) F_{s,s'}(\mathbf{k}_\perp, \omega)\varphi_{s'}(z') \ . \tag{2.3}$$

In the case of a constant electric field, $U(z) = eEz$ and Eq. (2.2) has solutions represented by the stationary states[30]

$$\psi_{\mathbf{k}_\perp, s}(\mathbf{r}) + \frac{1}{2\pi L} e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} Ai\left(\frac{z-s}{L}\right) \tag{2.4}$$

where $Ai(x)$ is the Airy function of the first kind and $L = (\hbar^2/2meE)^{1/3}$ the normalization length defined by the condition

$$\int dz \varphi_s^*(z)\varphi_{s'}(z) = \delta(s - s') \ .$$

The corresponding eigenvalues are

$$\varepsilon_s(\mathbf{k}_\perp) = \frac{\hbar^2\mathbf{k}_\perp^2}{2m} + eEs \ .$$

The Airy variable s, defined as $s = \varepsilon_z/eE$, with ε_z the energy eigenvalue in the direction of the field, has the physical interpretation as the quantum-mechanical analogue of the classical electron turning point in z. This solution is exact, but does not include the possibility of Zener tunnelling from one band to another, and effect that can be significant at very high electric fields, but which we ignore in the present treatment.

The transformation (2.3) in this case becomes the Airy transform

$$F(\mathbf{k}_\perp, z, z', \omega) = \int \frac{dsds'}{L^2} Ai\left(\frac{z-s}{L}\right) Ai\left(\frac{z'-s'}{L}\right) F(\mathbf{k}_\perp, s, s', \omega) \ , \tag{2.5}$$

which connects the two coordinate systems $(\mathbf{r}_\perp, z, z')$ and $(\mathbf{k}_\perp, s, s')$. Thus, working in the Hilbert space defined by $\Psi_{\mathbf{k}_\perp, s}(\mathbf{r})$, (i.e., plane waves in the plane perpendicular to the field and Airy functions along the direction of the field) enables us to define a coordinate system $(\mathbf{k}_\perp, s, s')$ for Fourier transforming to momentum in the transverse directions and "Airy transforming" to s-coordinates along the field.

Using the s-variable corresponds to a total energy representation where the kinetic and potential energy of the carriers along the applied field are considered simultaneously and indistinguishably. Some useful properties of the Airy transform are demonstrated in Appendix A.

We can now define the field operators in the interaction picture by

$$\hat{\Psi}(\mathbf{r}, t) = \int d\mathbf{k}_\perp ds \psi_{\mathbf{k}_\perp, s}(\mathbf{r}) \hat{a}_{\mathbf{k}_\perp, s}(t) \ , \tag{2.6a}$$

with an inverse transform

$$\hat{a}_{\mathbf{k}_\perp, s}(t) = \int d\mathbf{k}_\perp ds \psi_{\mathbf{k}_\perp, s}(\mathbf{r}) \hat{\Psi}(\mathbf{r}, t) \ . \tag{2.6b}$$

The creation and annihilation operators satisfy the properties

$$\begin{aligned} \left[\hat{a}_{\mathbf{k}_\perp, s}(t), \hat{a}^\dagger_{\mathbf{k}'_\perp, s'}(t)\right]_+ &= \delta(\mathbf{k}_\perp - \mathbf{k}'_\perp)\delta(s - s') \\ \left[\hat{a}_{\mathbf{k}_\perp, s}(t), \hat{a}_{\mathbf{k}'_\perp, s'}(t)\right]_+ &= 0 \ , \end{aligned} \tag{2.7}$$

since we are working with normalized basis functions.

The time dependence of the operators is given by

$$\hat{a}_{\mathbf{k}_\perp, s}(t) = \hat{a}_{\mathbf{k}_\perp, s} e^{-\frac{i}{\hbar}\varepsilon_s(\mathbf{k}_\perp)t} \ . \tag{2.8}$$

As a simple example, let us consider the Airy representation of the free-particle propagator at zero temperature. This is easily evaluated by using Eqs. (2.6)–(2.8) into definition (1.1):

$$\begin{aligned} G^r_E(\mathbf{r}, t; \mathbf{r}', t') = -\frac{i}{\hbar} d\mathbf{k}_\perp ds \int d\mathbf{k}'_\perp ds' \psi_{\mathbf{k}_\perp, s}(\mathbf{r}) \psi^*_{\mathbf{k}'_\perp, s}(\mathbf{r}') \vartheta(t - t') \\ \times \left\langle \Phi_0 \middle| \left[\hat{a}_{\mathbf{k}_\perp, s}(t), \hat{a}^\dagger_{\mathbf{k}'_\perp, s}(t')\right]_+ \middle| \Phi_0 \right\rangle \end{aligned}$$

with $|\Phi_0\rangle$ indicating the vacuum state. In $(\mathbf{k}_\perp, s)$-space we immediately obtain the simple expression

$$G^r_E(\mathbf{k}_\perp, s, t - t') = -\frac{i}{\hbar} \vartheta(t - t') e^{-\frac{i}{\hbar}\varepsilon_s(\mathbf{k}_\perp)(t - t')} \ . \tag{2.9}$$

The spectral density function is also immediately derived

$$A_E(\mathbf{k}_\perp, s, \omega) = -2 \operatorname{Im} G^r_E(\mathbf{k}_\perp, s, \omega) = 2\pi\delta(\hbar\omega - \varepsilon_s(\mathbf{k}_\perp)) \ . \tag{2.10}$$

Notice here that, although both $G^r_E(\mathbf{k}_\perp, s, t - t')$ and $A_E(\mathbf{k}_\perp, s, \omega)$ have forms analogous to the unperturbed, field-free expressions, yet they contain the full field-dependence through the eigenvalue $\varepsilon_s(\mathbf{k}_\perp)$.

The very same expressions (2.9) and (2.10), however, although exact, already pose some questions about the interpretation of the results that can be obtained in the total-energy (Airy) representation. Indeed, the resulting physical picture could be dependent on the gauge (scalar) used, as can be understood, for instance, by comparing (2.10) with its gauge-invariant counterpart[11]

$$\tilde{A}_E(\mathbf{k}, \omega) = \frac{1}{\Theta} Ai\left(-\frac{\hbar\omega - \varepsilon(\mathbf{k})}{\Theta}\right) , \tag{2.11}$$

where now $(\mathbf{k} = k_x, k_y, k_z)$, $\varepsilon(\mathbf{k}) = \hbar^2\mathbf{k}^2/2m$ and $\Theta = eEL$. Here, as well as in the remainder of the paper, an overtilde denotes gauge-invariant functions.

This problems will become even more severe when more complicated functions will be evaluated because of the possibility that the approximations made could be gauge dependent, and therefore physically incorrect. The Airy formalism, therefore, must be improved in order to formulae a gauge-invariant theory of wider and more general validity.

2.2. *Gauge-invariant transform*

Let us consider the product $g(1, 2) = \hat{\Psi}(1)\hat{\Psi}^\dagger(2)$ of field operators. In terms of the Wigner coordinates

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \; ; \quad \tau = \tau_1 - \tau_2$$
$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \; ; \quad T = \frac{\tau_1 + \tau_2}{2}$$

it can also be expressed as

$$g(\mathbf{r}, \tau; \mathbf{R}, T) = \hat{\Psi}\left(\mathbf{R} + \frac{\mathbf{r}}{2}, T + \frac{\tau}{2}\right)\hat{\Psi}^\dagger\left(\mathbf{R} - \frac{\mathbf{r}}{2}, T - \frac{\tau}{2}\right) . \tag{2.12}$$

We now want to prove that, for a particle of charge q, if ϕ and $\mathbf{A}$ are the scalar and vector potentials, respectively, the function $\tilde{g}(\mathbf{k}, \tau; \mathbf{R}, T)$ defined as

$$\tilde{g}(\mathbf{k}, \tau; \mathbf{R}, T) = \int \frac{d\mathbf{r}}{(2\pi)^{3/2}} \int \frac{d\tau}{\sqrt{2\pi}} e^{iw(\omega, \tau, T, \mathbf{k}, \mathbf{r}, \mathbf{R})} g(\mathbf{r}, \tau; \mathbf{R}, T) \tag{2.13}$$

$$w(\omega, \tau, T, \mathbf{k}, \mathbf{r}, \mathbf{R}) = \int_{-1/2}^{1/2} d\lambda \Big\{ \tau\left[\omega + \frac{q}{\hbar}\phi(\mathbf{R} + \lambda\mathbf{r}, \mathbf{T} + \lambda\tau)\right] - \mathbf{r} \cdot \left[\mathbf{k} + \frac{q}{\hbar c}\mathbf{A}(\mathbf{R} + \lambda\mathbf{r}, \mathbf{T} + \lambda\tau\right] \Big\}$$

remains unchanged under the gauge transformation

$$\mathbf{A} \to \mathbf{A}'(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}, t) + \nabla\chi(\mathbf{x}, t) , \quad \phi \to \phi'(\mathbf{x}, t) = \phi(\mathbf{x}, t) - \frac{1}{c}\frac{\partial\chi(\mathbf{x}, t)}{\partial t} , \tag{2.14}$$

where $\chi(\mathbf{x}, t)$ is an arbitrary scalar function. The proof goes as follows.

From elementary quantum mechanics[32] we know that the wave function in the new gauge is related to the wave function in the original gauge by

$$\tilde{\psi}(\mathbf{x}, t) = e^{i\frac{q}{\hbar c}\chi(\mathbf{x}, t)}\psi(\mathbf{x}, t) . \tag{2.15}$$

By substituting this into Eq. (2.12), and Eq. (2.14) into Eq. (2.13), we have

$$\begin{aligned} \tilde{g}(\mathbf{k}, \omega, \mathbf{R}, T) = & \int \frac{d\mathbf{r}}{(2\pi)^{3/2}} \int \frac{d\tau}{\sqrt{2\pi}} e^{iw'} \\ & \times e^{i\frac{q}{\hbar c}\chi(\mathbf{R} + \mathbf{r}/2.T + \tau/2)} e^{-i\frac{q}{\hbar c}\chi(\mathbf{R} - \mathbf{r}/2.T - \tau/2)} g(\mathbf{r}, \tau, \mathbf{R}, T) \\ w' = & \, w - \int_{-1/2}^{1/2} d\lambda \left[\left(\frac{q}{\hbar c}\right) \tau \frac{\partial\chi(\mathbf{x}, t)}{\partial t} + \left(\frac{q}{\hbar c}\right) \mathbf{r} \cdot \nabla\chi(\mathbf{x}, t) \right] \\ \equiv & \, w + \Delta w . \end{aligned} \tag{2.16}$$

In order to obtain a gauge invariant $\tilde{g}$, Δw must cancel the factor $e^{i\frac{q}{\hbar c}\chi - i\frac{q}{\hbar c}\chi}$ in (2.16). Indeed, by remembering, from (2.13), that $\mathbf{x} = \mathbf{R} + \lambda\mathbf{r}$ and $t = T + \lambda\tau$ we can write Δw as the total derivative

$$\begin{aligned} \Delta w = & - \left(\frac{q}{\hbar c}\right) \int_{-1/2}^{1/2} d\lambda \frac{\partial\chi(\mathbf{x}, t)}{\partial t} \\ = & - \left(\frac{q}{\hbar c}\right) [\chi(\mathbf{R} + \mathbf{r}/2, T + \tau/2) - \chi(\mathbf{R} - \mathbf{r}/2, T - \tau/2)] , \end{aligned}$$

and we see that the cancellation occurs.

Thus, we have proved that even though the wave functions and the electromagnetic potentials change with the gauge, products like (2.12) and therefore the various Green's functions, are independent of the gauge, provided we transform them by the prescription (2.13). Special cases of (2.13) have been considered by several authors.[12,15,19,33,34] For an electron ($q = -e$) in homogeneous, steady-state fields Eq. (2.13) reduces to

$$\tilde{g}(\mathbf{k}, \omega, \mathbf{R}, T) = \int \frac{d\tau}{\sqrt{2\pi}} e^{i(\omega + \frac{e}{\hbar}\mathbf{E} \cdot \mathbf{R})\tau} \int \frac{d\mathbf{r}}{(2\pi)^{3/2}} e^{-i\mathbf{k} \cdot \mathbf{r}} g_\phi(\mathbf{r}, \tau, \mathbf{R}, T) \tag{2.17}$$

for g calculated in the scalar-potential gauge (g_ϕ) with $\phi = -\mathbf{E} \cdot \mathbf{R}$, and to

$$\tilde{g}(\mathbf{k}, \omega, \mathbf{R}, T) = \int \frac{d\tau}{\sqrt{2\pi}} e^{i\omega\tau} \int \frac{d\mathbf{r}}{(2\pi)^{3/2}} e^{-i(\mathbf{k} + \frac{e}{\hbar}\mathbf{E}T) \cdot \mathbf{r}} g_A(\mathbf{r}, \tau, \mathbf{R}, T) \tag{2.18}$$

for g calculated in the vector-potential gauge (g_A) with $\mathbf{A} = -c\mathbf{E}T$. In Appendix B, we give to simple examples of how (2.17) and (2.18) may be applied.

