Airy-coordinate Green's-function technique for high-field transport in semiconductors

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(Received 17 February 1989)

We introduce an Airy-coordinate formulation of the Kadanoff-Baym-Keldysh Green's-function techniques to treat electron-phonon coupling in a high electric field. The resulting Dyson's equation is simpler than those found in purely momentum-coordinate formulations, and suggests a natural approximation. We observe oscillations due to phonon coupling which are incommensurate with those due to standing waves in the unperturbed problem.

Recent efforts to understand the physics of semiconductor devices at ultrasubmicrometer dimensions have brought into focus the limits and weaknesses of traditional semiclassical transport phenomena based upon the Boltzmann transport equation.[1] This theory assumes that the electrons exist in nearly stationary, free-particle-like states of momentum $\mathbf{k}$. Scattering is treated as weak and infrequent, so that an approach based upon perturbation theory can be utilized, while the applied electric field is assumed to be weak, and slowly varying on both space and time scales. In submicron devices, however, ordinary applied voltages lead to very high electric fields, and at these field strengths the scattering rates can be above 10^{14} $\sec^{-1}$.[2] In fact, when the spatiotemporal scales of the physical system under study begin to approach those of the microscopic interactions, we cannot expect any single collision to be completed before other processes occur and therefore interfere with it.[3] A transport theory is therefore needed which can overcome the semiclassical limits. Two important quantum effects that should be described by such a theory are collisional broadening (CB) and the intracollisional field effect (ICFE).[3] Collisional broadening has been treated alone for high fields and incorporated within a Monte Carlo process,[4,5] while only a formalism has been proposed for the ICFE.[6]

The development of a tractable quantum transport theory incorporating both CB and the ICFE, and capable of dealing with the length and time scales relevant to modern submicron devices, has proven to be a difficult task. Several approaches are based upon the Kadanoff-Baym-Keldysh (KBK) nonequilibrium Green's-function technique.[7] This technique is rigorous in principle, although current approximations have been limited to weak fields and/or slowly varying systems.[8] Such approximations have been used, for instance, to obtain the kinetic equation for the Wigner distribution function (required for comparison with the previously derived formalism for the ICFE).[9] In this paper as well, we utilize the KBK Green's functions, but describe an approach appropriate for high, homogeneous fields. We will concentrate mainly on the properties of the spectral density function $A(\mathbf{k},\omega)$ which gives a "probability" distribution for finding an electron with energy $\hbar\omega$ in a momentum state $\mathbf{k}$.

A constant electric field breaks the translation symmetry of the system along the field direction, so momentum along the field is no longer a good quantum number.[10] Many authors, in the attempt to overcome this difficulty, have represented the electric field $\mathbf{E}$ by a vector potential $\mathbf{A}(t)=-\int dt'\mathbf{E}(t')$. This breaks the time translation invariance, which is equally important in the proof of conservation laws. Low-field treatments can ignore this, since the field may be treated as a perturbation of a homogeneous system. Treating phonon interactions in an arbitrary field, on the other hand, leads to an intertwining of space and time coordinates in the Dyson equation, so the usual simplifications do not occur on transformation to momentum-energy Green's functions. Describing the system in terms of shifted coordinates,[11] such as $z-\hbar\omega/eE$, also does not deconvolve the Dyson equation. The use of center-of-mass (Wigner) coordinates does not simplify the task, as they have no preferred status in the theory, and a coordinate transformation is required to account for the translation–energy-shift symmetry.[8] The approach which we have found workable is to introduce an Airy transform of the coordinate (z) parallel to the field. We emphasize that previous treatments have found solutions in terms of Airy functions,[3,9,11] while the present use of an Airy transform differs by the incorporation of the symmetry of the problem at an early stage, diagonalizing the unperturbed Green's function and leading to a considerably simpler expression of Dyson's equation.

