Airy-coordinate technique for nonequilibrium Green's-function approach to high-field quantum transport

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(Received 1 May 1989)

We develop a formalism for studying the motion of nondegenerate electrons in semiconductors, which allows a nonperturbative description of the effects of an external high electric field on electron-phonon scattering within the Kadanoff-Baym-Keldysh nonequilibrium Green's-function approach. Based on the exact solutions of Schrödinger's equation, we solve Dyson's equation for the single-particle retarded Green's function $G^r(\mathbf{k}_\perp,z,z',\omega)$. Recognizing that high fields break the translational symmetry of the system and that momentum is no longer a good quantum number, we use Airy transforms to handle the position dependence parallel to the applied high field. From this we are able to derive a model for the spectral density function $A(\mathbf{k}_\perp,s,\omega)$ through which we can account for quantum effects such as collisional broadening and the intracollisional field effect in a simple and rigorous way. We demonstrate the theory by considering only weak scattering with nonpolar optical phonons and restrict ourselves to fields that are constant in space and time. Our formulation suggests the presence of a novel quantum effect induced by the simultaneous presence of scattering and electric field which produces a discontinuous trajectory of the electron path along the field direction.

I. INTRODUCTION

The technological possibility of fabricating devices of nanometer dimensions[1] and the subsequent recent rapidly increasing interest in the physics of ultrasmall semiconductor electronics components have motivated the formulation of a quantum theory of transport phenomena capable of overcoming the limits of the semiclassical approach based on the Boltzmann equation.[2] This latter theory is based on the validity of the adiabatic approximation and on perturbation theory. It assumes the conduction electrons to be in nearly stationary and free-particlelike states with a well-defined momentum $\mathbf{k}$. Nonstationarity arises from the assumption that the perfect-crystal periodicity is altered by imperfections, impurities, and phonons. Collisions with phonons, in particular, are assumed to be independent and to occur instantaneously in space and time, thus causing weak and infrequent scattering of the electrons among the states $\{\mathbf{k}\}$. Any applied electric field is treated as weak and slowly varying and its effect is only to accelerate the carriers through the momentum states without distorting the states or interfering with the scattering processes.

In nanometer devices, however, both the electric field and the scattering rates can reach very high values[3] and the spatio-temporal variations of the phenomena involved become comparable to those of the microscopic interactions. In these regimes, encountered especially when processes such as impact ionization and carrier injection into insulators are investigated, we cannot expect each individual collision to be completed before other processes occur and therefore interfere with them.[4] The limits of applicability of the Boltzmann theory are thus surpassed and transport must be considered from a fully quantum-mechanical viewpoint, since neglecting the uncertainty relations can now lead to erroneous results.[5] Two important quantum effects that appear as a consequence of the position-momentum uncertainty relation and of finite lifetime are collisional broadening (CB) and the intracollisional field effect (ICFE), and these should be taken into account in a proper treatment of quantum transport.[4,6]

Collisional broadening reflects the finite lifetime of the carriers interacting with impurities, phonons, etc., thus violating the assumption of the effective-mass model, according to which there is a unique relation between the carrier energy $\varepsilon_{\mathbf{k}}=\hbar\omega$ and its wave vector $\mathbf{k}$ ($\varepsilon_{\mathbf{k}}=\hbar^2\mathbf{k}^2/2m$). $\hbar\omega$ and $\mathbf{k}$ must now be taken as independent variables; the relation between them is described by a spectral density function $A(\mathbf{k},\omega)$.[7-9]

The intracollisional field effect deals with the fact that a carrier is accelerated by the field during a collision whose duration can no longer be treated as instantaneous.[4,10,11] This effect, which can be present even in the semiclassical regime,[12,13] becomes significant in submicrometer devices characterized by mean collision durations and mean free times that are not negligible compared to the transit times through the device. This is expected to produce a shift of the threshold energy for the emission or absorption of phonons.[14]

The formulation of a scheme capable of describing nonlinear transport phenomena is a long-standing and much-debated theoretical problem,[14,15] and most existing Green's-function formalisms have been limited by the use of gradient expansions in the external fields.[7,16] Several models have been proposed[6,17-29] to include collisional broadening and the intracollisional field effect within a Monte Carlo approach, but they are far from being satisfactory since they do not have any solid first-principles

justification that goes beyond the gradient expansion.

Other approaches[30] are based upon the Kadanoff-Baym-Keldysh (KBK) nonequilibrium Green's-function technique.[7,31–33] By including the field in the "unperturbed" (absence of scattering) Hamiltonian, this technique makes possible a nonperturbative calculation, at least in principle. However, current applications of the KBK methods have been limited to weak fields and/or slowly varying systems and have not been applied successfully to problems beyond the linear response.

The aim of this paper is to derive a spectral density model which can account for both the energy dependence of the collision rate and ICFE. In Sec. II, we give a very brief review of the general theory based on the KBK methods, whereas in Sec. III and the Appendix we present the details of our formalism and how it differs from a treatment based on center-of-mass coordinates. We will show how, by solving the appropriate Dyson's equation for the case of scattering mechanisms described by a momentum-independent self-energy, we can obtain an analytical expression for $A(\mathbf{k}_\perp,s,\omega)$, as well as for the quantum-mechanical distribution function $f(\mathbf{k}_\perp,\omega)$, capable of accounting for CB and the ICFE.

II. THE SPECTRAL FUNCTION AND THE NONEQUILIBRIUM GREEN'S FUNCTIONS

The spectral function $A(\mathbf{r},t;\mathbf{r}',t')$ can be defined in terms of the anticommutator[34] of the fermion-creation and -annihilation field operators $\hat{\Psi}^\dagger(\mathbf{r},t)$ and $\hat{\Psi}(\mathbf{r},t)$ as

$$A(\mathbf{r},t;\mathbf{r}',t')=\langle\{\hat{\Psi}(\mathbf{r},t),\hat{\Psi}^\dagger(\mathbf{r}',t')\}\rangle , \tag{1}$$

where the angular brackets $\langle\ldots\rangle$ indicate the nonequilibrium expectation value.[32,35] The spectral function defined above becomes

$$A(\mathbf{r};t;\mathbf{r}',t)=\delta(\mathbf{r}-\mathbf{r}') , \tag{2}$$

as a consequence of the equal-time commutation of the field operators. If A is a function only of the difference of its arguments, it can be Fourier transformed and Eq. (2) leads to the sum rule

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A(\mathbf{k},\omega)=1 . \tag{3}$$

It is also easily seen that the summation over all momentum states provides the density of states[7,9]

$$\rho(\omega)=\frac{1}{2\pi}\int\frac{d^3k}{(2\pi)^3}A(\mathbf{k},\omega) . \tag{4}$$

$A(\mathbf{k},\omega)$ also satisfies higher-order sum rules.[9,34] All of these properties make the spectral function an essential quantity to calculate, since it has a clear interpretation as a weighting function (with total weight unity), giving the conditional probability that a particle in state $\mathbf{k}$ will have energy $\hbar\omega$.