2.3. *The two transformations combined*

Assume that s and ω be not independent variables and consider functions of the type (see Sec. 3 for an example of a function of this kind)

$$F\left(\mathbf{k}_\perp, \omega - \frac{eE}{\hbar}s, \omega - \frac{eE}{\hbar}s'\right) .$$

In order to put this function into gauge-invariant form, we have to apply (2.5) and then (2.17), namely

$$\begin{aligned}\tilde{F}(\mathbf{k}_\perp, k_z, k_{z'}, \tau) = \int \frac{d\omega}{\sqrt{2\pi}} e^{i\left(\omega + \frac{eE}{\hbar}Z\right)\tau} \int \frac{dz}{\sqrt{2\pi}} \int \frac{dZ}{\sqrt{2\pi}} e^{ik_z(Z+z/2)} e^{ik_{z'}(Z-z/2)} \\ \times \int \frac{ds ds'}{L^2} Ai\left(\frac{Z + z/2 - s}{L}\right) Ai\left(\frac{Z - z/2 - s'}{L}\right) \\ \times F\left(\mathbf{k}_\perp, \omega - \frac{eE}{\hbar}s, \omega - \frac{eE}{\hbar}s'\right) , \end{aligned} \tag{2.19}$$

where z and z' in (2.5) have been replaced by $(Z + z/2)$ and $(Z - z/2)$ in the center-of-mass coordinate space.

By writing

$$\begin{aligned} F\left(\mathbf{k}_\perp, \omega - \frac{eE}{\hbar}s, \omega - \frac{eE}{\hbar}s'\right) \\ = \int \frac{dt}{\sqrt{2\pi}} e^{i\left(\omega - \frac{eE}{\hbar}s\right)t} \int \frac{dt'}{\sqrt{2\pi}} e^{-i\left(\omega - \frac{eE}{\hbar}s'\right)t'} F(\mathbf{k}_\perp, t, t') , \end{aligned}$$

and using the integral representation (A.2) for the Airy function, Eq. (2.19) reduces to

$$\tilde{F}(\mathbf{k}, \tau) = \sqrt{2\pi} L \frac{\hbar}{eE} F\left(\mathbf{k}_\perp, \frac{\hbar k_z}{eE} + \frac{\tau}{2}, \frac{\hbar k_z}{eE} - \frac{\tau}{2}\right) \tilde{A}_E(k_z, \tau) , \tag{2.20}$$

with

$$\tilde{A}_E(k_z, \tau) = \frac{1}{\hbar} e^{-i\left[\frac{(eE)^2}{24\hbar m}\tau^3 + \frac{\epsilon(\mathbf{k})}{\hbar}\tau\right]}$$

the Fourier transform of Eq. (2.11). In Eq. (2.20), we notice that $\hbar k_z/eE$ can be regarded as the k_z-dependent "center-of-mass" time $T(k_z)$ since $\hbar k_z$ is the electron momentum in the field direction and eE the accelerating force due to the field. Thus, in our formalism, the unperturbed (absence of scattering), field-dependent spectral function $\tilde{A}_E$ can be exactly factored out of all the functions (Green's functions,

self-energies, correlation functions) we will be dealing with. This bears a formal analogy with Eq. (2.21) of Ref. 19 for the definition of the "reduced functions". In the present case, however, $\tilde{A}_E$ contains information about the motion along the field direction only. This motion is also described partly (through $T(k_z)$) by the F-function on the RHS of Eq. (2.20), which also gives us information about the motion on the plane perpendicular to the field direction.

By the same procedure, a function $F(\omega - eEs/\hbar)$, of a single $(\omega - eEs/\hbar)$ argument, can be put into gauge-invariant form. In this case we have

$$\tilde{F}(\mathbf{k}, \tau) = F(\mathbf{k}_\perp, \tau)\tilde{A}_E(k_z, \tau) , \tag{2.21}$$

where

$$F(\tau) = \int \frac{d\Omega}{\sqrt{2\pi}} e^{-i\Omega\tau} F(\Omega)$$

and

$$\Omega = \omega - \frac{eE}{\hbar} s .$$

The k_z-dependence is now carried only by the unperturbed, field-dependent spectral density function $\tilde{A}_E$ which also contains an explicit dependence on the electric field. This is an interesting result: it tells that the transverse and parallel components of the motion are separated and can be treated independently. Equation (2.21) also implies that the Fourier transform from τ to ω of Eq. (2.21) is just the convolution product

$$\tilde{F}(\mathbf{k}, \tau) = \int d\Omega F(\mathbf{k}_\perp, \Omega)\tilde{A}_E(k_z, \omega - \Omega) . \tag{2.22}$$

This property will be very useful in calculating the quantities of interest. Furthermore, remembering the expression (2.11) for $\tilde{A}_E(k_z, \omega)$, we have

$$\tilde{F}(\mathbf{k}, \omega) = \int d\Omega F(\mathbf{k}_\perp, \Omega) \frac{1}{\Theta} Ai\left[\frac{\hbar\Omega - (\hbar\omega - \varepsilon(k_z))}{\Theta}\right] . \tag{2.23}$$

This result states that in order to transform a function f defined in (s, ω)-space into gauge-invariant form, we simply have to take its single Airy transform

$$f(s) = \int dz \frac{1}{L} Ai\left(\frac{z - s}{L}\right) f(z)$$

with L, z and s replaced by Θ, $\hbar\Omega$ and $(\hbar\omega - \varepsilon(k_z))$ respectively.

We can also establish a connection between Eq. (2.22) and (2.20). Let us take the average of (2.20) over the k_z-dependence of the center-of-mass time $T(k_z)$. This

means that we only have to average the function $F(T(k_z)+\tau/2,\, T(k_2)-\tau/2)$:

$$\langle F(T(k_z)+\tau/2,\, T(k_z)-\tau/2)\rangle = \int \frac{dk_z}{\nu_z} F(T(k_z)+\tau/2,\, T(k_z)-\tau/2) \qquad (2.24)$$

where $\nu_z = \sqrt{2\pi}L$ is the field-dependent volume-element in $(k_z,\, s)$-space which reflects the different metric obeyed by the Airy space. Again, by writing

$$F(T(k_z)+\tau/2,\, T(k_z)-\tau/2) = \int \frac{d\Omega}{\sqrt{2\pi}} e^{-i\left(\frac{\hbar k_z}{eE}+\frac{\tau}{2}\right)\Omega} \int \frac{d\Omega'}{\sqrt{2\pi}} e^{-i\left(\frac{\hbar k_z}{eE}-\frac{\tau}{2}\right)\Omega'} F(\Omega,\, \Omega') \,,$$

the above average (2.24) becomes

$$\langle F(T(k_z)+\tau/2,\, T(k_z)-\tau/2)\rangle = \frac{1}{\nu_z}\frac{eE}{\hbar} F(\tau) \,. \qquad (2.25)$$

By inserting this in place of $F(T(k_z)+\tau/2,\, T(k_z)-\tau/2)$ in Eq. (2.20), we obtain precisely Eq. (2.21) which is valid for functions diagonal in $(\omega - eEs/\hbar)$ in s-space.

As a simple example of how the above procedure is employed, let us transform G_E^r given in Eq. (2.9) into gauge-invariant form.

Using the prescription (2.21), and $\varepsilon(\mathbf{k}) = \varepsilon(\mathbf{k}_\perp) + \varepsilon(k_z)$, we immediately obtain

$$\tilde{G}_E^r(\mathbf{k}_\perp,\, \tau) = -\frac{i}{\hbar}\vartheta(\tau) e^{-i\left[\frac{(eE)^2}{24\hbar m}\tau^3 + \frac{\varepsilon(\mathbf{k})}{\hbar}\tau\right]} \,, \qquad (2.26)$$

in agreement with previous results and, by Fourier-transforming the τ variable,

$$\tilde{G}_E^r(\mathbf{k}_\perp,\, \omega) = -\frac{\pi}{\Theta}\left[Gi\left(-\frac{\hbar\omega - \varepsilon(\mathbf{k})}{\Theta}\right) + iAi\left(-\frac{\hbar\omega - \varepsilon(\mathbf{k})}{\Theta}\right)\right] \,, \qquad (2.27)$$

where $Gi(\chi)$ can be evaluated in terms of Airy functions.[31]

3. A Model for the Self-Energy

In order to solve Dyson's equation for G^r, we need a model for the retarded self-energy Σ^r.

The operator ordering in $G^<$ is such that it vanishes as the density goes to zero. As a result, for a nondegenerate system, the term containing $G^<$ in the expression for Σ^r, as given in Eq. (1.2), is a negligible correction[16,19] to that containing G^r and

$$\Sigma^r \cong D^> G^r \,.$$

This is a standard approximation which decouples Dyson's equation for G^r from that for $G^<$, thus solving one of the difficulties mentioned in the Introduction.

Also, at low-particle densities, the electrons are not expected to influence the phonon states, so we can assume that the phonons remain in equilibrium and are not affected by the electric field. We therefore use the familiar expression[10]

$$D_0^{>}(\mathbf{q}, \omega) = -\frac{i}{\hbar} \sum_{\eta=\pm 1} |V_{\mathbf{q}}|^2 \left(N_{\mathbf{q}} + \frac{\eta + 1}{2} \right) \delta(\omega - \eta\omega_{\mathbf{q}}) \tag{3.1}$$

for the phonon correlation function. Here $\mathbf{q}$ and $N_{\mathbf{q}}$ are the phonon wave vector and occupation number, respectively, and $|V_{\mathbf{q}}|$ is the electron-phonon interaction matrix element.[35] The term with $\eta = +1(-1)$ corresponds to emission (absorption) of a phonon of frequency $\hbar\omega_{\mathbf{q}}$. Within this model, the retarded self-energy in reciprocal space reads

$$\begin{aligned} \Sigma^r(\mathbf{k}_\perp, k_z, k_{z'}, \omega) = -\frac{i}{2\pi} \int \frac{d\mathbf{q}}{(2\pi)^3} \times \sum_{\eta=\pm 1} |V_{\mathbf{q}}|^2 \left(N_{\mathbf{q}} + \frac{\eta + 1}{2} \right) \\ \times G^r(\mathbf{k}_\perp - \mathbf{q}_\perp, k_z - q_z, k_{z'} - q_{z'}\omega - \eta\omega_{\mathbf{q}}) \, . \end{aligned} \tag{3.2}$$

By Airy transforming along the z-direction we obtain

$$\begin{aligned} \Sigma^r(\mathbf{k}_\perp, s, s', \omega) = -i \int \frac{d\mathbf{k}_\perp}{(2\pi)^3} \sum_{\eta=\pm 1} |V_{\mathbf{q}}|^2 \left(N_{\mathbf{q}} + \frac{\eta + 1}{2} \right) \\ \times \int \frac{ds'' ds'''}{L^2} G^r(\mathbf{k}_\perp - \mathbf{q}_\perp, s'', s''', \omega - \eta\omega_{\mathbf{q}}) \\ \times \int \frac{dz}{L} e^{iq_z z} Ai\left(\frac{z - s}{L} \right) Ai\left(\frac{z - s''}{L} \right) \\ \times \int \frac{dz'}{L} e^{-iq_{z'} z'} Ai\left(\frac{z' - s'}{L} \right) Ai\left(\frac{s' - s'''}{L} \right) \, . \end{aligned} \tag{3.3}$$

We consider scattering with nonpolar optical phonons, characterized by a dispersion spectrum and a momentum-independent coupling matrix element. Since scattering is relatively weak in most semiconductors, we also evaluate (3.2) only in the lowest-order, one-phonon scattering processes by taking $G^r \approx G_E^r$. With these simplifications, Σ^r turns out to be independent of the transverse momentum, namely

$$\begin{aligned} \Sigma^r(s, s', \omega) = -i \sum_{\eta=\pm 1} |V|^2 \left(N_0 + \frac{\eta + 1}{2} \right) \int \frac{dz}{L} Ai\left(\frac{z - s}{L} \right) Ai\left(\frac{z - s'}{L} \right) \\ \times \int \frac{ds''}{L^2} Ai^2\left(\frac{z - s''}{L} \right) \int \frac{d(\mathbf{k}_\perp - \mathbf{q}_\perp)}{(2\pi)^2} G_E^r(\mathbf{k}_\perp - \mathbf{q}_\perp, s', \omega - \eta\omega_0) \, . \end{aligned} \tag{3.4}$$

This equation is exact in the sense that, within the present physical model, no mathematical approximations were made to obtain it. Furthermore, Σ^r is a function only of the difference, Ω, of the ω and s variables, as can be easily verified.