Using this formulation, we solve Dyson's equation for the single-particle retarded Green's function $G^r(\mathbf{k}_\perp,z,z',\omega)$. For this, we are able to derive a spectral density function for the weak electron-phonon interaction which accounts for both collisional broadening and the intracollisional field effect. Using Airy coordinates we are also able to distinguish straightforwardly between two kinds of oscillatory effects that are combined in other representations: In real space, the potential of the electric field acts as a sharp barrier, and standing waves are generated on the real-momentum side of the classical turning point. This leads to nodes in the spectral density, when that is viewed as a function of coordinate z. These first oscillations are absent when the spectral density is viewed as a function of Airy coordinate. When the phonon interactions are included the oscillations are changed as a conse-

quence of the interaction between the field and the scatterers, and oscillations are present in the real part of the self-energy. These latter oscillations are the only ones present in the self-energy in the Airy coordinate representation. As a result, it is possible to see clearly the oscillations which are due to the electron-phonon interaction. These oscillations are *incommensurate* with the standing-wave oscillations.

The spectral function can be defined in terms of the anticommutator of the fermion creation and annihilation field operators $\psi(\mathbf{r},t)$ and $\psi^{\dagger}(\mathbf{r},t)$ as[13]

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

where the angular bracket $\langle\cdots\rangle$ indicates the nonequilibrium expectation value. If the system is translationally invariant in space and time, we can Fourier transform the spectral function into $(\mathbf{k},\omega)$ space. Then $A(\mathbf{k},\omega)$ obeys sum rules that give it the meaning of a weighting function: $A(\mathbf{k},\omega)/2\pi$ represents the probability that a particle with momentum $\hbar\mathbf{k}$ has energy $\hbar\omega$. The spectral function is calculated from the nonequilibrium retarded Green's function:[13]

$$A(\mathbf{k},\omega)=-2\,\mathrm{Im}[G^{r}(\mathbf{k},\omega)] . \tag{2}$$

The retarded Green's function satisfies the familiar Dyson's equation, which can be formally written as

$$G^{r}=G_0^{r}+G_0^{r}\Sigma^{r}G^{r} , \tag{3}$$

where G_0^{r} is the retarded free-particle propagator and the self-energy Σ^{r} describes the scattering processes.

The electric field is usually included with the scattering processes in Σ^{r}. As noted above, this leads to a perturbed Green's function G^{r} that is no longer translationally invariant. The usual Fourier transformations then yield a Dyson's equation in terms of a center-of-mass time T and a center-of-mass $\mathbf{R}$, in addition to $\mathbf{k}$ and ω. These "Wigner coordinates" have been used in many earlier attempts to go beyond perturbatively small fields. The coordinates are convolved in a way that depends on the gauge used to describe the electric field, and both scalar and vector gauges have been used in attempts to solve the equation.

We take a different approach, including the electric field (represented by a scalar potential $\phi=-Ez$) as a part of the unperturbed Hamiltonian. While this has been done previously, we choose as a basis set the eigenstates of the Hamiltonian: plane waves in the plane normal to the field and Airy functions of the first kind along the direction of the field. This allows us to define a coordinate system $(\mathbf{k}_{\perp},s)$, where $\mathbf{k}_{\perp}=(k_x,k_y)$. The transformation that connects the two coordinate systems (x,y,z) and $(\mathbf{k}_{\perp},s)$ is defined by the integral operation

$$F(\mathbf{k}_{\perp},s)=\int\frac{dxdy}{2\pi}\int\frac{dz}{L}e^{i\mathbf{k}_{\perp}\cdot\boldsymbol{\rho}}\mathrm{Ai}\left[\frac{z-s}{L}\right]f(\boldsymbol{\rho},z) , \tag{4}$$

where $L=(\hbar^2/2mE)^{1/3}$ and $\boldsymbol{\rho}$ is the transverse position vector. The Airy transform variable s has a physical interpretation as the turning point in z of a (noncoupled) electron with energy $\varepsilon(\mathbf{k}_{\perp},s)=\hbar^2\mathbf{k}_{\perp}^2/2m+eEs$. 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.