In the Boltzmann theory, where the electrons are in the free-particle states

$$\psi(\mathbf{r})=\frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}} , \tag{5}$$

the spectral function reduces to

$$A(\mathbf{k},\omega)=2\pi\delta(\hbar\omega-\varepsilon_{\mathbf{k}}) , \tag{6}$$

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

In the case of electrons interacting with phonons, on the other hand, uncertainties in the momentum-energy relationship must be taken into account. The nonequilibrium Green's-function method is particularly suitable for determining not only this renormalization of the electron eigenvalues due to the interactions, but also the effect of an applied external field on the interactions themselves. This formalism is based on the double-time correlation functions[33,36]

$$G^<(\mathbf{r},t;\mathbf{r}',t')=\frac{i}{\hbar}\langle\hat{\Psi}^\dagger(\mathbf{r}',t')\hat{\Psi}(\mathbf{r},t)\rangle , \tag{7a}$$

$$G^>(\mathbf{r},t;\mathbf{r}',t')=-\frac{i}{\hbar}\langle\hat{\Psi}(\mathbf{r},t)\hat{\Psi}^\dagger(\mathbf{r}',t')\rangle \tag{7b}$$

(the field operators are expressed in the interaction representation) which describe the propagation of an extra particle (or hole) added to the system. From these we can define the retarded and advanced Green's functions

$$G^r(\mathbf{r},t;\mathbf{r}',t')=-\frac{i}{\hbar}\vartheta(t-t')\langle\{\hat{\Psi}(\mathbf{r},t),\hat{\Psi}^\dagger(\mathbf{r}',t')\}\rangle , \tag{8a}$$

$$G^a(\mathbf{r},t;\mathbf{r}',t')=\frac{i}{\hbar}\vartheta(t'-t)\langle\{\hat{\Psi}(\mathbf{r},t),\hat{\Psi}^\dagger(\mathbf{r}',t')\}\rangle , \tag{8b}$$

respectively. Analogous relations hold for the various phonon Green's functions $D^\alpha(\mathbf{r},t;\mathbf{r}',t')$ with $\alpha=<,>,r,a$.

The definition (1) for the spectral function is then equivalent to that usually given in terms of the retarded and advanced Green's functions,[7]

$$A=i(G^>-G^<)=i(G^r-G^a)=-2\,\mathrm{Im}G^r . \tag{9}$$

This allows us to calculate A from the solution of Dyson's equation for G^r, which can be formally written as

$$G^r=G_0^r+G_0^r\Sigma^rG^r , \tag{10}$$

where integration over intermediate variables is implied throughout. Here G_0^r is the retarded free-particle propagator and the retarded self-energy Σ^r desribes the interactions of the electrons with the crystal, as well as with any applied external field. Σ^r, however, is a functional not only of G^r, but also of $G^<$, which makes (10) an equation coupled to Dyson's equation for $G^<$.[32,35,37]

III. THE AIRY-REPRESENTATION FORMALISM

A. The Airy representation

The solution of Dyson's equation is a difficult task, especially in the presence of high external fields that cannot be handled perturbatively. In order to describe high-

field effects, we must be able to overcome the difficulties associated with an electron system that is no longer translationally invariant along the direction of the applied electric field.[2] As a consequence, momentum along the field is no longer a good quantum number and Dyson's equation cannot be diagonalized in the space of the unperturbed, free-particle Hamiltonian.

Many authors,[27,37–40] have attempted to overcome these difficulties by representing the electric field E by a vector potential $\mathbf{A}(t)=-\int \mathbf{E}(t')\,dt'$. This breaks time-translation invariance, which is equally important in the proof of conservation laws. A kind of translational symmetry *does* persist in the presence of a constant field: a real-space translation along the field, combined with a shift in the *energy*, preserves the form of the problem.[39,40] However, describing the system in terms of shifted coordinates, like $z-\hbar\omega/eE$, also does not deconvolve the Dyson's equation. The introduction of the Wigner coordinates, used in many earlier attempts to go beyond small perturbative fields, does not make the problem simpler, but actually complicates it by artificially introducing the unphysical extra center-of-mass time T in a vector-potential gauge or the extra center-of-mass coordinate $\mathbf{R}$ if a scalar potential is used.

We have used a different approach. As stated earlier, when an external potential $\phi(\mathbf{r})$ is applied, the unperturbed (absence of scattering) Dyson equation cannot be diagonalized by Fourier transforming in space. It is possible, however, to diagonalize it in the space defined by the normalized eigenfunctions $\{\psi_i(\mathbf{r})\}$ of the field-dependent unperturbed Hamiltonian $H=H_0+\phi$.[7]

We restrict ourselves to electrons in a single band and represent the uniform, applied electric field E along the z direction of motion through a scalar potential $\phi(z)=eEz$, so that the system is described by the effective-mass Schrödinger equation

$$\left[-\frac{\hbar^2\nabla^2}{2m^*}+eEz\right]\psi(z)=\varepsilon\psi(z)\ . \tag{11}$$

This has solutions represented by the stationary states

$$\psi_{\mathbf{k}_\perp,s}(\mathbf{r})=\frac{1}{2\pi L}e^{i\mathbf{k}_\perp\cdot\boldsymbol{\rho}}\mathrm{Ai}[(z-s)/L]\ , \tag{12}$$

corresponding to the energies

$$\varepsilon_{\mathbf{k}_\perp,s}=\frac{\hbar^2\mathbf{k}_\perp^2}{2m^*}+eEs\ , \tag{13}$$

where ρ and $\mathbf{k}_\perp$ are, respectively, the position and wave vector of the electron in the plane normal to the field, $L=(\hbar^2/2m^*eE)^{1/3}$, and $\mathrm{Ai}(x)$ is the Airy function of the first kind.[41] Airy variable s, defined as $s=\varepsilon_z/eE$, with ε_z the electron kinetic energy in the direction of the field, has a physical interpretation as the electrons turning point in z. This solution is exact,[42] but does not include the possibility of Zener tunneling from one band to another, an effect that can be significant at very high electric fields, but which we ignore in the present treatment. The case of more general fields is discussed in the conclusions.

We work in the Hilbert space defined by the normalized eigenfunctions (12), i.e., plane waves in the plane perpendicular to the field and Airy functions along the direction of the field. This enables us to define a coordinate system $(\mathbf{k}_\perp,s)$ for Fourier transforming to momentum in the transverse directions and "Airy transforming" (see the Appendix) to s coordinates along the field. The transformation that connects the two coordinate systems $(\boldsymbol{\rho},z)$ and $(\mathbf{k}_\perp,s)$ is defined by the integral operation

$$g(\mathbf{k}_\perp,s)\equiv\int\frac{d\boldsymbol{\rho}}{2\pi}\int\frac{dz}{L}e^{i\mathbf{k}_\perp\cdot\boldsymbol{\rho}}\mathrm{Ai}[(z-s)/L]f(\boldsymbol{\rho},z)\ , \tag{14}$$

where $f(\boldsymbol{\rho},z)$ is an arbitrary function. As demonstrated in the Appendix, in this space, a function diagonal in both $\mathbf{k}_\perp$ and s variables is translationally invariant in the transverse direction, but not along the z direction. This is a very appealing property since it implies the possibility of dealing with diagonal functions without requiring an assumption of translational invariance along the direction of the applied field.