Let us consider the "averaged" self-energy

$$\int ds' \Sigma^r(s, s', \omega) = \left(\frac{3}{2}\right)^{1/2} \frac{\rho_{2D}}{2\pi} \left(\frac{eE}{3^{1/3}\Theta}\right) \sum_\eta |V|^2 \left(N_0 + \frac{\eta+1}{2}\right) \times \int_0^\infty \frac{dt}{t^{3/2}} e^{i\left(\frac{t^3}{12} + \zeta t + \frac{\pi}{4}\right)} = \Sigma^r(\Omega) \tag{3.5}$$

where $\zeta = -(\hbar\omega - eEs - \eta\hbar\omega_0)/3^{1/3}\Theta$ and $\rho_{ND} = \pi V(2m/\hbar^2)^{N/2}$ is the Nth dimensional free-electron density-of-states factor. Equation (3.5) can be transformed into gauge-invariant form by the prescription (2.22). The result reads

$$\begin{aligned} \tilde{\Sigma}(k_z, \omega) &= \sum_\eta |V|^2 \left(N_0 + \frac{\eta+1}{2}\right) \tilde{F}(k_z, \omega) \ , \\ \mathrm{Re}[\tilde{F}(k_z, \omega)] &= \frac{\rho_{3D}}{(2\pi)^2}\Theta^{1/2}\left[Ai'(\xi)Bi'(\xi) - \xi Ai(\xi)\dot{B}i(\xi) + \frac{\sqrt{\xi}}{\pi}\vartheta(\xi)\right] \ , \\ \mathrm{Im}[\tilde{F}(k_z, \omega)] &= -\frac{\rho_{3D}}{(2\pi)^2}\Theta^{1/2}[Ai'^2(\xi) - \xi Ai^2(\xi)] \ , \end{aligned} \tag{3.6}$$

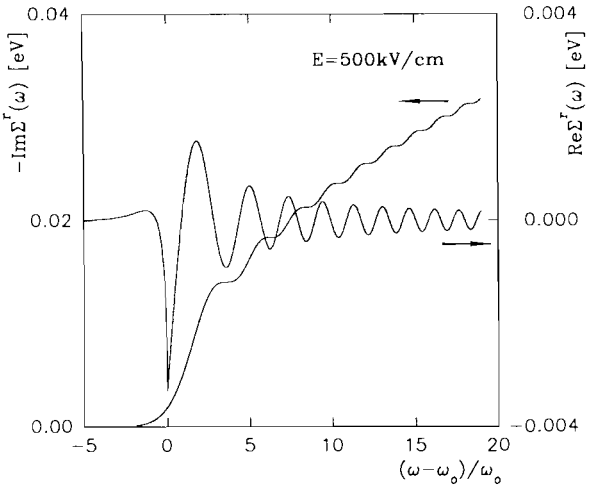
where now $\xi = -[\hbar\omega - \varepsilon(k_z) - \eta\hbar\omega_0)/2^{1/3}\Theta$. This expression has to be compared with Eq. (20) of Ref. 28. The two models have a very similar behavior. The model considered in Ref. 28, however, neglects the real part of the self-energy, which determines the renormalization of the quasiparticle energies caused by the presence of the interactions (including the electric field). Also, because of the averaging procedure over $\mathbf{k}$, it ignores the dependence on the electron momentum along the field direction. Both features are retained in the present model of Eq. (3.6). Furthermore, the above self-energy has the correct limit for vanishing fields. In fact, when $E \to 0$ (or equivalently, $\xi \to \infty$), its imaginary part, which the optical theorem relates to the scattering rate Γ by

$$\Gamma(\omega) = \frac{1}{\tau(\omega)} = -\frac{2}{\hbar}\mathrm{Im}\,\Sigma^r(\omega) \ , \tag{3.7}$$

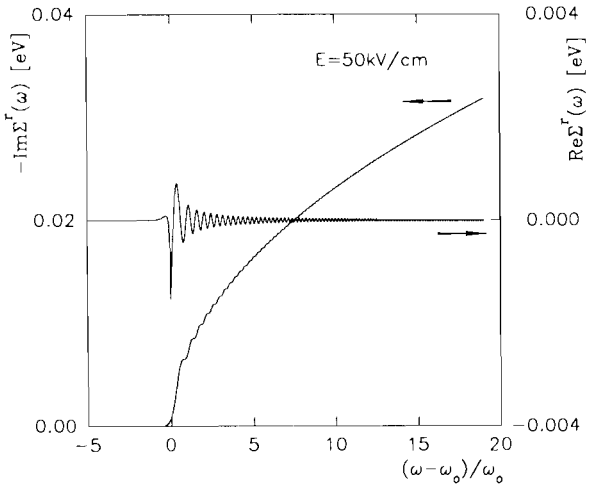
reduces to that obtained by considering one-phonon emission processes in the Born approximation:

$$\lim_{\xi\to\infty} \frac{1}{\hbar}\mathrm{Im}\,\Sigma^r(\omega) = \frac{4}{\hbar}\frac{\rho_{3D}}{(2\pi)^3} \sum_\eta |V|^2 \left(N_0 + \frac{\eta+1}{2}\right) \sqrt{\hbar\omega - \varepsilon(k_z) - \eta\hbar\omega_0} \ . \tag{3.8}$$

On the other hand, the real part of the self-energy vanishes when $E = 0$. This indicates that our lowest-order approximation fails to describe fully the energy renormalization caused by collisional broadening alone, but it represents a quite



(a)



(a)

Fig. 1. The real and imaginary part of the self-energy for 500 kV/cm (a) and 50 kV/cm (b) for phonon-emission processes. We use parameters appropriate to Si: and optical-phonon energy $\hbar\omega_0 = 64.04\,\mathrm{meV}$; deformation potential $D_t = 11.0 \cdot 10^8\,\mathrm{eV/cm}$; density $\rho = 2.33\,\mathrm{g/cm^3}$ and effective mass $m^* = .3282\,m_e$. The longitudinal momentum k_z is taken to be equal to zero.

reasonable model for the ICFE. Figure 1 shows the real and imaginary part of the self-energy for emission processes as a function of the argument ξ for two different values of the field. The oscillatory nature of the self energy has not been seen in previous treatments of the high-field behavior and is a consequence of the nonper-

turbative inclusion of the electric field in the problem. These oscillations indicate the existence of regions in which the electron energy is alternately lowered (negative values of the self-energy) and raised (positive values of the self-energy), suggesting the existence of preferred energies for the electron, with every other zero crossing in the figure representing a quantized level towards which the quasi particle energy tends to concentrate. In the solution (2.4) the zero crossings would occur asymptotically where $\xi = [3\pi(2n - 1/2)/4]^{2/3}$. In $\mathrm{Re}\Sigma^r(\omega)$, on the other hand, because of the presence of phonons, and of the irrational factor $2^{1/3}\Theta$, the oscillations are incommensurate with those occurring in the phonon-decoupled problem. The validity of the interpretation is reinforced by the step-like oscillations present in $\mathrm{Im}\Sigma^r(\omega)$. Since this quantity is proportional to the scattering rate $\Gamma(\omega)$, the plateaus, which occur precisely at the negative values of $\mathrm{Re}\Sigma^r(\omega)$, are an indication the the quasi-two-dimensional sub-band tendencies mentioned above. Furthermore, the presence of the ICFE and of CB is found to generate a tail in $\Gamma(\omega)$ for $\xi < 0$. The existence of such a tail to negative energies corresponds to the part with $\xi > 0$ in the Airy function $Ai(\xi)$, and represents tunnelling into the classically forbidden region. This smooths out the sharp threshold in energy of the scattering rate, making possible transitions that cannot occur in the absence of the field.

4. Dyson's Equation and its Gauge-Invariant Solution

As explained in the Introduction, the calculation of static properties such as the spectral function and the density of states of the system interacting with the environment, requires the solution of the full Dyson's equation (1.10) for the retarded Green's function.

If the electric field is applied along the z direction, Dyson's equation can be written as

$$G^r(\mathbf{k}_\perp, z, z', \omega) = G^r_E(\mathbf{k}_\perp, z, z', \omega) + \int dz_1 dz_2 G^r_E(\mathbf{k}_\perp, z, z_1, \omega) \times \Sigma^r(\mathbf{k}_\perp, z_1, z_2, \omega) G^r(\mathbf{k}_\perp, z_2, z', \omega) \; . \tag{4.1}$$

By using the transformation (2.5) and the self-energy model of the previous section, Eq. (4.1) simplifies to

$$G^r(\mathbf{k}_\perp, s, s', \omega) = G^r_E(\mathbf{k}_\perp, s, \omega)\delta(s - s') + G^r_E(\mathbf{k}_\perp, s, \omega) \int ds_2 \Sigma^r(s, s_2, \omega) G^r(\mathbf{k}_\perp, s_2, s', \omega) \; . \tag{4.2}$$

The approximation $G^r \approx G^r_E$ in Σ^r does not neglect essential physical effects such as collisional broadening, as one might be led to think, because the retarded Green's function must still be determined self-consistently in (4.2) and the presence of G^r_E introduces high-field effects in the total Green's function G^r (see below).

Due to the singular behavior of the self-energy (3.4) in s-s_2, the s_2 dependence of the product $\Sigma^r(s, s_2, \omega)G^r(\mathbf{k}_\perp, s_2, s', \omega)$ in Eq. (4.2) is dominated by Σ^r, and we can, therefore, move $G^r(\mathbf{k}_\perp, s_2, s', \omega)$ outside of the integral. This results in the replacement of the self-energy (3.4) by its average over the variable s_2 whose expression is given in Eq. (3.5).

Equation (4.2) can now be solved immediately, and we obtain

$$G^r(\mathbf{k}_\perp, \Omega) = \frac{\delta(\Omega - \Omega')}{\hbar\Omega - \varepsilon(\mathbf{k}_\perp) - \Sigma^r(\Omega)} \tag{4.3}$$

a function diagonal in the Ω variable.

Since the full retarded Green's function above is only a function of the difference $(\omega - eEs/\hbar)$ we can again use Eq. (2.22) to transform it into gauge-invariant form, namely

$$\tilde{G}^r(\mathbf{k}, \omega) = \int d\Omega G^r(\mathbf{k}_\perp, \Omega)\tilde{A}_E(k_z, \omega - \Omega) \ . \tag{4.4}$$

The gauge-invariant spectral density can now be immediately calculated, and it is given by

$$\tilde{A}(\mathbf{k}, \omega) = \int d\Omega A(\mathbf{k}_\perp, \Omega)\tilde{A}_E(k_z, \omega - \Omega) \ , \tag{4.5}$$

with

$$A(\mathbf{k}_\perp, \Omega) = -2\,\mathrm{Im}\,\tilde{G}^r = \frac{-2\,\mathrm{Im}\,\Sigma^r(\Omega)}{[\hbar\Omega - \varepsilon(\mathbf{k}_\perp) - \mathrm{Re}\,\Sigma^r(\Omega)]^2 + [\mathrm{Im}\,\Sigma^r(\Omega)]^2} \ . \tag{4.6}$$

In the absence of an electric field, even if $\mathrm{Re}\Sigma^r(\Omega) \to 0$, the above expression gives a finite width which accounts for collisional broadening (see Eq. (3.8)).

$\tilde{A}(\mathbf{k}, \omega)$ satisfies the normal sum rules because (4.6) does[24] and because of the normalization properties of the Airy functions (see Eq. (2.11)).

The zero-field, zero-scattering limit can also be evaluated. From (4.6) and (3.8) we have

$$\lim_{E\to 0} A(\mathbf{k}_\perp, \Omega) = \sqrt{2\pi}\delta(\hbar\Omega - \varepsilon(\mathbf{k}_\perp)) \ ,$$

and from Eq. (2.11)[32]

$$\lim_{E\to 0} \tilde{A}_E(k_z, \omega - \Omega) = \sqrt{2\pi}\delta(\hbar\omega - \hbar\Omega - \varepsilon(k_z)) \ ;$$

therefore,

$$\begin{aligned}\tilde{A}_{\mathrm{free}}(\mathbf{k}, \omega) &= 2\pi \int d\Omega \delta(\hbar\Omega - \varepsilon(\mathbf{k}_\perp))\delta(\hbar\omega - \hbar\Omega - \varepsilon(k_z)) \\ &= 2\pi\delta(\hbar\omega - \varepsilon(\mathbf{k})) \ ,\end{aligned} \tag{4.7}$$

as in the semiclassical theory.