The unperturbed, field-dependent Green's function can now be written down quickly as

$$G_E^{r}(\mathbf{k}_{\perp},s,t-t')=-i\theta(t-t')\exp\left[-\frac{i}{\hbar}\varepsilon_{\mathbf{k}_{\perp},s}(t-t')\right] . \tag{5}$$

Dyson's equation becomes

$$G^{r}(k_{\perp},s,s',\omega)=G_E^{r}(\mathbf{k}_{\perp},s,\omega)\delta(s-s')+G_E^{r}(\mathbf{k}_{\perp},s,\omega)\int ds_2\Sigma^{r}(\mathbf{k}_{\perp},s,s_2,\omega)G^{r}(\mathbf{k}_{\perp},s_2,s',\omega) , \tag{6}$$

and the self-energy Σ^{r} now contains only information about the scattering mechanisms. For a nondegenerate system, this can be approximated as

$$\Sigma^{r}(\mathbf{r},t;\mathbf{r}',t')=iD_0^{>}(\mathbf{r},t;\mathbf{r}',t')G^{r}(\mathbf{r},t;\mathbf{r}',t') , \tag{7}$$

where $D_0^{>}$ is the equilibrium phonon correlation function

$$D_0^{>}(\mathbf{r},t;\mathbf{r}',t')=\langle\varphi(\mathbf{r},t)\varphi(\mathbf{r}',t)\rangle$$

with φ and $\varphi^{\dagger}$ the phonon field operators.

We consider nonpolar optical processes, and consider only one-phonon scattering with the approximation $G^{r}=G_E^{r}$ in (7). Because G_E^{r} is diagonal and $\Sigma^{r}(\mathbf{k}_{\perp},s,s',\omega)$ is highly peaked about $s=s'$, a diagonal approximation for Σ^{r} is appropriate here. We then obtain the expression

$$\begin{aligned}
&\Sigma^{r}(s,\omega)=\frac{2\pi}{\hbar}|V|^2\sum_{\eta=\pm1}\left[N_0+\frac{\eta+1}{2}\right]F(s,\omega) ,\\
&\mathrm{Re}[F(s,\omega)]=-\frac{2\pi}{\sqrt{2}}\frac{m^{3/2}}{\hbar^2}\Theta^{1/2}\left[\mathrm{Ai}'(\zeta)\mathrm{Bi}'(\zeta)-\zeta\mathrm{Ai}(\zeta)\mathrm{Bi}(\zeta)+\frac{\sqrt{\zeta}}{\pi}\theta(\zeta)\right] ,\\
&\mathrm{Im}[F(s,\omega)]=-\frac{2\pi}{\sqrt{2}}\frac{m^{3/2}}{\hbar^2}\Theta^{1/2}[\mathrm{Ai}'^2(\zeta)-\zeta\mathrm{Ai}^2(\zeta)] ,
\end{aligned} \tag{8}$$

where $\Theta=[3(\hbar eE)^2/2m]^{1/3}$, $\zeta=[eEs-\hbar(\omega-\eta\omega_0)]/\Theta$, and $|V|^2$ is the square of the electron-phonon matrix element. The terms with $\eta=+1$ correspond to emission and $\eta=-1$ to absorption of a phonon of frequency ω_0 by the electron.

Dysons's equation (6) is now a multiplicative equation and an expression for the full, retarded Green's function is obtained as

$$\mathrm{Re}[G^r(\mathbf{k}_\perp,s,\omega)] = \frac{\hbar\omega-\varepsilon_{\mathbf{k}_\perp,s}-\mathrm{Re}\Sigma^r(s,\omega)}{[\hbar\omega-\varepsilon_{\mathbf{k}_\perp,s}-\mathrm{Re}\Sigma^r(s,\omega)]^2+[\mathrm{Im}\Sigma^r(s,\omega)]^2}, \tag{9}$$

$$\mathrm{Im}[G^r(\mathbf{k}_\perp,s,\omega)] = \frac{\mathrm{Im}\Sigma^r(s,\omega)}{[\hbar\omega-\varepsilon_{\mathbf{k}_\perp,s}-\mathrm{Re}\Sigma^r(s,\omega)]^2+[\mathrm{Im}\Sigma^r(s,\omega)]^2}. \tag{10}$$