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

$$\hat{\Psi}(\mathbf{r},t)=\int d^2\mathbf{k}_\perp\int ds\,\Psi_{\mathbf{k}_\perp,s}(\mathbf{r})\hat{a}_{\mathbf{k}_\perp,s}(t)\ , \tag{15a}$$

with an inverse transformation

$$\hat{a}_{\mathbf{k}_\perp,s}(t)=\int d\mathbf{r}\,\psi^*_{\mathbf{k}_\perp,s}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\ , \tag{15b}$$

with

$$\begin{aligned}&[\hat{a}_{\mathbf{k}_\perp,s}(t),\hat{a}^\dagger_{\mathbf{k}'_\perp,s'}(t)]_\pm=\delta(\mathbf{k}_\perp-\mathbf{k}'_\perp)\delta(s-s')\ ,\\&[\hat{a}_{\mathbf{k}_\perp,s}(t),\hat{a}_{\mathbf{k}'_\perp,s'}(t)]_\pm=0\ .\end{aligned} \tag{16}$$

as a consequence of the fact that the basis is normalized. Here the negative sign on the subscript indicates commutation for bosons and the plus sign indicates anticommutation for fermions. The time dependence of the operators is given by

$$\hat{a}_{\mathbf{k}_\perp,s}(t)=\hat{a}_{\mathbf{k}_\perp,s}e^{-i/\hbar\varepsilon_{\mathbf{k}_\perp,s}t}\ . \tag{17}$$

B. Nonequilibrium field-dependent Green's functions

As emphasized in the previous sections, we want to treat the electric field exactly. In order to do this, we follow the suggestion of Ref. 38 and take the free-particle propagator G_0^r in (10) to be the Green's function for an electron in the presence of the electric field, but without scattering, and denote it by G_E^r. One of the advantages of our formalism is that now, using (15)–(17) in (8a), the unperturbed, field-dependent, single-particle propagator at zero temperature,

$$G_E^r(\mathbf{r},t;\mathbf{r}',t')=\frac{i}{\hbar}\int d^2\mathbf{k}_\perp ds\int d^2\mathbf{k}'_\perp\int ds'\,\psi_{\mathbf{k}_\perp,s}(\mathbf{r})\psi^*_{\mathbf{k}'_\perp,s'}(\mathbf{r}')\vartheta(t-t')\langle\Phi_0|\{\hat{a}_{\mathbf{k}_\perp,s}(t),\hat{a}^\dagger_{\mathbf{k}'_\perp,s'}(t')\}|\Phi_0\rangle\ , \tag{18}$$

in $(\mathbf{k}_\perp,s)$ space has the simple expression

$$G_E^r(\mathbf{k}_\perp,s;t-t')=-\frac{i}{\hbar}\vartheta(t-t')e^{-i/\hbar\varepsilon_{\mathbf{k}_\perp,s}(t-t')}, \tag{19}$$

or, in the frequency domain,

$$G_E^r(\mathbf{k}_\perp,s,\omega)=\frac{1}{\hbar\omega-\varepsilon_{\mathbf{k}_\perp,s}+i\eta}. \tag{20}$$

In (18) $|\Phi_0\rangle$ indicates the vacuum state and η in (20) is an infinitesimal positive convergence factor.

Transforming Dyson's equation into the Airy representation leaves only one integration over intermediate variables, namely

$$G^r(\mathbf{k}_\perp,s,s';\omega)=G_E^r(\mathbf{k}_\perp,s;\omega)\delta(s-s')+G_E^r(\mathbf{k}_\perp,s;\omega)\int ds_2\,\Sigma^r(\mathbf{k}_\perp,s,s_2;\omega)\times G^r(\mathbf{k}_\perp,s_2,s';\omega) \tag{21}$$

(here the development of the appropriate integration paths follows the description of Ref. 33). This is a vast improvement over the many integrations (they add in pairs) that one gets by using ordinary coordinates or momenta.

C. Self-energies

In order to solve the Dyson equation (21), we need a model for the retarded self-energy Σ^r in $(\mathbf{k}_\perp,s)$ coordinates. If the system is weakly coupled, we can write the electron-phonon interaction in the Born approximation,[7]

$$\Sigma(\mathbf{r},t;\mathbf{r}',t')=iD(\mathbf{r},t;\mathbf{r}',t')G(\mathbf{r},t;\mathbf{r}',t'), \tag{22}$$

which includes the vertex matrix elements and corresponds to the diagrams shown in Fig. 1.[9] The retarded self-energy is then given by[32,35]

$$\Sigma^r=i(D^>G^r+D^rG^<). \tag{23}$$

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 $G^<$ is a negligible[33,37] correction to that containing G^r, and

$$\Sigma^r=iD^>G^r. \tag{24}$$

This approximation decouples Dyson's equation for G^r from that for $G^<$, thus solving the difficulty mentioned in Sec. II.

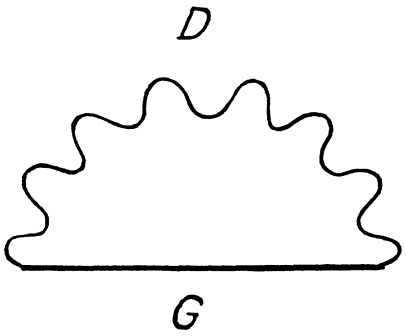

FIG. 1. Born approximation to the self-energy from electron-phonon scattering.

The phonon Green's function is given by

$$D_0(\mathbf{r},t;\mathbf{r}',t')=-\frac{i}{\hbar}\langle T[\hat{\varphi}(\mathbf{r},t),\hat{\varphi}^\dagger(\mathbf{r}',t')]\rangle, \tag{25}$$

where $\hat{\varphi}$ and $\hat{\varphi}^\dagger$ are the phonon field operators.

In the limit of low particle concentration, the electrons are not expected to affect the phonon states,[9] so we can assume that the phonons remain in equilibrium, and are not affected by the electric field. We therefore use the familiar expression[36]

$$D_0^>(\mathbf{q})=-i\sum_{\eta=\pm1}|V_{\eta\mathbf{q}}|^2[N_\mathbf{q}+(\eta+1)/2]\delta(\omega-\eta\omega_{\eta\mathbf{q}}) \tag{26}$$

for the phonon correlation function. Here $\mathbf{q}$ and $N_\mathbf{q}$ are the phonon wave vector and occupation number, respectively, and $|V_{\eta\mathbf{q}}|$ is the electron-phonon interaction matrix element.[43] The term with $\eta=+1$ corresponds to emission, and $\eta=-1$ to absorption, of a phonon of frequency $\omega_\mathbf{q}$ by the electron of energy $\hbar\omega$.

