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Microscopic Theory of Quantum-Transport Phenomena in Mesoscopic Systems: A Monte Carlo Approach

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(Received 14 October 1997)

A theoretical investigation of quantum-transport phenomena in mesoscopic systems is presented. In particular, a generalization to "open systems" of the well-known semiconductor Bloch equations is proposed. The presence of spatial boundary conditions manifests itself through self-energy corrections and additional source terms in the kinetic equations, whose forms are suitable for a solution via a generalized Monte Carlo simulation. The proposed approach is applied to the study of quantum-transport phenomena in double-barrier structures as well as in superlattices, showing a strong interplay between phase coherence and relaxation. [S0031-9007(98)05753-6]

PACS numbers: 73.23.–b, 02.70.Lq, 72.10.–d, 73.40.–c

The Monte Carlo (MC) method, which has been applied for more than 25 years for calculation of semiclassical charge transport in semiconductors, is the most powerful numerical tool for microelectronics device simulation [1]. However, present-day technology pushes device dimensions toward limits where the traditional semiclassical transport theory can no longer be applied, and a more rigorous quantum transport theory is required [2]. To this end, various quantum-kinetic formulations of charge transport have been proposed, based on Green's function [3] or Wigner function [4] approaches. While such quantum-mechanical formalisms allow for a rigorous treatment of phase coherence, they typically describe energy-relaxation and dephasing processes via purely phenomenological models. A full quantum-mechanical simulation scheme for the analysis of transient-transport phenomena in the presence of carrier-phonon interaction has also been proposed [5]. However, due to the huge amount of computation required, its applicability is still limited to short time scales and extremely simplified situations. As a result, despite many efforts and despite the unquestionable intellectual progress associated with the study of these quantum-kinetic formulations, their application to realistic devices in the presence of a strong scattering dynamics is still an open problem. Recent results by Datta, Lake, and co-workers seem to be rather promising [6]. However, their steady-state Green's function formulation cannot be applied to the analysis of time-dependent nonequilibrium phenomena, which play a crucial role in modern optoelectronic devices.

In this letter we propose a generalized MC approach for the analysis of hot-carrier transport and relaxation phenomena in quantum devices. The method is based on a MC solution of the set of kinetic equations governing the time evolution of the single-particle density matrix; it can be regarded as an extension to open systems of the generalized MC approach recently proposed for the analysis of the coupled coherent and incoherent carrier dynamics in photoexcited semiconductors [7]. Compared to more academic quantum-kinetic approaches [3–5]—whose application is often limited to highly simplified physical models and conditions—the proposed simulation scheme allows one to maintain all the well known advantages of the MC method in describing a large variety of scattering mechanisms on a microscopic level [1].

In order to properly describe carrier-transport phenomena in mesoscopic structures, an electron-phonon system can be considered, whose Hamiltonian can be schematically written as $\mathbf{H} = \mathbf{H}_0 + \mathbf{H}'$. Here, the single-particle term $\mathbf{H}_0$ includes the phonon and free-carrier Hamiltonians as well as the potential profile (including possible external fields), while the many-body contribution $\mathbf{H}'$ accounts for all possible interaction mechanisms, e.g., carrier-carrier and carrier-phonon coupling. By denoting with $\phi_\alpha(\mathbf{r}) = \langle \mathbf{r} \mid \alpha \rangle$ the wave functions of the single-particle states α [8] and with ϵ_α the corresponding energies, the equations of motion for the single-particle density matrix ρ [9] in this α representation—known as semiconductor Bloch equations (SBE) [10,11]—can be schematically written as

$$\frac{d}{dt}\rho_{\alpha\beta} = \frac{d}{dt}\rho_{\alpha\beta}|_{\mathbf{H}_0} + \frac{d}{dt}\rho_{\alpha\beta}|_{\mathbf{H}'} . \qquad (1)$$