In Fig. 1, we plot the real part of the self-energy Σ^r as a function of the argument ζ. The oscillations in the self-energy have not been seen previously in other treatments of the high field behavior, and arise from the Airy functions in (8). The oscillatory nature means that we have regions in which the energies are lowered, and other regions where the energy is raised, and that these regions alternate with one another. In fact, the negative-slope zero crossings in Fig. 1 are quantized energies towards which the quasiparticle energy concentrates. The zero crossings occur asymptotically where $\zeta=[(3\pi/8)(2n+1)]^{2/3}$. Because of the irrational factor in $\Theta=3^{1/3}eEL$, these oscillations are incommensurate with those due to standing waves of the phonon-decoupled problem. The redistribution of spectral density is also reflected in the imaginary part of the self-energy, plotted in Fig. 2, where the appearance of steplike behavior signals the onset of additional densities of final states corresponding to the subbands generated by each quantized level.

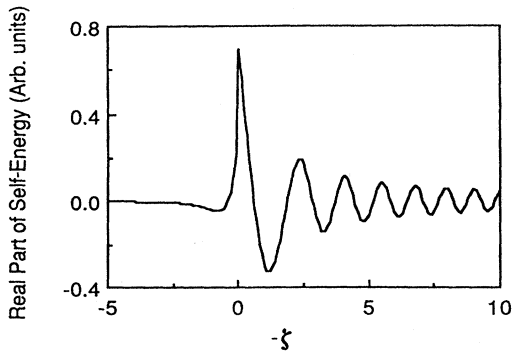

FIG. 1. The real part of the self-energy, in arbitrary units, is plotted as a function of the reduced coordinate ζ [defined following Eq. (8)].

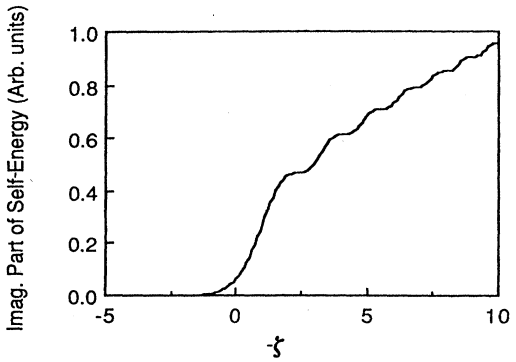

FIG. 2. The imaginary part of the self-energy, which is the scattering rate in normal circumstances, as a function of the reduced coordinate ζ. The steps in the scattering rate are essentially the onset of new quasi-two-dimensional structures corresponding to the zeroes of the real part of the self-energy in Fig. 1.

The spectral density found in (10), using definition (2), satisfies the normal sum rules in that in Airy coordinate it is positive definite and integrates properly. However, in the real space along the field this does not carry through, and nonpositive definiteness is found as in the case of earlier work.[9,10,12,14] Here, however, we believe the results suggest that the oscillations (which are Airy-function-like) are related to the "subband" tendencies discussed above in relation to the real part of the self-energy. The structure in the imaginary part of the self-energy reinforces this view. In addition, the spectral density in the Airy coordinates exhibits an unusual double peak near the zero point (where the limiting δ function occurs, which is the semiclassical turning point). This double-peak structure suggests that there is a length scale associated with the motion along the electric 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. A state-counting argument then implies the need for another quantum number. (An approximately analogous situation occurs in crystals. The continuous reciprocal-space coordinate is replaced by a quasimomentum restricted to the first Brillouin zone, and is augmented by a band index.) The levels represented by zero crossings of the real part of the self-energy in Fig. 1 could serve as a kind of sub-banding in which the particular crossing, or subband, plays the analogous role of the band index.

We have introduced a treatment in which the momentum coordinate representation along the field direction is replaced by a representation in terms of an Airy coordinate. This yields the mathematical advantage of simplified Dirac equations involving fewer coordinates. It also yields the heuristic advantage of separating phonon-coupled from phonon-free effects in the Green's function and spectral density. We have applied this to the case of nonpolar optical-phonon scattering in semi-

conductors in high electric fields. The results provide new insight to the coupled electron-phonon system in these high fields.

This work was supported by the Office of Naval Research and the North Atlantic Treaty Organization. The authors wish to thank A. Jauho (Copenhagen), C. Jacoboni (Modena), and L. Reggiani (Modena) for helpful suggestions that led to this work.

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