Within this model, the retarded self-energy in reciprocal space reads

$$\Sigma^r(\mathbf{k},\mathbf{k}';\omega)=\frac{2\pi}{\hbar}\int d\mathbf{q}\sum_\eta|V_{\eta\mathbf{q}}|^2[N_\mathbf{q}+(\eta+1)/2]\times G^r(\mathbf{k}-\mathbf{q},\mathbf{k}'-\mathbf{q};\omega-\eta\omega_\mathbf{q}). \tag{27}$$

Fourier transforming in time and transverse coordinates, and Airy transforming along the z direction, we obtain the following expression:

$$G^r(\mathbf{k}_\perp,s,s';\omega)=\frac{2\pi}{\hbar}\sum_\eta\int d\mathbf{q}\,|V_{\eta\mathbf{q}}|^2[N_0+(\eta+1)/2]\times\int ds''\int ds'''\,G^r(\mathbf{k}_\perp-\mathbf{q}_\perp,s'',s''';\omega-\eta\omega_\mathbf{q})\times\int dz\,e^{iq_zz}\mathcal{A}(z-s)\mathcal{A}(z-s'')\int dz'\,e^{-iq_zz'}\mathcal{A}(z'-s')\mathcal{A}(z'-s''') \tag{28}$$

for the electron-phonon interaction in $(\mathbf{k}_\perp,s;\omega)$ space. For nonpolar optical phonons, $\Sigma^r(s,s')$ is highly peaked about $s=s'$, so that we can make the approximation

$$\Sigma^r(s,s')=\Sigma^r(s)\delta(s-s'),\quad G^r(s,s')=G^r(s)\delta(s-s'). \tag{29}$$

By integrating (28) over the s' values, we finally obtain

$$\Sigma^r(\mathbf{k}_\perp,s;\omega)=\frac{2\pi}{\hbar}|V|^2\left[-\frac{(2\pi)^2}{3^{1/6}}\right]\sum_\eta[N_0+(\eta+1)/2]\int d^2\mathbf{q}_\perp\int ds''\mathcal{A}^2((s-s'')/3^{1/3}l)G^r(\mathbf{k}_\perp-\mathbf{q}_\perp,s'';\omega-\eta\omega_0)\ . \tag{30}$$

Equation (30), together with Dyson's equation (21), is now a self-consistent problem, since knowledge of the full Green's function G^r, obtainable by solving (21), is needed for the calculation of Σ^r present in (21) itself. As a first estimate, we consider only the lowest-order, one-phonon scattering by taking $G^r\sim G_E^r$ in (30), which can now be evaluated explicitly and reads

$$\Sigma^r(s,\omega)=\frac{2\pi}{\hbar}|V|^2\sum_{\eta=\pm1}[N_0+(\eta+1)/2]F(s,\omega)\ ,$$

$$\mathrm{Re}[F(s,\omega)]=\frac{2\pi}{\sqrt{2}}\frac{m^{*3/2}}{\hbar^2}\Theta^{1/2}\left[\mathrm{Ai}'(\zeta)\mathrm{Bi}'(\zeta)-\zeta\,\mathrm{Ai}(\zeta)\mathrm{Bi}(\zeta)+\frac{\sqrt{\zeta}}{\pi}\vartheta(\zeta)\right]\ , \tag{31}$$

$$\mathrm{Im}[F(s,\omega)]=\frac{2\pi}{\sqrt{2}}\frac{m^{*3/2}}{\hbar^2}\Theta^{1/2}[\mathrm{Ai}'^2(\zeta)-\zeta\,\mathrm{Ai}^2(\zeta)]\ ,$$

where $\Theta=[3(\hbar eE)^2/2m^*]^{1/3}$, $\zeta=[eEs-\hbar(\omega-\eta\omega_0)]/\Theta$.

The self-energy above has the correct limit for vanishing field. In fact, for $\eta=1$, its imaginary part, which the optical theorem relates to the scattering rate Γ by

$$\Gamma(\omega)=\frac{1}{\tau(\omega)}=-\frac{2}{\hbar}\mathrm{Im}\Sigma^r(\omega)\ , \tag{32}$$

reduces to that obtained by considering one-phonon emission processes in the Born approximation, when $\zeta\to\infty$ (or equivalently, $E\to0$):

$$\lim_{\zeta\to\infty}\left[\frac{1}{\hbar}\mathrm{Im}\Sigma^r(s,\omega)\right]=\frac{\pi}{\hbar}g^2(\hbar\omega-\varepsilon_z-\hbar\omega_0)^{1/2}$$

$$=\frac{\Gamma(\varepsilon_z,\omega)}{2}\ , \tag{33}$$

where $g^2=(2m^*)^{3/2}|V|^2/\hbar^2$. Even in the absence of an electric field, therefore, we have a finite linewidth which accounts for collisional broadening.

On the other hand, the real part of the self-energy, which represents the deviation, due to the interactions, of the electron energy from the free-electron energy ε_k vanishes when $E=0$. This indicates that our lowest-order approximation fails to describe fully the energy renormalization caused by collisional broadening alone, but that it represents a quite reasonable model for the ICFE. Figure 2 shows the real part of the self-energy as a function of the argument ζ for three 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 nonperturbative inclusion of the electric field in the problem. These oscillations indicate the existence of regions in which the electron energy is alternately lowered and raised, suggesting the presence of quantization in space, with every other zero crossing in the figure representing a quantized level towards which the quasiparticle energy concentrates. The zero crossings occur asymptotically where $\zeta=[3\pi(2n+1)/8]^{2/3}$. Because of the irrational factor in $\Theta=3^{1/3}eEL$, the oscillations are incommensurate with those occurring in the