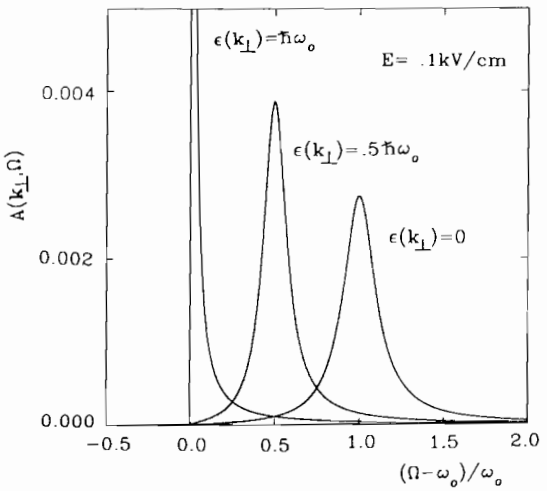
For phonon emission processes, Fig. 2a shows the role of $\mathrm{Re}\Sigma^r(\Omega)$ in removing the semiclassical peak from $\varepsilon(\mathbf{k}_\perp) = \hbar\Omega$, and placing it with one closer to the energy corresponding to the phonon interaction, according to the solutions of

$$\hbar\Omega - \varepsilon(\mathbf{k}_\perp) - \mathrm{Re}\,\Sigma^r(\Omega) = 0 \ .$$

For the given electric field, $\mathrm{Re}\,\Sigma^r(\Omega)$ plays no essential role when $\varepsilon(\mathbf{k}_\perp)$ equals the phonon energy $\hbar\omega_0$, at least compared with the cases of smaller transverse kinetic energies, where its increasing important in further distorting $A(\mathbf{k}_\perp, \Omega)$ is evident.

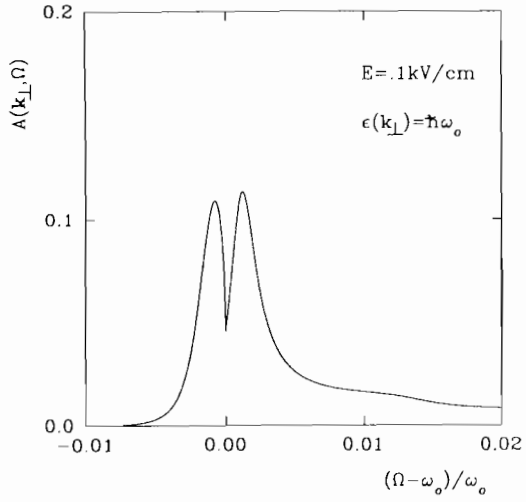
However, even when $\varepsilon(\mathbf{k}_\perp) = \hbar\omega_0$, a finer scale reveals a more complex behavior with the electric field (Fig. 2b): the narrow peak is split, at $\Omega = \omega_0$, into a left and a right peak indicating the role played by the discontinuity of $\mathrm{Re}\Sigma^r(\Omega)$ at this value of the total energy (see Fig. 1).

The behavior of $A(\mathbf{k}_\perp, \Omega)$ for $\varepsilon(\mathbf{k}_\perp) = \hbar\omega_0$, is further analyzed in Fig. 3 as a function of the electric field. At the very small fields, $A(\mathbf{k}_\perp, \Omega)$ reduces to the half Lorentzian shape caused mainly by CB (Fig. 3a). Increasing the electric field, the narrow CB peak broadens into the double-peak structure seen in Fig. 2. We interpret this as an indication of the increased distorsion, caused by the field, in the momentum-energy relationship. The right peak would describe the probability that the carrier has of being forward-scattered, and accelerated even during the emission of a phonon. The electron loses less energy to the phonon and exits the scattering process with a total-energy change greater than $\hbar\omega_0$. The left-hand peak, on the other hand, indicates the possibility for the electron of being decelerated by the



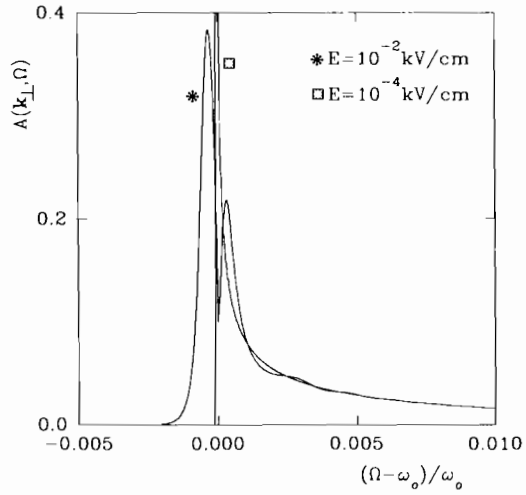
(a)

Fig. 2. The normalized spectral density function $A(\mathbf{k}_\perp, \Omega)$ in Airy representation for different values of the transverse kinetic energy $\varepsilon(\mathbf{k}_\perp)$.



(b)

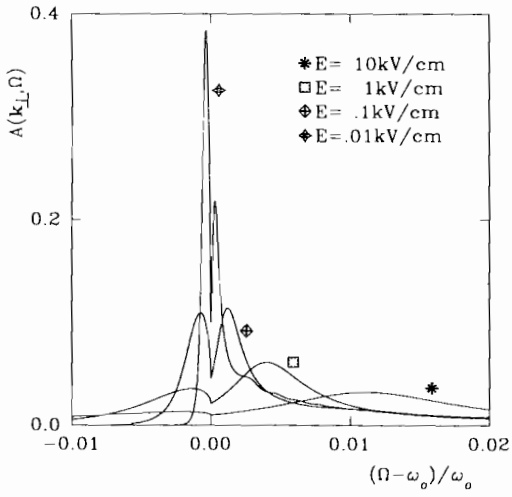
Fig. 2. (*Continued*)



(a)

Fig. 3. The normalized spectral density function $A(\mathbf{k}_\perp, \Omega)$ in Airy representation for different values of the electric field.

field during the emission process. In this case, the collision ends with an energy loss greater than $\hbar\omega_0$. The energy change in the lattice is always just the phonon energy, but the electron sees a modified energy by virtue of the field acting during the collision. This interpretation is supported by the fact that, by increasing the field



(b)

Fig. 3. (*Continued*)

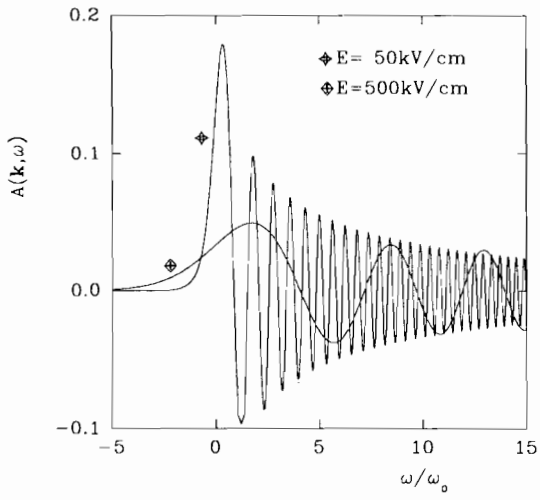
(Fig. 3b), the height of the left-hand peak, relative to the right-hand one, decreases, and their relative separation increases. At high fields ($E \leq 10\,\mathrm{kV/cm}$) only the right peak survives in a broad Lorentzian-type spectral density whose shift towards high energies would, then, indicate the role of high fields in reducing scattering efficiency.

Figure 4 shows the spectral density function $\tilde{A}(\mathbf{k}, \omega)$ for different values of the electric field, as a function of the dimensionless variable ω/ω_0. Because of the approximately equal weight that $A(\mathbf{k}_\perp, \Omega)$ and $\tilde{A}_E(k_z, \omega - \Omega)$ give to the integral (4.5) at these values of the field, $\tilde{A}(\mathbf{k}, \omega)$ is not a positive semi-definite quantity, and its interpretation as a probability function pose some problems. However, at the very high electric fields ($\leq 500\,\mathrm{kV/cm}$), or for higher scattering rates, where the dominating contribution in (4.5) arises from the broad Lorentzian-type shape of $A(\mathbf{k}_\perp, \Omega)$, the oscillatory behavior of $\tilde{A}$ is characterized by a rather large period, with the amplitude of the oscillations decaying very slowly as the energy increases (Fig. 4a). As the field strength is reduced, the oscillations are compressed to a much smaller range of energies and their amplitude now decreases very rapidly. Finally, the oscillatory behavior dies out at the very low fields where $\tilde{A}_E$ approaches its δ-function behavior, and the more familiar[4,18,36] Lorentzian-type shape of $\tilde{A}$ reappears (Fig. 4b).

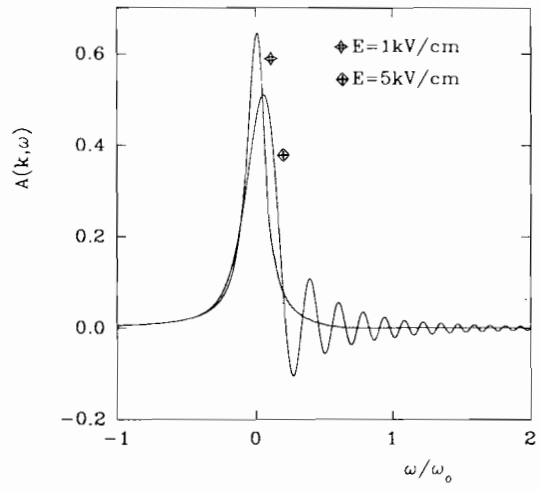
Once the spectral density is known, we can calculate the density of states per spin as follows;

$$\tilde{\rho}(\omega) = \int \frac{d\mathbf{k}}{(2\pi)^3} \tilde{A}(\mathbf{k}, \omega) = \int \frac{d\mathbf{k}}{(2\pi)^3} \int d\Omega A(\mathbf{k}_\perp, \Omega) \tilde{A}_E(k_z, \omega - \Omega)$$

$$= \int d\Omega \rho_\perp(\Omega) \rho_\parallel(\omega - \Omega) \,, \tag{4.8}$$



(a)



(b)

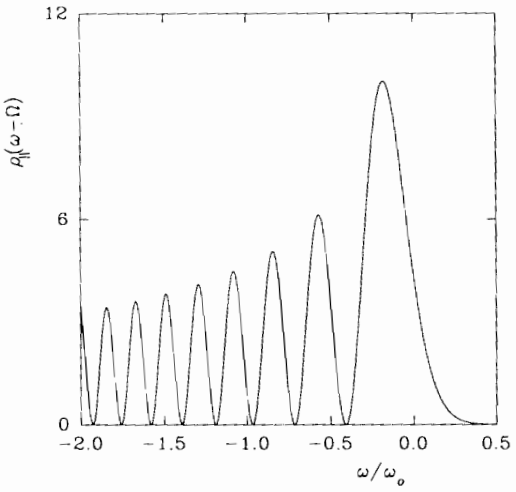
Fig. 4. The normalized spectral density function $\tilde{A}(\mathbf{k}, \omega)$ as a function of ω/ω_0 for different field values.

where

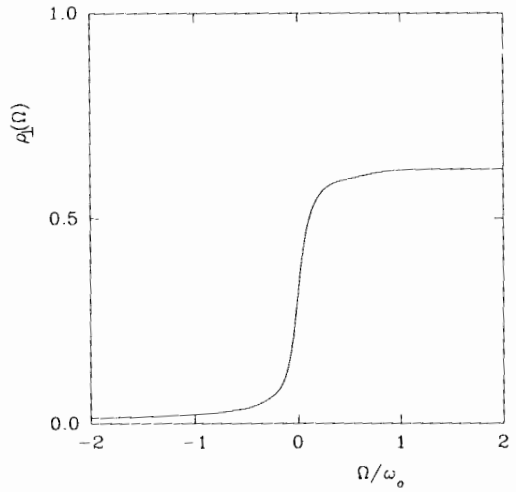
$$\rho_{\perp}(\Omega) = \int \frac{d\mathbf{k}_{\perp}}{(2\pi)^2} A(\mathbf{k}_{\perp}, \Omega) = \frac{\rho_{2D}}{2\pi^2} \left[\frac{\pi}{2} + \tan^{-1} \left[\frac{\hbar\Omega - \mathrm{Re}\,\Sigma^r(\Omega)}{\mathrm{Im}\,\Sigma^r(\Omega)} \right] \right] , \qquad (4.9)$$

and

$$\rho_{\parallel}(\omega - \Omega) = \int \frac{dk_z}{2\pi} \tilde{A}_E(k_z, \omega - \Omega) = \frac{\rho_{1D}}{(2\pi)^2} \frac{1}{\sqrt{\Theta}} Ai^2 \left[-\frac{\hbar(\omega - \Omega)}{\Theta} \right] . \qquad (4.10)$$



(a)



(b)

Fig. 5. The density of states $\rho_{\|}$ (a) and $\rho_{\perp}$ (b) as functions of the dimensionless variable ω/ω_0 and Ω/ω_0 respectively.