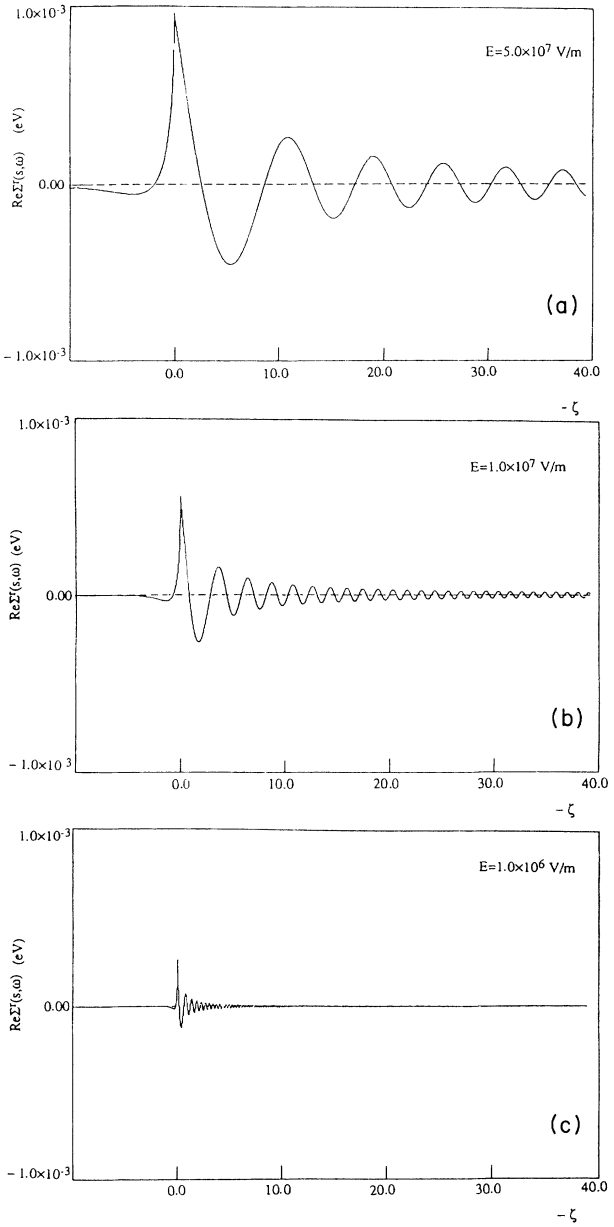

FIG. 2. The real part of the self-energy as a function of the reduced coordinated ζ [defined following Eq. (32)] for three different values of the applied electric field.

phonon-decoupled problem.

In Fig. 3, we plot the imaginary part of the self-energy. The presence of the ICFE is found to generate a tail in the scattering rate for $\zeta<0$ and a series of damped steps at $\zeta>0$ associated with the oscillations in the real part of the self-energy and reflecting the influence of the quantized levels through the Airy functions. The existence of such a tail smooths out the sharp threshold in energy of the scattering rate, making possible transitions which cannot occur in the absence of the field. The appearance of steplike oscillations, on the other hand, signals the onset of additional densities of final states corresponding to the subbands generated by the quantized levels described above.

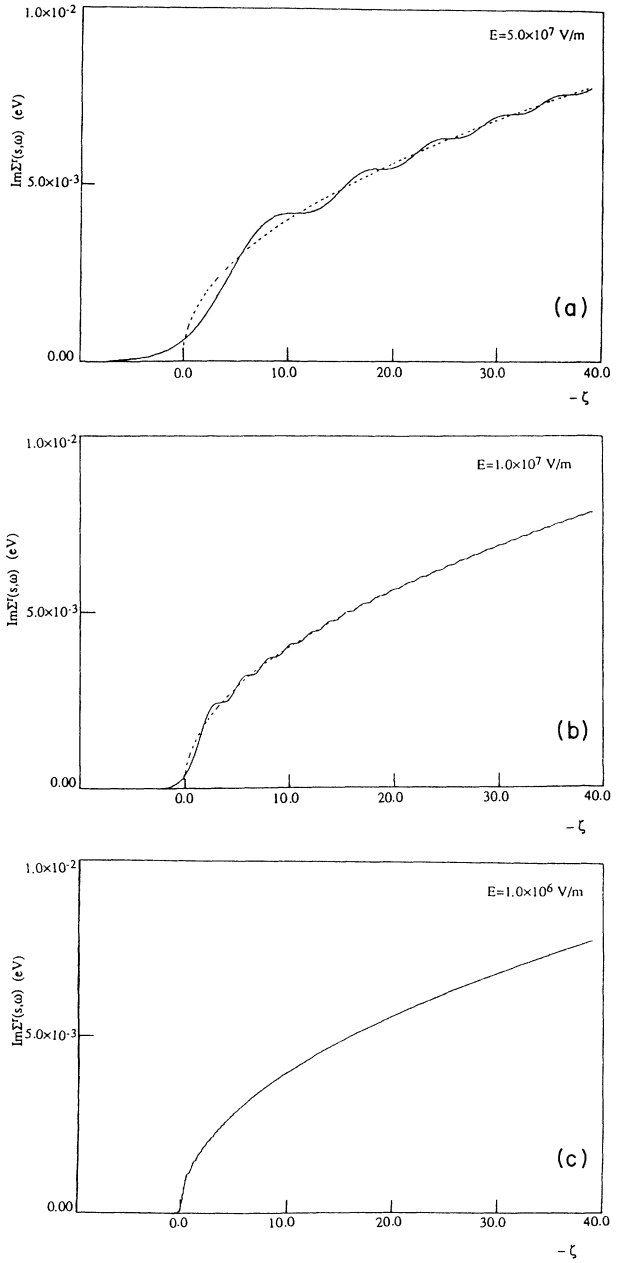

FIG. 3. The imaginary part of the self-energy, which is proportional to the scattering rate, for three different values of the applied electric field. The continuous curve refers to the case when the ICFE is accounted for and the dashed curve to the case when the ICFE is neglected.

D. The spectral density function

With this model for the self-energy, Dyson's equation (21) is a multiplicative equation and can be solved immediately for the retarded Green's function

$$G^r(\mathbf{k}_\perp,s,s';\omega)=\frac{\delta(s-s')}{\hbar\omega-\varepsilon_{\mathbf{k}_\perp,s}-\Sigma^r(s,\omega)}\ , \tag{34}$$

whose imaginary part is proportional to the spectral density function $A(\mathbf{k}_\perp,s,\omega)$. According to the definition (9), we have

$$A(\mathbf{k}_\perp,s;\omega)=\frac{-2\,\mathrm{Im}\Sigma^r(s,\omega)}{[\hbar\omega-\varepsilon_{\mathbf{k}_\perp,s}-\mathrm{Re}\Sigma^r(s,\omega)]^2+[\mathrm{Im}\Sigma^r(s,\omega)]^2}\ . \tag{35}$$

This is plotted in Fig. 4 for different values of the electric field. It is positive definite and integrates properly, satisfying the normalization condition (3). $A(\mathbf{k}_\perp,s;\omega)$ exhibits an unusual double-peak structure near the zero point (where, in the semiclassical limit, there is a δ function representing the semiclassical turning point). The depth of the valley between the peaks increases as the electric field decreases. On the other hand, the height of the right peak relative to the left one decreases, as does their relative separation, until they merge to form the Lorenztian shape typical of the collisional broadening effect in the absence of a field. This can be seen analytically by taking the limit of (35) for vanishing fields, which is

$$\begin{aligned}\lim_{\zeta\to\infty}A(\mathbf{k}_\perp,s;\omega)&=\frac{\hbar\Gamma(\varepsilon_z,\omega)}{(\hbar\omega-\varepsilon_{\mathbf{k}_\perp}-\varepsilon_z)^2+\left[\frac{\hbar\Gamma(\varepsilon_z,\omega)}{2}\right]^2}\\&=A^{\mathrm{CB}}(\mathbf{k}_\perp,\varepsilon_z,\omega)\ .\end{aligned} \tag{36}$$