Figure 5 shows the density of states $\rho_{\|}$. This is the density of states for a one-dimensional system corresponding to the component of the motion along the field direction. As the electron energy $\hbar\omega$ is increased, $\rho_{\|}$ oscillates between zero and twice the free-electron form of the density of states

$$\rho_{\|} = \frac{\rho_{1D}}{(2\pi)^3} \frac{1}{\sqrt{\hbar(\omega - \Omega)}} \,.$$

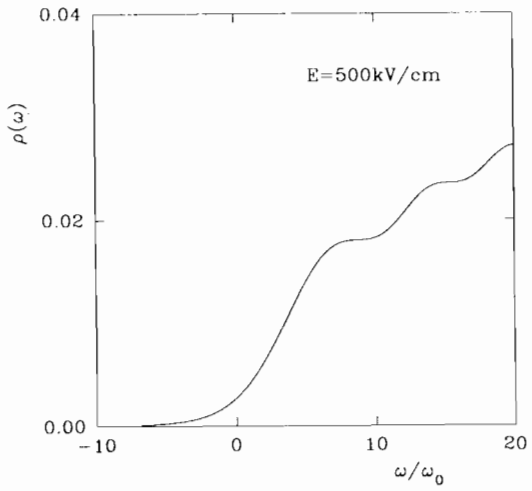
Explicitly,

$$\lim_{\hbar\omega\to\infty} \rho_{\parallel}(\omega-\Omega) = \frac{\rho_{1D}}{4\pi^3}\frac{1}{\sqrt{\hbar(\omega-\Omega)}}\sin^2\left[\frac{2}{3}\left[\frac{\hbar(\omega-\Omega)}{\Theta}\right]^{3/2}+\frac{\pi}{4}\right] .$$

On the other hand, at very small energies, namely for vanishing electric fields, $\rho_{\parallel}$ does show the free-electron behavior since

$$\lim_{E\to 0} \rho_{\parallel}(\omega-\Omega) = \frac{\rho_{1D}}{(2\pi)^3}\frac{1}{\sqrt{\hbar(\Omega-\omega)}}\vartheta(\hbar\Omega-\hbar\omega) .$$

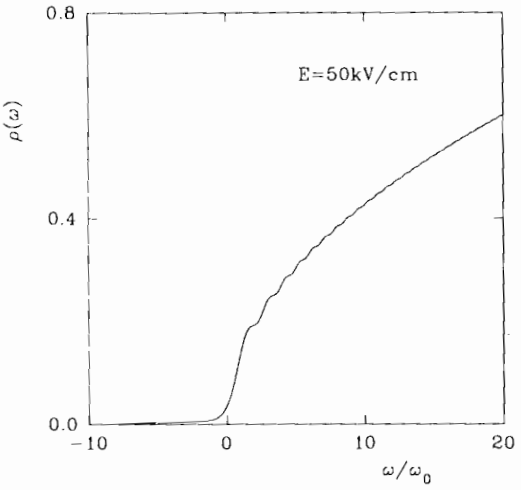
Figure 5 also shows the density of states $\rho_{\perp}$ corresponding to the component of the motion on the plane perpendicular to the field direction. This is the density of states for a two-dimensional system. Here, however, the sharp step-function behavior, typical of the free-electron system, is smeared by the presence of the interactions.



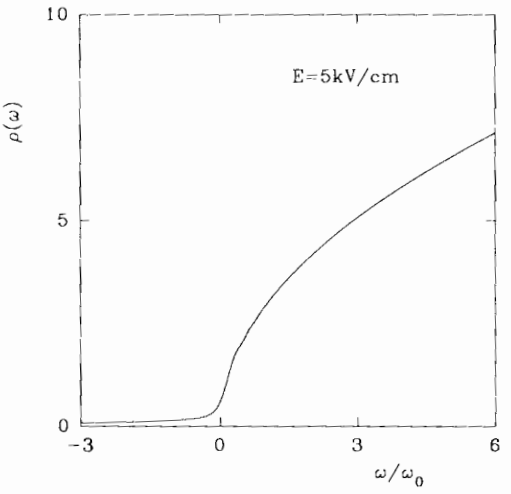
(a)

Fig. 6. The gauge-invariant density of states $\tilde{\rho}$ as given in Eq. (4.8) versus ω/ω_0 for three different values of the electric field.

Figure 6 shows the total density of states (4.8) for different values of the electric fields. Here again, the oscillations denote the existence of preferred energies (rather, energy subbands) for the electron, caused by the presence of the electric field. These subbands, however, are compressed to a very small energy range as the electric field decreases, until they collapse to form a continuous spectrum at $E \leq 5\,\mathrm{kV/cm}$. The



(b)



(c)

Fig. 6. (*Continued*)

zero-field behavior is restored at high electron energies. The negative-energy tail, also present at low fields where the oscillations have already disappeared, on the other hand, shows the effect of the collisional broadening. All this essentially confirms the interpretation given previously to the gauge-invariant self-energy (3.6).

5. Quantum Kinetic Equations

The ultimate goal is to find a solution for the quantum distribution function, such as the Wigner function, from which observables like number or current density can be extracted. There are at least three possible ways to proceed. The first one would be to construct a joint spectral density, as suggested by Reggiani *et al.*[18] and apply the quantum Monte Carlo technique.[20] However, the nonpositive definiteness of the spectral density would require either an approximation scheme, or nonstandard simulation techniques. Another possibility is to construct a simulation technique directly in the Airy-coordinate representation (Ref. 37 is an attempt to pursue this approach). A third method is to apply the techniques explained in Sec. 2, and directly solve the KBK equations for the correlation function $G^<$. Explicitly, they read

$$\left(i\hbar\frac{\partial}{\partial t'} - H\right) G^<(\mathbf{r}, t; \mathbf{r}', t') = \int_{-\infty}^{\infty} dt_1 d\mathbf{r}_1 \left[\Sigma^r(\mathbf{r}, t; \mathbf{r}_1, t_1)G^<(\mathbf{r}_1, t_1; \mathbf{r}', t') + \Sigma^<(\mathbf{r}, t; \mathbf{r}_1, t_1)G^a(\mathbf{r}_1, t_1; \mathbf{r}, t)\right] \tag{5.1a}$$

$$\left(-i\hbar\frac{\partial}{\partial t'} - H'\right) G^<(\mathbf{r}, t; \mathbf{r}', t') = \int_{-\infty}^{\infty} dt_1 d\mathbf{r}_1 \left[G^r(\mathbf{r}, t; \mathbf{r}_1, t_1)\Sigma^<(\mathbf{r}_1, t_1; \mathbf{r}', t') + G^<(\mathbf{r}, t; \mathbf{r}_1, t_1)\Sigma^a(\mathbf{r}_1, t_1; \mathbf{r}, t)\right] \tag{5.1b}$$

By Fourier transforming the transverse variable $(\mathbf{r}-\mathbf{r}')_\perp$ and Airy transforming the longitudinal variables z and z', as well as Fourier transforming to frequency variable ω on both sides of (5.1), these can be written in $(\mathbf{k}_\perp, s)$-space as

$$[\hbar\omega - \varepsilon_s(\mathbf{k}_\perp)]\, G^<(\mathbf{k}_\perp, s, s', \omega) = \int ds_1 \left[\Sigma^r(\mathbf{k}_\perp, s, s_1, \omega)G^<(\mathbf{k}_\perp, s_1, s', \omega) + \Sigma^<(\mathbf{k}_\perp, s, s_1, \omega)G^a(\mathbf{k}_\perp, s_1, s', \omega)\right]$$

$$[\hbar\omega - \varepsilon_s(\mathbf{k}_\perp)]\, G^<(\mathbf{k}_\perp, s, s', \omega) = \int ds_1 \left[G^r(\mathbf{k}_\perp, s, s_1, \omega)\Sigma^<(\mathbf{k}_\perp, s_1, s', \omega) + G^<(\mathbf{k}_\perp, s, s_1, \omega)\Sigma^a(\mathbf{k}_\perp, s_1, s', \omega)\right] .$$

This is a vast important over the many integrations one gets by using ordinary coordinate and momenta. Furthermore, by employing the model (3.5) for the retarded self-energy and, consequently, using Eq. (4.3) for G^r, the above equations become the simple multiplicative equations

$$[\hbar\omega - \varepsilon_s(\mathbf{k}_\perp)]\, G^<(\mathbf{k}_\perp, \Omega, \Omega') = \Sigma^r(\Omega)G^<(\mathbf{k}_\perp, \Omega, \Omega') + \Sigma^<(\Omega, \Omega')G^a(\mathbf{k}_\perp, \Omega') \tag{5.2a}$$

$$[\hbar\omega - \varepsilon_s(\mathbf{k}_\perp)]\, G^<(\mathbf{k}_\perp, \Omega, \Omega') = \Sigma^r(\mathbf{k}_\perp, \Omega)\Sigma^<(\Omega, \Omega') + G^<(\mathbf{k}_\perp, \Omega, \Omega')\Sigma^a(\Omega') . \tag{5.2b}$$

Each of the above equations can be solved for $G^<$ independently, and both give (compare with Eq. (1.11))

$$G^<(\mathbf{k}_\perp, \Omega, \Omega') = G^r(\mathbf{k}_\perp, \Omega)\Sigma^<(\Omega, \Omega')G^a(\mathbf{k}_\perp, \Omega') \ . \tag{5.3}$$

The same result can be obtained by subtracting the two equations (5.2a) and (5.2b). Analogously, by adding, instead of subtracting, the two equations, we always arrive at the same result.[14] All this can be proved by simple algebra, and it tells the equivalence of the two KBK equations.

An important point worth mentioning here is the following. Equation (5.3) relies on the approximation discussed below Eq. (4.2), which involves only retarded and advanced functions, but no less-than functions. Now, in Eq. (5.3), $\Sigma^<$ contains scattering "in", but scattering "out" is carried over by G^r and G^a. One can then wonder whether approximating G^r and $G^<$ in different ways would introduce an asymmetry between scattering "in" and "out". In this case, the resulting equation would be likely to violate conservation laws such as, for instance, conservation of particles. To convince ourselves that this is not the case here, we recall that, as mentioned above, Eq. (5.3) is entirely equivalent to

$$\begin{aligned}\hbar(\Omega - \Omega')G^<(\mathbf{k}_\perp, \Omega, \Omega') = [\Sigma^r(\Omega) - \Sigma^a(\Omega')]\, G^<(\mathbf{k}_\perp, \Omega, \Omega') \\ - [G^r(\mathbf{k}_\perp, \Omega) - G^a(\mathbf{k}_\perp, \Omega')]\, \Sigma^<(\Omega, \Omega') \ ,\end{aligned} \tag{5.4}$$

obtained by subtracting (5.2b) from (5.2a). In (5.4) the first term on the RHS corresponds to scattering "out", whereas the second term is the scattering "in" piece. Written in this way, the (generalized) scattering rates $[\Sigma^r(\Omega) - \Sigma^a(\Omega')]$ and $[G^r(\mathbf{k}_\perp, \Omega) - G^a(\mathbf{k}_\perp, \Omega')]$ appear entirely symmetric, and are clearly evaluated on the same level of approximation.

In order to put Eq. (5.3) into gauge-invariant form, we have to use rule (2.20) for nondiagonal functions, which we can rewrite as

$$\begin{aligned}\tilde{G}^<(\mathbf{k}, \tau) = \sqrt{2\pi}L\frac{\hbar}{eE}\int \frac{d\Omega d\Omega'}{2\pi} e^{-i\left[T(k_z)+\frac{\tau}{2}\right]\Omega'} e^{i\left[T(k_z)-\frac{\tau}{2}\right]\Omega'} \\ \times G^<(\mathbf{k}_\perp, \Omega, \Omega')\tilde{A}_E(k_z, \tau) \ .\end{aligned}$$

According to Eq. (1.13), the distribution function is obtained by taking the frequency integral of the correlation function

$$\begin{aligned}\tilde{f}(\mathbf{k}) &= \hbar\int \frac{d\omega}{\sqrt{2\pi}}\tilde{G}^<(\mathbf{k}, \omega) = \hbar\tilde{G}^<(\mathbf{k}, \tau = 0) \\ &= \sqrt{2\pi}L\frac{\hbar}{eE}\int \frac{d\Omega d\Omega'}{2\pi} e^{-iT(k_z)(\Omega-\Omega')}G^<(\mathbf{k}_\perp, \Omega, \Omega') \ ,\end{aligned} \tag{5.5}$$

and thus the knowledge of $G^<$ in Airy representation suffices to determine the full $\tilde{f}(\mathbf{k})$. In (5.5) we also observe that the transformation into gauge-invariant form restores the k_z-dependence through the "center-of-mass" time $T(k_z)$ discussed in Sec. 2.

5.1. *Formal properties*

Let us now consider some properties of $G^<$ in Airy representation. By substituting the explicit expression (4.3) for G^r, Eq. (5.3) can be manipulated to give

$$G^<(\mathbf{k}_\perp, \Omega, \Omega') = A(\mathbf{k}_\perp, \Omega) f_1(\mathbf{k}_\perp, \Omega, \Omega') \ , \tag{5.6a}$$

with

$$f_1(\mathbf{k}_\perp, \Omega, \Omega') = \frac{G^a(\mathbf{k}_\perp, \Omega')}{G^a(\mathbf{k}_\perp, \Omega)} \left[\frac{\Sigma^<(\Omega, \Omega')}{\hbar\Gamma(\Omega)} \right] \ . \tag{5.6b}$$

Equations (5.6) satisfy both (5.2a) and (5.2b) as can be verified by substitution.

Expression (5.6a) for $G^<$ is quite interesting. It is derived exactly from Eq. (5.3) and has the same formal structure of the nonequilibrium *ansätze* introduced in many earlier attempts to solve both the high-field and the linear-response-regime problem.[12,15,18,22,38] Equation (5.6a) expresses a direct relationship between the correlation function $G^<$ and a quantum mechanical distribution function f_1. In the present form, however, f_1 has no practical advantage with respect to $G^<$ since it contains the same number of variables, and we might as well solve (5.6a) directly for $G^<$, as can be easily realized by recalling expression (1.2) for $\Sigma^<$.

The separation given in (5.6), however, is not unique since, by substituting G^a, instead of G^r, we can write

$$G^<(\mathbf{k}_\perp, \Omega, \Omega') = A(\mathbf{k}_\perp, \Omega') f_2(\mathbf{k}_\perp, \Omega, \Omega') \ ,$$

$$f_2(\mathbf{k}_\perp, \Omega, \Omega') = \frac{G^r(\mathbf{k}_\perp, \Omega)}{G^r(\mathbf{k}_\perp, \Omega')} \left[\frac{\Sigma^<(\Omega, \Omega')}{\hbar\Gamma(\Omega')} \right] \ .$$

A unique expression is, however, obtained for the modulus of $G^<$:

$$|G^<(\mathbf{k}_\perp, \Omega, \Omega')| = A(\mathbf{k}_\perp, \Omega, \Omega') \mathcal{F}(\mathbf{k}_\perp, \Omega, \Omega') \ ,$$

with

$$\mathcal{F}(\mathbf{k}_\perp, \Omega, \Omega') = \frac{|\Sigma^<(\Omega, \Omega')|}{\hbar\Gamma(\Omega, \Omega')} \ ,$$

which is now independent of the transverse momentum $\mathbf{k}_\perp$, and

$$A(\mathbf{k}_\perp, \Omega, \Omega') = \sqrt{A(\mathbf{k}_\perp, \Omega) A(\mathbf{k}_\perp, \Omega')} \ , \quad \Gamma(\Omega, \Omega') = \sqrt{\Gamma(\Omega)\Gamma(\Omega')}$$

the geometric means of the two spectral density functions and scattering rates, respectively.

Also the diagonal elements $G^<(\mathbf{k}_\perp, \Omega)$ have a unique factorization

$$G^<(\mathbf{k}_\perp, \Omega) = A(\mathbf{k}_\perp, \Omega) f(\Omega) \ , \tag{5.7a}$$

with

$$f(\Omega) = -\frac{\Sigma^<(\Omega)}{\hbar\Gamma(\Omega)} \ , \tag{5.7b}$$

again a momentum-independent function.

By a procedure similar to that leading to Eq. (3.5) for $\Sigma^r(\Omega)$, we obtain the Airy representation of $\Sigma^<$, namely

$$\begin{aligned}\Sigma^>(\Omega) = -\hbar\frac{\rho_{1D}}{\sqrt{2\pi}}\frac{1}{\sqrt{3^{1/3}\Theta}}\sum_\eta |V|^2 \left(N_o + \frac{\eta+1}{2}\right)\int \frac{d(\mathbf{k}_\perp - \mathbf{q}_\perp)}{(2\pi)^2} \\ \times \int_{-\infty}^{\infty} \frac{d\Omega}{\sqrt{2\pi}} Ai^2\left(\frac{\hbar\Omega - \hbar\Omega')}{3^{1/3}\Theta}\right) G^<(\mathbf{k}_\perp - \mathbf{q}_\perp, \Omega' + \eta\omega_0) \ .\end{aligned} \tag{5.8}$$

Therefore, by using Eq. (5.7a), and performing the momentum integration, $f(\Omega)$ defined in (5.7b) satisfy the homogeneous integral equation

$$f(\Omega) = \int d\Omega' K(\Omega, \Omega') f(\Omega') \ , \tag{5.9a}$$

with

$$\begin{aligned}K(\Omega, \Omega') = \frac{\rho_{1D}}{\sqrt{3^{1/3}\Theta}}\sum_\eta |V|^2 \left(N_0 + \frac{\eta+1}{2}\right) \\ \times \int \frac{dt}{2\pi} e^{-\Gamma(\Omega)t} Ai^2\left(\frac{\hbar\Omega - \hbar\Omega'}{3^{1/3}\Theta}\right) \rho_\perp(\Omega')\end{aligned} \tag{5.9b}$$

and $\rho_\perp(\Omega')$ given in Eq. (4.9) with $\zeta = -(\hbar\Omega' + \eta\hbar\omega_0)/3^{1/3}\Theta$. In Eq. (5.9), the variable Ω' always appears as $\Omega' + \eta\omega_0$, and thus represents the total electronic energy before the scattering events has occurred. On the other hand, Ω always appears as $\Omega - \eta\omega_0$. The kernel $K(\Omega, \Omega')$, therefore, acting on the function $f(\Omega')$ calculated before the scattering, transforms it to $f(\Omega)$ evaluated after the scattering has occurred. Here we recall that in equilibrium $\Sigma^<_{eq}(\omega) = f_{FD}(\omega)\Gamma_{eq}(\omega)$, and hence, in this limit, $f(\Omega)$ reduces to the Fermi-Dirac distribution f_{FD}.[6]

The function $f(\Omega)$ turns out to play a crucial role in the future development.

6. Average Values

6.1. *Density of particles*

Once the distribution function $\tilde{f}(\mathbf{k})$ is obtained, the average values of the observables of interest can be calculated as its moments.

The number density n, for instance, is obtained as

$$n = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \tilde{f}(\mathbf{k}) ,$$

where $\mathcal{V}$ is the crystal volume.

Applying Eq. (5.5), and going to the continuous $\mathbf{k}$-variable, the required k_z-integrations are readily performed and we obtain

$$n = \int \frac{d\mathbf{k}_\perp}{(2\pi)^2} \int d\Omega G^<(\mathbf{k}_\perp, \Omega) = \int d\Omega \rho_\perp(\Omega) f(\Omega) \equiv \int d\Omega n(\Omega) , \qquad (6.1)$$

where Eq. (5.7a) has been used, and the $\mathbf{k}_\perp$-integration has been performed.

Here we would like to stress that $\tilde{f}(\mathbf{k})$ contains the full, nondiagonal correlation function $G^<(\mathbf{k}_\perp, \Omega, \Omega')$ (a diagonal $G^<$ gives no current) and that this was employed to obtain Eq. (6.1). However, as a result of the k_z-integration, one needs only to explicitly evaluate the simpler diagonal $G^<(\mathbf{k}_\perp, \Omega)$, or, equivalently, $f(\Omega)$.

The kernel $K(\Omega, \Omega')$ in Eq. (5.9b), though quite complicated, is expressed in terms of standard functions and therefore Eq. (5.9a) is well suited for a numerical solution. We have solved Eq. (5.9a) iteratively with a Maxwell-Boltzmann distribution as the initial guess. Since Eq. (5.9a) is a homogeneous equation, it requires a boundary condition. This is provided by Eq. (6.1). Namely, at each iteration $f(\Omega)$ was normalized so that the density of particles stayed at a constant value of $n = 10^{28}$ cm^{-3}. In the numerical work, the truncation of the infinite Ω-integral had to be carefully optimized in order to obtain a convergent distribution function $n(\Omega)$. Once the proper ('converging') integration interval was identified, the final results were not sensitive to the choice of the seed of the iteration, and the normalization procedure described above was carried out to take care of roundoff errors. One should also note that since we are working with a homogeneous equation, which has a trivial solution $f(\Omega) = 0$, one must also be on guard against a collapse towards this direction.

Figure 7 shows the function $n(\Omega)$ for two different field strengths. For comparison, we also show the corresponding equilibrium function. An important feature of $n(\Omega)$ is the pronounced high-energy tail, which is consistent with the results of Refs. 18 and 20. It suggests that the carriers can increase its kinetic energy even when it emits a phonon because of CB and ICFE. We also find the existence of particles with negative total energy, as well as a series of preferred energy levels indicated by the damped oscillations occurring at $\Omega > 0$. The period of the oscillations exactly scales with the field strength (this feature is also present in the gauge invariant spectral density function) confirming the sub-bands formation caused by the field.

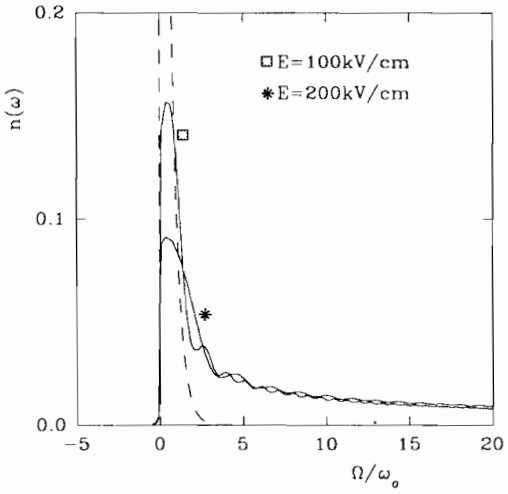


Fig. 7. The local density of particles as a function of the electron energy.

6.2. *Current density*

The electron current density is calculated from the distribution function $\tilde{f}(\mathbf{k})$ as

$$\mathbf{J} = -e\langle \nu \rangle = -\frac{e\hbar}{m}\frac{1}{\mathcal{V}}\mathbf{k}\tilde{f}(\mathbf{k}) \ ,$$

that is, by the same procedure as in the previous subsection,

$$\mathbf{J} = -\sqrt{2\pi}\frac{\hbar^2}{mE}\int \frac{d\mathbf{k}_\perp}{(2\pi)^{3/2}}(\mathbf{k}_\perp \hat{\mathbf{r}}_\perp + k_z\hat{\mathbf{z}})\int \frac{d\Omega d\Omega'}{2\pi}e^{-iT(k_z)(\Omega-\Omega')}G^<(\mathbf{k}_\perp, \Omega, \Omega')$$
$$= \mathbf{J}_\perp \hat{\mathbf{r}}_\perp + J_z\hat{\mathbf{z}} \ ,$$

with $\hat{\mathbf{r}}_\perp$ and $\hat{\mathbf{z}}$ the unit vectors along the transverse and longitudinal direction, respectively.