A^{CB} is shown in Fig. 5 for different ratios of the transverse energy to the optical-phonon energy. A similar behavior is shown in Fig. 6 for $A(\mathbf{k}_\perp,s,\omega)$ of (35). Furthermore, $A(\mathbf{k}_\perp,s,\omega)$ reduces to the free-particle δ function of (6) in the absence of the electric field and scattering:

$$\begin{aligned}A^{\mathrm{free}}(\mathbf{k},\omega)&=\lim_{\Gamma\to0}\lim_{\zeta\to\infty}A(\mathbf{k}_\perp,s;\omega)\\&=\lim_{\Gamma\to0}A^{\mathrm{CB}}(\mathbf{k}_\perp,\varepsilon_z;\omega)\\&=2\pi\delta(\hbar\omega-\varepsilon_{\mathbf{k}_\perp}-\varepsilon_z)\ .\end{aligned} \tag{37}$$

E. The quantum-mechanical distribution function

The next step is to calculate the correlation function (7a). The density of particles is, in fact, given by

$$\begin{aligned}\langle n(\mathbf{r},t)\rangle&=\langle\hat{\Psi}^\dagger(\mathbf{r},t),\Psi(\mathbf{r},t)\rangle\\&=-i\hbar G^<(\mathbf{r},t;\mathbf{r},t)\\&=-i\hbar\int\frac{d\omega}{2\pi}\int\frac{d\mathbf{k}}{(2\pi)^3}G^<(\mathbf{k},\omega)\ ,\end{aligned} \tag{38}$$

so that $G^<(\mathbf{k},\omega)$ can really be identified as the average density of particles in the system with momentum $\hbar\mathbf{k}$ and energy $\hbar\omega$.[7] $G^<(\mathbf{k},\omega)$, therefore, must be closely related to the distribution function $f(\mathbf{k},\omega)$ which describes the physical system. As a matter of fact, the quantum-mechanical Wigner distribution function $f_W(\mathbf{k})$ is defined in terms of $G^<$ as[34]

$$f_W(\mathbf{k})=-i\hbar\int\frac{d\omega}{2\pi}G^<(\mathbf{k},\omega)\ , \tag{39}$$

and the knowledge of $G^<$ would then represent the solution of the transport problem. In equilibrium, $G^>$ and $G^<$ obey

$$G^<(\mathbf{k},\omega)=iA(\mathbf{k},\omega)f_{\rm FD}(\omega)\ , \tag{40}$$

$$G^>(\mathbf{k},\omega)=-iA(\mathbf{k},\omega)[1-f_{\rm FD}(\omega)]\ , \tag{41}$$

where $f_{\rm FD}(\omega)$ is the Fermi-Dirac distribution function. No similar relation holds in nonequilibrium situations, and an equation of motion is needed for $G^<$ (Ref. 44) (and/or for $G^>$). In the Kadanoff-Baym formulation, with the prescriptions given by Langreth[32,35] for the time-contour integration, this is represented by the two integro-differential equations

$$\left[i\hbar\frac{\partial}{\partial t}-H\right]G^<(\mathbf{r},t;\mathbf{r}',t')=\int_{-\infty}^{\infty}dt_1\int d\mathbf{r}_1[\Sigma^r(\mathbf{r},t;\mathbf{r}_1,t_1)G^<(\mathbf{r}_1,t_1;\mathbf{r},t)+\Sigma^<(\mathbf{r},t;\mathbf{r}_1,t_1)G^a(\mathbf{r}_1,t_1;\mathbf{r},t)]\ , \tag{42a}$$

and

$$\left[-i\hbar\frac{\partial}{\partial t'}-H'\right]G^<(\mathbf{r},t;\mathbf{r}',t)=\int_{-\infty}^{\infty}dt_1d\mathbf{r}_1[G^r(\mathbf{r},t;\mathbf{r}_1,t_1)\Sigma^<(\mathbf{r}_1,t_1;\mathbf{r}',t')+G^<(\mathbf{r},t;\mathbf{r}_1,t_1)\Sigma^a(\mathbf{r}_1,t_1;\mathbf{r}',t')]\ , \tag{42b}$$

where H and H' act on the unprimed and primed variables, respectively. By Fourier transforming the transverse variable $\boldsymbol{\rho}=(\mathbf{r}-\mathbf{r}')_\perp$ and Airy transforming the longitudinal variables z and z' on both sides of (42a) and (42b), these can be