The transverse component $\mathbf{J}_\perp$ vanish identically because of the angular integration. The longitudinal component, after the variable change $k_z \rightarrow T(k_z)$, can be rewritten as

$$J_z = \sigma(E)E \ ,$$

generalizing Ohm's law through the field-dependent, steady-state conductivity

$$\sigma(E) = -\frac{e^2}{m}\int \frac{d\mathbf{k}_\perp}{(2\pi)^2}\int TdT\int \frac{d\Omega d\Omega'}{2\pi}e^{-iT(\Omega-\Omega')}G^<(\mathbf{k}_\perp, \Omega, \Omega') \ . \qquad (6.2)$$

This expression can be put in a more transparent form by noting that

$$\left(\frac{\partial}{\partial\Omega}-\frac{\partial}{\partial\Omega'}\right)\delta(\Omega-\Omega')=\int_{-\infty}^{\infty}\frac{dT}{2\pi}(-2iT)e^{-iT(\Omega-\Omega')}$$

and substituting this into (6.2). An integration by parts then, leads to

$$\sigma=\frac{e^2}{m}\int\frac{d\mathbf{k}_\perp}{(2\pi)^2}\int d\Omega\left[-\frac{i}{2}\left(\frac{\partial}{\partial\Omega}-\frac{\partial}{\partial\Omega'}\right)G^<(\mathbf{k}_\perp,\Omega,\Omega')\right]_{\Omega-\Omega'}.$$

From this expression we understand why a diagonal $G^<$ would lead to a vanishing current. Indeed $(\partial/\partial\Omega-\partial/\partial\Omega')$ measures how G^r changes as $(\Omega-\Omega')$ varies. For $G^<\propto\delta(\Omega-\Omega')$ this variation is precisely zero if one understand $\delta(\Omega-\Omega')$ as the limit of symmetric, highly peaked functions. Therefore, while a simpler, diagonal model for G^r can lead to physically meaningful results, the full, nonlocal total energy dependence of $G^<$ must be retained. The situation is quite analogous to what is encountered in standard linear-response theory: there, simple forms for G^r suffice, while for the vertex part, the full frequency dependence must be considered.

Using Eq. (5.3)

$$\left(\frac{\partial}{\partial\Omega}-\frac{\partial}{\partial\Omega'}\right)G^<(\mathbf{k}_\perp,\Omega,\Omega')\Big|_{\Omega=\Omega'}$$
$$=\left(\frac{\partial}{\partial\Omega}-\frac{\partial}{\partial\Omega'}\right)G^r(\mathbf{k}_\perp,\Omega)\Sigma^r(\Omega,\Omega')G^a(\mathbf{k}_\perp,\Omega')\Big|_{\Omega=\Omega'},$$

and noting that for the present type of scattering mechanism $[(\partial/\partial\Omega-\partial/\partial\Omega')\Sigma^<(\Omega,\Omega')]_{\Omega-\Omega'}=0$ (see Eq. (3.3) with $r\to<$, and $-\eta\omega_{\mathbf{q}}\to+\eta\omega_{\mathbf{q}}$), we have

$$\left(\frac{\partial}{\partial\Omega}-\frac{\partial}{\partial\Omega'}\right)G^<(\mathbf{k}_\perp,\Omega,\Omega')\Big|_{\Omega=\Omega'}$$
$$=\left[\frac{\partial G^r(\mathbf{k}_\perp,\Omega)}{\partial\Omega}G^a(\mathbf{k}_\perp,\Omega')-G^r(\mathbf{k}_\perp,\Omega)\frac{\partial G^a(\mathbf{k}_\perp,\Omega')}{\partial\Omega'}\right]\Sigma^<(\Omega,\Omega')\Big|_{\Omega=\Omega'}.$$

By Eq. (4.3) the derivative of G^r and G^a are easily performed and, finally, one obtains

$$\sigma=\frac{\hbar e^2}{2m}\int\frac{d\mathbf{k}_\perp}{(2\pi)^2}\int d\Omega\left[\left(1-\frac{1}{\hbar}\frac{\partial\,\mathrm{Re}\,\Sigma^r}{\partial\Omega}\right)\right.$$
$$\left.+(\hbar\Omega-\varepsilon(\mathbf{k}_\perp)-\mathrm{Re}\Sigma^r)\left(\frac{1}{\hbar}\frac{\partial\ln\mathrm{Im}\,\Sigma^r}{\partial\Omega}\right)\right]\times A^2(\mathbf{k}_\perp,\Omega)f(\Omega)\,. \tag{6.3}$$

This expression for the nonlinear conductivity is the central analytical result of our work. Equation (6.3) bears formal similarities to the *linear* Quantum Boltzmann Equation derived by Mahan[12,15]: some of the mass-renormalization factors have the

same structure (but recall that there are nonequilibrium quantities), and we also get the square of the spectral density.

The $\mathbf{k}_\perp$-integration can also be performed analytically and we obtain

$$\sigma = \frac{e^2}{m}\int d\Omega \left(1 - \frac{1}{\hbar}\frac{\partial \operatorname{Re}\Sigma^r}{\partial\Omega}\right)\rho_\perp(\Omega)\tau(\Omega)f(\Omega)$$
$$- \frac{e^2}{m}\int d\Omega \left(\frac{\rho_{2D}}{4\pi^2}\right)\left(1 - \frac{1}{\hbar}\frac{\partial \operatorname{Re}\Sigma^r}{\partial\Omega}\right)(\hbar\Omega - \operatorname{Re}\Sigma')\tau(\Omega)G^<(\Omega)$$
$$+ \frac{e^2}{m}\int d\Omega \left(\frac{\rho_{2D}}{4\pi^2}\right)\left(\frac{1}{2\hbar}\frac{\partial \operatorname{Im}\Sigma^r}{\partial\Omega}\right)G^<(\Omega)\,, \tag{6.4}$$

where $[\tau(\Omega)]^{-1} = -\frac{2\operatorname{Im}\Sigma^r(\Omega)}{\hbar}$ is the scattering rate and $G^<(\Omega) \equiv A(\mathbf{k}_\perp = 0, \Omega)$ $f(\Omega)$.

Equation (6.4) effectively reduces the evaluation of the nonlinear current to the solution of the one-dimensional integral equation (5.9) obeyed by $f(\Omega)$ and already discussed in Sec. 6.1.

An important question concerns the relation between our result and the well-known results in linear-response theory. Taking the linear-response limit of $f(\Omega)$ in our formulation is not straightforward. We trace the difficulty to the fact that in the zero-field limit the Airy functions do not approach plane waves uniformly (but they do in the distribution sense, see Ref. 38). Consequently, we have not been able to demonstrate *in general* that the linear limit of our result coincides with those obtained with, say, the Kubo formula, or the Quantum Boltzmann Equation of Mahan[12,39] and others. However, it is not difficult to demonstrate that the semiclassical Boltzmann equation result is contained in our theory. To see this, note first that in linear response, we can evaluate all the quantities appearing in Eq. (6.3) in equilibrium. Next, according to the Boltzmann picture, we make the quasiparticle approximation

$$\int \frac{d\Omega}{2\pi} A^2(\varepsilon(\mathbf{k}_\perp), \Omega) f(\Omega) = \frac{f(\varepsilon(\mathbf{k}_\perp))}{\Gamma(\varepsilon(\mathbf{k}_\perp))}\,.$$

Recalling the connection between the relaxation time and the imaginary part of the Green's function (3.7), and using expression (6.1) for the number density, we see that the Boltzmann equation result $\sigma = ne^2\tau/m$ is recovered.

In Fig. 8 we compare the drift velocities obtained with quantum approach, and semiclassical simulations.[40] To our knowledge, this is the first time such a comparison has been made. Our quantum-mechanical calculation results in a larger drift velocity than what is found in the semiclassical case; confirming the predictions of other quantum transport simulations.[18,20] Finally, in Fig. 9a, we display the effect of temperature, and in Fig. 9b calculations corresponding to two different values of the deformation-potential constant are shown. The qualitative trends seen in Figs. 9a and 9b are the same as found in experiment and in the semiclassical

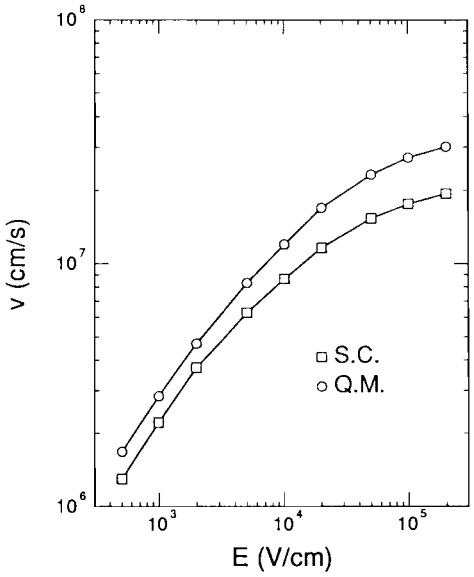


Fig. 8. The electron drift velocity vs. electric field. S. C. refers to semiclassical cellular automata simulation.[40]

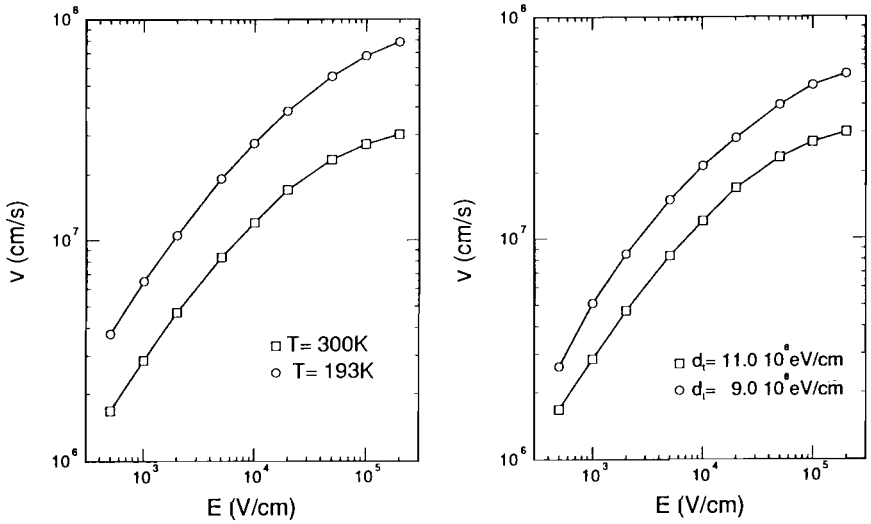


Fig. 9. a) Effect of temperature for quantum drift velocities. b) Effect of coupling constant for quantum drift velocities.

theory. It would be, however, premature to assign quantitative significance to the actual numbers of interpret experiments in the light of our model calculations: to do

so one would also have to consider other scattering mechanisms as well as realistic band structures.

7. Calculations

We presented a new formulation of the Kadanoff-Baym-Keldysh nonequilibrium Green's function methods to develop a fully quantum mechanical formalism that can be used for high, homogeneous fields. The aim was to derive a spectral density model and a quantum kinetic equation which account for both the energy dependence of the collision rate and the intracollisional field effect in a relatively simple and rigorous way.

Spectral density is an object of central interest in theories of interacting many-body systems. On the other hand, it gives information about the quasi-particle spectrum of the system, such as densities of states of life-times. On the other hand, quantum kinetic theories on nonequilibrium Green's function techniques, often require the knowledge of the spectral density as a prerequisite. Solutions for the spectral density for nontrivial systems under highly nonequilibrium conditions, such as those encountered in many semiconductor microstructures, are scarce, and in most cases restricted to limiting cases only (e.g. weak fields or weak scattering).

In order to find a spectral density model which treat scattering and field effects on equal footing, we replaced the usual momentum representation along the field direction by a representation in terms of a convenient set of variables ('Airy coordinates'). We have to point out technique differs from the previous ones that have found solutions in terms of Airy functions. The introduction of the Airy transform, in fact, introduces the proper symmetry of the system from the beginning, thus yielding mathematically simpler equations with fewer coordinates and convolutions. We have applied this technique to the case of silicon with nonpolar optical phonon scattering, under a homogeneous electric field of arbitrary strength.

However, the interpretation of results given in Airy coordinates is not straightforward because of the explicit gauge dependence. Therefore, we have undertaken a general analysis of the interrelationship between the Airy coordinate results and their counterparts in a gauge invariant formulation. Our main formal results are contained in Eqs. (2.20) and (2.22), which allow one to transform any function found in Airy coordinates to a gauge-invariant form. As an illustration of the techniques, we consider a number of examples, the results for some of which were known previously. As a nontrivial application, we consider the model electron-phonon system mentioned above.

The result is the appearance of a series of damped oscillations in both the real and imaginary parts of the electron self-energy. They indicate the existence of preferred energy levels for the electron, represented by the alternate zero-crossings of the real part of the self-energy, and reflected in the plateau-structure of the scattering rate.

The solution of Dyson's equation, obtained by making use of the singular nature of the self-energy function in the Airy representation, preserves the sum rules any proposal for the spectral density must obey. We have analyzed the resulting spectral density and density of states as a function of the applied field (Figs. 2–6). We find a transition from a collision dominated regime for low fields (pure collisional broadening) to a field dominated regime for high fields.

Next, we applied our techniques to the Kadanoff and Baym quantum kinetic equations in order to derive a gauge-invariant distribution function $\tilde{f}(\mathbf{k})$ and evaluate the average values of experimentally accessible quantities.

Our calculations involve neither assumptions of the form of the nonequilibrium correlation function, nor gradient expansions, as in the case of many older theories. This represents a significant improvement with respect to previous formulations, most of which have resulted either in formal results only, or have required nonstandard Monte Carlo techniques for their solution. The only (and in our view, not essential) approximation was made in the choice of the model for the retarded self-energy for the electron-phonon interaction. The main consequence of this approximation is that the retarded and advanced Green functions are diagonal in the variable Ω. Given this property, the KBK equations for the correlation function can be manipulated analytically without introducing additional approximations.

Nonunique solutions of the KBK equations were obtained in the Airy representation for the nonlocal correlation function $G^<(\Omega, \Omega')$, whereas a unique solution could be obtained only for the local $G^<(\Omega)$ from which, however, a straightforward evaluation of the current is not possible.

An interesting feature of the Airy representation is existence of the relation $G^< = Af$ which generalizes to high fields the equilibrium relation (1.12). This relation is the expression of the "fluctuation-dissipation" theorem:[41] It relates the mean-square fluctuation

$$\langle \hat{\psi}(\omega)\hat{\psi}^\dagger(\omega)\rangle = \int d\tau e^{i\omega\tau}\langle \hat{\psi}(\tau)\hat{\psi}^\dagger(0)\rangle \approx G^<(\omega)$$

of the field operators (or, more generally, of any appropriate operator) to Im $G^r(\omega)$, which is often proportional to the dissipation in the system.[42] This is a celebrated result, and because of its generally it is believed (although debated in the literature[22,38]) to hold also for nonequilibrium systems. However, for these cases, none of the previous approaches has been able to derive an expression that, through the distribution function, exactly relate the correlation function and the spectral function. Even in the near-equilibrium gradient approximation only ansätze are available.

Finally, by employing a gauge-invariant formulation, we have cast nonlinear quantum transport theory in a form which appears well suited for the numerical evaluation of the distribution function $\tilde{f}(\mathbf{k})$. An important result of the theory presented here, however, is that it is not necessary to compute $\tilde{f}(\mathbf{k})$ to extract the averaged physical quantities: The vastly simpler object $f(\Omega)$ can be singled

out as a unique function with a direct connection to physical observables. The final result for the nonlinear conductivity goes beyond the quasiparticle limit by including renormalization effects explicitly.

We have not treated inhomogeneous fields. However, we know that by transforming to a basis of states found in the absence of phonon scattering, but with a nontrivial field included, a simplified form of the KBK equations results.

It remains to be seen how much of the above analysis can be carried over to less restrictive mechanisms of electron-phonons interaction and/or experimentally relevant geometries. This will be a topic of future work.

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Appendix A

We define the Airy transform $\mathcal{A}_s[a(z)]$ of a general function $a(z)$ by

$$A(s) \equiv \mathcal{A}_s[a(z)] \equiv \int_{-\infty}^{\infty} dz Ai(z-s)a(z) \ . \tag{A.1}$$

The problem is to find the inverse transform of the Airy transform. Using the integral representation[31]

$$Ai(x) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\left(\frac{t^3}{3}+xt\right)} \ , \tag{A.2}$$

we find that

$$\int_{-\infty}^{\infty} dz Ai(z-s)Ai(z-s') = \delta(s-s') \ . \tag{A.3}$$

We can therefore define the inverse of the Airy transform as

$$a(z) \equiv \mathcal{A}_z^{-1}[A(z)] \equiv \int_{-\infty}^{\infty} dz Ai(z-s)A(s) \ . \tag{A.4}$$

The Airy transform is in the form of a convolution and, therefore, the Fourier transform of the Airy transform is the simple product

$$\mathcal{F}_k[A(s)] = Ai(k)a(k) \ . \tag{A.5}$$

A function $f(z, z')$ is translationally invariant if its value depends only on the variable difference $z - z'$, that is

$$f(z, z') = f(z - z', 0) \equiv f(z - z') \ .$$

A function $f(z, z')$ is diagonal if it can be written as

$$f(z, z') \equiv f(z)\delta(z - z') \ .$$

If $f(z, z')$ is translationally invariant, then it is diagonal in reciprocal space. In fact,

$$\begin{aligned} f(k, k') &= \int \frac{dz}{\sqrt{2\pi}} \int \frac{dz}{\sqrt{2\pi}} e^{-ikz} e^{ikz'} f(z, z') = \int \frac{dz dz'}{2\pi} e^{-ik(z-z')} e^{i(k-k')z'} f(z, z') \\ &= \int d(z - z') e^{-ik(z-z')} f(z - z') \int \frac{dz'}{2\pi} e^{i(k-k')z} \\ &= \int d(z - z') f(z - z') \delta(k - k') \\ &= f(k)\delta(k - k') \ . \end{aligned} \tag{A.6}$$

However, a similar relation does not hold between translational invariance in real space and diagonality in the Airy coordinate space. Indeed, if a function is translationally invariant in z, then it is also translationally invariant in s:

$$\begin{aligned} f(s, s') &= \int dz dz' Ai(z - s) Ai(z' - s') f(z, z') \\ &= \int dz dz' Ai(z - s + s') Ai(z') f(z + s', z' + s') \\ &= \int dz dz' Ai[z - (s - s')] Ai(z') f(z, z') = f(s - s', 0) \equiv f(s - s') \ . \end{aligned} \tag{A.7}$$

This last property was somehow expected since the s-space has the same nature of real z-space, but it allows to include nonperturbatively in the problem the proper symmetry features of an inhomogeneous system.

Appendix B

Example 1. Let us apply the transformation (2.13) to the retarded Green's function[32]

$$\begin{aligned} G^r_\phi(\mathbf{k}_1, t_1; \mathbf{k}_2, t_2) = -\frac{i}{\hbar} \vartheta(t_1 - t_2) \delta \left(\mathbf{k}_1 - \mathbf{k}_2 + \frac{e\mathbf{E}}{\hbar}(t_1 - t_2) \right) \\ \times e^{-\frac{i}{\hbar} \int_0^{t_1 - t_2} dt' \varepsilon \left(\mathbf{k}_1 + \frac{e\mathbf{E}}{\hbar} t' \right)} \end{aligned} \tag{B.1}$$

calculated in the scalar potential gauge.

First, let us Fourier-transform (B.1)

$$G^r_\phi(\mathbf{k}_1, t_1; \mathbf{k}_2, t_2) = -\frac{i}{\hbar}\vartheta(t_1 - t_2)\int \frac{d\mathbf{k}_1 d\mathbf{k}_2}{(2\pi)^3} e^{i\mathbf{k}_1 \cdot \mathbf{r}_1 - i\mathbf{k}_2 \cdot \mathbf{r}_2}$$
$$\times \delta\left(\mathbf{k}_1 - \mathbf{k}_2 + \frac{e\mathbf{E}}{\hbar}(t_1 - t_2)\right) e^{-\frac{i}{\hbar}\int_0^{t_1 - t_2} dt'\varepsilon\left(\mathbf{k}_1 + \frac{e\mathbf{E}}{\hbar}t'\right)}$$
$$= -\frac{i}{\hbar}\vartheta(t_1 - t_2)\int \frac{d\mathbf{k}_1}{(2\pi)^3} e^{i\mathbf{k}_1 \cdot \mathbf{r}_1 - i\left[\mathbf{k}_1 + \frac{e\mathbf{E}}{\hbar}(t_1 - t_2)\right] \cdot \mathbf{r}_2}$$
$$\times e^{-\frac{i}{\hbar}\int_0^{t_1 - t_2} dt'\varepsilon\left(\mathbf{k}_1 + \frac{e\mathbf{E}}{\hbar}t'\right)} ,$$

or, using the center-of-mass coordinates,

$$G^r_\phi(\mathbf{r}, \tau, \mathbf{R}, T) = -\frac{i}{\hbar}\vartheta(\tau)\int \frac{d\mathbf{k}_1}{(2\pi)^3} e^{i\mathbf{k}_1 \cdot \mathbf{r}_1 - i\frac{e}{\hbar}\mathbf{E} \cdot \left(\mathbf{R} - \frac{\mathbf{r}}{2}\right)\tau} e^{-\frac{i}{\hbar}\int_0^\tau dt'\varepsilon\left(\mathbf{k}_1 + \frac{e\mathbf{E}}{\hbar}t'\right)} .$$

Now we can apply (2.17)

$$\tilde{G}^r(\mathbf{k}, \omega, \mathbf{R}, T) = \int_{-\infty}^{\infty} \frac{d\tau}{\sqrt{2\pi}} e^{i\left(\omega + \frac{e}{\hbar}\mathbf{E} \cdot \mathbf{R}\right)\tau} \int \frac{d\mathbf{r}}{(2\pi)^{3/2}} e^{-i\mathbf{k} \cdot \mathbf{r}} G^r_\phi(\mathbf{r}, \tau, \mathbf{R}, T)$$
$$= -\frac{i}{\hbar}\int_0^\infty \frac{d\tau}{\sqrt{2\pi}} e^{i\omega\tau}\int d\mathbf{k}_1 \delta\left(\mathbf{k}_1 + \frac{e\mathbf{E}}{2\hbar}\tau - \mathbf{k}\right) e^{-\frac{i}{\hbar}\int_0^\tau dt'\varepsilon + \left(\mathbf{k}_1 + \frac{e\mathbf{E}}{\hbar}t'\right)}$$
$$= -\frac{i}{\hbar}\int_0^\infty \frac{d\tau}{\sqrt{2\pi}} e^{i\omega\tau} e^{-\frac{i}{\hbar}\int_0^\tau dt'\varepsilon\left(\mathbf{k}_1 + \frac{e\mathbf{E}}{2\hbar}\tau + \frac{e\mathbf{E}}{2\hbar}t'\right)}$$
$$-\frac{i}{\hbar}\int_0^\infty \frac{d\tau}{\sqrt{2\pi}} e^{i\omega\tau} e^{-\frac{i}{\hbar}\int_{-\tau/2}^{\tau/2} dt'\varepsilon\left(\mathbf{k}_1 + \frac{e\mathbf{E}}{2\hbar}\tau'\right)}$$
$$= \tilde{G}^r(\mathbf{k}, \omega) . \tag{B.2}$$

Example 2. Let us now transform the Green's function

$$G^r_{\mathbf{A}}(\mathbf{p}_1, t_1, \mathbf{p}_2, t_2) = -\frac{i}{\hbar}\vartheta(t_1 - t_2)\delta(\mathbf{p}_1 - \mathbf{p}_2) e^{-\frac{i}{\hbar}\int_{t_2}^{t_1} dt'\varepsilon\left[\mathbf{p}_1 - \frac{e}{\hbar c}\mathbf{A}(t')\right]} ,$$

calculated in the vector-potential gauge.

By the same procedure as in Example 1, and applying (2.18), we can write

$$\tilde{G}(\mathbf{k}, \omega, \mathbf{R}, T) = -\frac{i}{\hbar}\int_0^\infty \frac{d\tau}{\sqrt{2\pi}} e^{i\omega\tau}\int \frac{d\mathbf{r}}{(2\pi)^{3/2}} e^{-i\left(\mathbf{k} + \frac{e}{\hbar}\mathbf{E}T\right) \cdot \mathbf{r}}$$
$$\times \int \frac{d\mathbf{p}_1}{(2\pi)^{3/2}} e^{i\mathbf{p}_1 \cdot \mathbf{r}} e^{-\frac{i}{\hbar}\int_{T - \tau/2}^{T + \tau/2} dt'\varepsilon\left(\mathbf{p}_1 - \frac{e}{\hbar}\mathbf{E}t'\right)}$$
$$= -\frac{i}{\hbar}\int_0^\infty \frac{d\tau}{\sqrt{2\pi}} e^{i\omega\tau}\int d\mathbf{p}_1 \delta\left(\mathbf{p}_1 - \mathbf{k} - \frac{e}{\hbar}\mathbf{E}T\right) e^{-\frac{i}{\hbar}\int_{T - \tau/2}^{T + \tau/2} dt'\varepsilon\left(\mathbf{p}_1 - \frac{e}{\hbar}\mathbf{E}t'\right)}$$

$$= -\frac{i}{\hbar}\int_0^\infty \frac{d\tau}{\sqrt{2\pi}} e^{i\omega\tau} e^{-\frac{i}{\hbar}\int_{-\tau/2}^{\tau/2} dt' \epsilon\left(\mathbf{k} - \frac{e}{\hbar}\mathbf{E}t'\right)}$$

$$= \tilde{G}^\tau(\mathbf{k}, \omega) \tag{B.3}$$

as in Eq. (B.2).

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