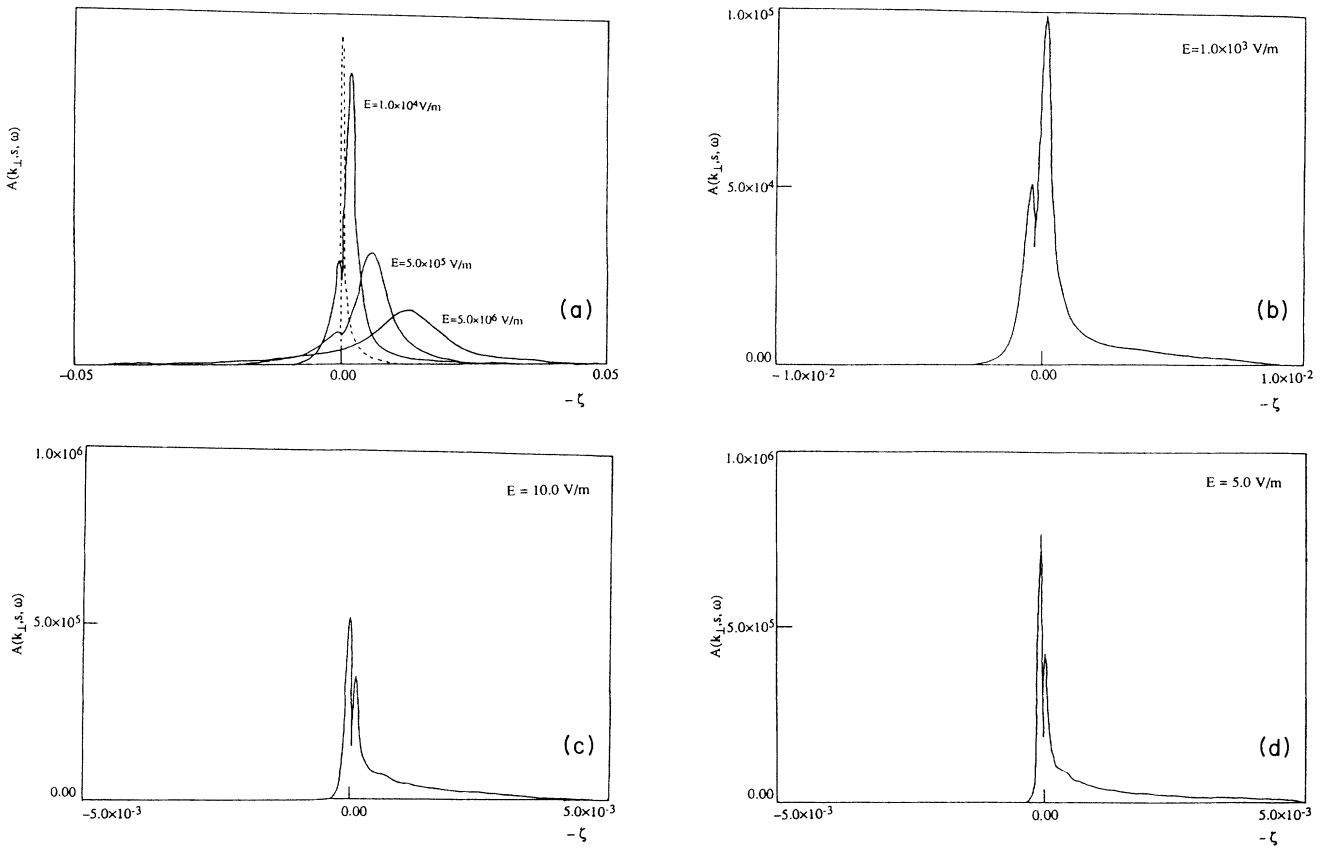

FIG. 4. (a) The spectral density function (continuous curve) in Airy coordinates as in Eq. (35) for three different values of the electric field. The dashed curve refers to calculations with collisional broadening only [see Eq. (36)]. The spectral function for (b) 1000 V/m, (c) 10 V/m, and (d) 5 V/m. Notice the change in the ζ scale. Here the electron transverse energy $\varepsilon_{\mathbf{k}_\perp}$ is taken to be equal to the phonon energy $\hbar\omega_0$.

written in $(\mathbf{k}_\perp,s)$ space as

$$\left[i\hbar\frac{\partial}{\partial\tau}-\varepsilon_{\mathbf{k}_\perp,s}\right]G^<(\mathbf{k}_\perp,s,s';\tau)=\int_{-\infty}^{\infty}d\tau_1[\Sigma^r(s;\tau-\tau_1)G^<(\mathbf{k}_\perp,s,s';\tau_1)+\Sigma^<(\mathbf{k}_\perp,s,s';\tau-\tau_1)G^a(\mathbf{k}_\perp,s;\tau_1)]\ , \tag{43a}$$

and

$$\left[i\hbar\frac{\partial}{\partial\tau}-\varepsilon_{\mathbf{k}_\perp,s'}\right]G^<(\mathbf{k}_\perp,s,s';\tau)=\int_{-\infty}^{\infty}d\tau_1[G^r(\mathbf{k}_\perp,s;\tau-\tau_1)\Sigma^<(\mathbf{k}_\perp,s,s';\tau_1)+G^<(\mathbf{k}_\perp,s,s';\tau-\tau_1)\Sigma^a(s;\tau_1)]\ , \tag{43b}$$

where the approximation (29) has been used and the change of variables $\tau=t-t'$ and $\tau_1=t_1-t'$ has been performed. The right-hand sides of both (43a) and (43b) are sums of convolution products so that the Fourier transform in the time domain can be trivially done. Furthermore, by summing them, we obtain

$$(2\hbar\omega-2\varepsilon_{\mathbf{k}_\perp}-2Es)G^<(\mathbf{k}_\perp,s;\omega)=2\,\mathrm{Re}[\Sigma^r(s;\omega)]G^<(\mathbf{k}_\perp,s;\omega)+2\,\mathrm{Re}[G^r(\mathbf{k}_\perp,s;\omega)]\Sigma^<(\mathbf{k}_\perp,s;\omega)\ , \tag{44}$$

where $\Sigma^r+\Sigma^a=2\,\mathrm{Re}\Sigma^r$ and $G^r+G^a=2\,\mathrm{Re}G^r$ have been used.

Equation (44) can be solved for $G^<$ and we obtain

$$G^<(\mathbf{k}_\perp,s,\omega)=A(\mathbf{k}_\perp,s,\omega)\left[-\frac{\Sigma^<(s,\omega)}{2\,\mathrm{Im}\Sigma^r(s,\omega)}\right]\ , \tag{45}$$

with A and $\mathrm{Im}\Sigma^r$ as given in (35) and (31), respectively. $\Sigma^<$ can be expressed in $(\mathbf{k}_\perp,s)$ space as

$$\Sigma^<(s,\omega)=\frac{2\pi}{\hbar}|V|^2\left[\frac{(2\pi)^2}{3^{1/6}}\right]\sum_\eta[N_0+(\eta+1)/2]\int d^2\mathbf{q}_\perp\int ds''\mathcal{A}^2((s-s'')/3^{1/3}L)G^<(\mathbf{k}_\perp-\mathbf{q}_\perp,s'';\omega+\eta\omega_0)\ , \tag{46}$$

with a procedure analogous to that used to obtain (30). In Eq. (45), the quantity in large parentheses can be identified as the quantum-mechanical distribution

$$f(s,\omega)=i\frac{\Sigma^<(s,\omega)}{\Gamma(s,\omega)}\ , \tag{47}$$

where $\Gamma(s,\omega)=-2\,\mathrm{Im}\Sigma^r(s,\omega)/\hbar$, and we can rewrite (45) as

$$G^<(\mathbf{k}_\perp,s,\omega)=iA(\mathbf{k}_\perp,s;\omega)f(s,\omega)\ . \tag{48}$$

This relation tells us that, within the limitation of the approximations involved in our approach, a separation analogous to (40) also holds in the nonequilibrium case without the loss of CB or the ICFE. Thus, the Airy coordinates allow us to *derive* the ansatz that has been introduced in earlier approaches.[34,37,38,44]

Substituting (45) into (46) and performing the $\mathbf{q}_\perp$ integration, the quantum-mechanical distribution function $f(s,\omega)$ reads

$$f(s,\omega)=\sum_\eta[(N_0+(\eta+1)/2]\times\int_{-\infty}^{\infty}ds''\,\mathcal{F}(s,s'';\omega+\eta\omega_0)\times f(s'';\omega+\eta\omega_0) \tag{49}$$

with

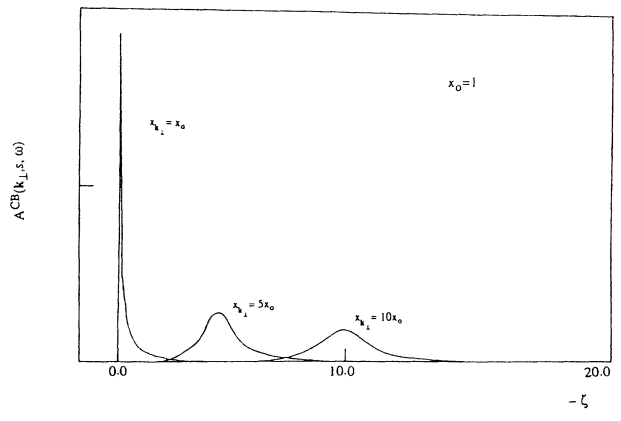

FIG. 5. The collisional broadening spectral density as a function of the scaled many-body energy ζ for three different values of the electron transverse kinetic energy $\varepsilon_{\mathbf{k}_\perp}$ (here the energies are expressed in dimensionless units $x_{\mathbf{k}_\perp}=\varepsilon_{\mathbf{k}_\perp}/\hbar\omega_0$ and $x_0=1$).

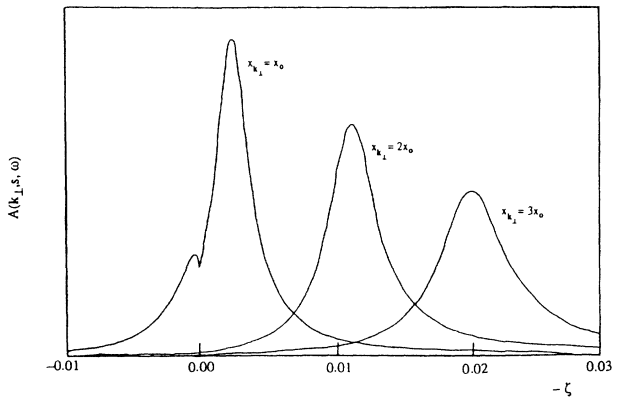

FIG. 6. The total (CB+ICFE) spectral density of Eq. (35) for three different values of the electron transverse energy (here, as in Fig. 5, the energies are in dimensionless units) at $E=10^4$ V/m.

$$\mathcal{F}(s,s'';\omega)\equiv\left[\frac{2\pi}{h}\right]^2|V|^2\frac{2\sqrt{3}\pi^2 m\mathcal{A}^2((s-s'')/3^{1/3}L)}{\mathrm{Im}\Sigma^r(s,\omega-\eta\omega_0)}\left[\frac{\pi}{2}+\tan^{-1}\left[\frac{\hbar\omega-eEs''-\mathrm{Re}\Sigma^r(s'';\omega)}{\mathrm{Im}\Sigma^r(s'';\omega)}\right]\right]. \quad (50)$$

Equation (49) is a homogeneous integral equation which can be solved by numerical integration. This solution procedure will be described elsewhere.

IV. CONCLUSIONS

We have introduced a treatment in which the momentum coordinate representation along the field direction is replaced by a new representation in terms of Airy coordinates. This yields the mathematical advantage of simplified Dyson's equations involving fewer coordinates. We have applied this to the case of nonpolar optical-phonon scattering in semiconductors in high electric fields.

The result is the appearance of a series of damped oscillations in both the real and imaginary parts of the electron self-energy, indicatinng the existence of preferred quantized energy levels for the electron. A state-counting argument would, then, imply the need for another quantum number. An approximately analogous situation occurs in crystals where the continuous reciprocal-space coordinate is replaced by a quasimomentum restricted to the first Brillouin zone and its augmented by a band index. The levels represented by zero crossings of the real part of the self-energy could serve as a kind of quasi-two-dimensional subbanding in which each crossing plays a role analogous to the subband index.

In addition, the double-peak structure of the spectral density function suggests that there is a length scale associated with the motion along the field direction. We conjecture that this motion might therefore be more appropriately treated in terms of "hopping" transport in the z direction between states described by discrete values of the Airy coordinate: the net effect of the field is to produce a discontinuity in the electron trajectory, which can be evaluated quantitatively using the new metric defined by the Airy transform. This discontinuity, which can be interpreted as a field-assisted scattering (hopping) from z to z', is ultimately responsible for the broadening of the carrier position after each scattering event along the field direction.

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. A diagonal approximation in the associated coordinate system may lead to similarly useful results.

We have also shown how, in our formalism, an expression generalizing the equilibrium $G^<=iAf$ relation (40) holds even at higher fields. This is generally expected (although debated in the literature[38,44]) since it is consistent with the definition (39): the frequency integral of A always equals unity by virtue of the equal-time (anti)commutation rules [see Eq. (3)].

The positive definiteness and normalization of $A(\mathbf{k}_\perp,s,\omega)$ also indicate the possibility of constructing a novel Monte Carlo simulation[45] able to provide a quantitative evaluation of this effect. This will be described in a later paper.

ACKNOWLEDGMENTS

The authors would like to thank L. Reggiani, A. P. Jauho, and P. Lipavsky for helpful discussions and comments. This work was supported by the U.S. Office of Naval Research.

APPENDIX

We define the Airy transform $A_\xi[a(t)]$ of a general function $a(t)$ by

$$A(\xi)\equiv A_\xi[a(t)]\equiv\int_{-\infty}^{\infty}dt\,\mathcal{A}(\xi-t)a(t)\,, \quad (A1)$$

where $\mathcal{A}$ is the normalized Airy function

$$\mathcal{A}(\xi-t)=\frac{1}{L}\mathrm{Ai}[(z-s)/L]\,.$$

The problem is to find the inverse transform of the Airy transform. Using the integral representation[41]

$$\mathrm{Ai}(\xi)=\int_{-\infty}^{\infty}\frac{dt}{2\pi}\exp(\tfrac{1}{3}it^3+i\xi t)\,, \quad (A2)$$

we find that

$$\int_{-\infty}^{\infty}dt\,\mathcal{A}(t-\xi)\mathcal{A}(t-\zeta)=\delta(\xi-\zeta)\,. \quad (A3)$$

We can therefore define the inverse of the Airy transform as

$$a(t)\equiv A_t^{-1}[A(\xi)]=\int_{-\infty}^{\infty}d\xi\,\mathcal{A}(\xi-t)A(\xi)\,. \quad (A4)$$

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

$$F_k[A(\xi)]=\mathcal{A}(k)a(k)\,. \quad (A5)$$

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,

$$f(\mathbf{k},\mathbf{k}')=\int\frac{dz}{\sqrt{2\pi}}\int\frac{dz'}{\sqrt{2\pi}}e^{-ikz}e^{ikz'}f(z,z')=\int\frac{dz\,dz'}{2\pi}e^{ik(z-z')-i(k-k')z'}f(z,z')$$
$$=\int d(z-z')e^{-ik(z-z')}\int\frac{dz'}{2\pi}e^{-i(k-k')z'}$$
$$=\int d(z-z')e^{-ik(z-z')}f(z-z')\delta(k-k')=f(k)\delta(k-k')\ . \tag{A6}$$

However, a similar relation does not hold between translational invariance in real space and diagonality in the Airy coordinate space.

If a function is translationally invariant in z, then it is also translationally invariant in s:

$$f(s,s')=\int dz\int dz'\mathcal{A}(z-s)\mathcal{A}(z'-s')f(z,z')$$
$$=\int dz\int dz'\mathcal{A}(z-s+s')\mathcal{A}(z')f(z+s',z'+s')$$
$$=\int dz\int dz'\mathcal{A}(z-(s-s'))\mathcal{A}(z')f(z+s',z'+s')$$
$$=\int dz\int dz'\mathcal{A}(z-(s-s'))\mathcal{A}(z')f(z,z')$$
$$=f(s-s',0)\equiv f(s-s')\ , \tag{A7}$$

where the fourth line follows by translational invariance in z.

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