The time evolution induced by the single-particle Hamiltonian $\mathbf{H}_0$ can be evaluated exactly. In contrast, the contribution due to the many-body Hamiltonian $\mathbf{H}'$ involves phonon-assisted as well as higher-order density matrices; thus, in order to "close" our set of equations, approximations are needed. In particular, as described in [11], the "mean-field" approximation together with the Markov limit leads to a closed set of equations still local in time. Within such an approximation scheme, the equations of

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motion in (1) can be written as

$$\frac{d}{dt}\rho_{\alpha\beta} = \sum_{\alpha'\beta'} L_{\alpha\beta,\alpha'\beta'}\rho_{\alpha'\beta'} \tag{2}$$

with

$$L_{\alpha\beta,\alpha'\beta'} = \frac{1}{i\hbar}(\epsilon_\alpha - \epsilon_\beta)\delta_{\alpha\beta,\alpha'\beta'} + \Gamma_{\alpha\beta,\alpha'\beta'}. \tag{3}$$

Here, the two terms correspond to the separation in (1).The explicit form of the scattering tensor Γ involves the microscopic in- and out-scattering rates for the various interaction mechanisms [12].

The analysis presented so far is typical of a so-called "closed" system, i.e., defined over the whole coordinate space. However, this is not the case of interest for the study of quantum-transport phenomena in mesoscopic devices, where the properties of the carrier subsystem are strongly influenced by the spatial boundaries with the external environment. This requires a real-space description, which can be obtained in terms of the phase-space formulation of quantum mechanics originally proposed by Wigner [13] and generalized to solids in the pioneering paper by Buot [14]. In our case, this corresponds to introducing the following unitary transformation u connecting our $\alpha\beta$ representation to the desired phase space $\mathbf{r}, \mathbf{k}$:

$$u_{\alpha\beta}(\mathbf{r},\mathbf{k}) = (2\pi)^{-3/2}\int d\mathbf{r}'\phi_\alpha\left(\mathbf{r} + \frac{1}{2}\mathbf{r}'\right)e^{-i\mathbf{k}\cdot\mathbf{r}'} \times \phi^*_\beta\left(\mathbf{r} - \frac{1}{2}\mathbf{r}'\right). \tag{4}$$

By applying the above Weyl transform to the single-particle density matrix ρ, we obtain the so-called Wigner function [4],

$$f^W(\mathbf{r},\mathbf{k}) = \sum_{\alpha\beta}\rho_{\alpha\beta}u_{\alpha\beta}(\mathbf{r},\mathbf{k}). \tag{5}$$

For a closed system, f^W is defined for any value of the real-space coordinate $\mathbf{r}$, and its time evolution is fully determined by its initial condition. In contrast, for an open system, f^W is defined only within a given region Ω of interest and its time evolution is determined by the initial condition inside such a region as well as by its values f^W_b on the boundary $\mathbf{r}_b$ of the domain at any time $t' > t_0$. More specifically, by applying the Green's function theory to the equation of motion for f^W—which is obtained by applying to Eq. (2) the Weyl-Wigner transform (5)—we get

$$f^W(\mathbf{r},\mathbf{k};t) = \int_\Omega d\mathbf{r}'\int d\mathbf{k}'G(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}';t - t_0)f^W(\mathbf{r}',\mathbf{k}';t_0) + \int d\mathbf{r}_b\int d\mathbf{k}'\int_{t_0}^{t} dt'G(\mathbf{r},\mathbf{k};\mathbf{r}_b,\mathbf{k}';t - t')f^W_b(\mathbf{r}_b,\mathbf{k}',t')v(\mathbf{k}'), \tag{6}$$

where

$$G(\mathbf{r},\mathbf{k};\mathbf{r}',\mathbf{k}';\tau) = \sum_{\alpha\beta,\alpha'\beta'} u_{\alpha\beta}(\mathbf{r},\mathbf{k})[e^{L\tau}]_{\alpha\beta,\alpha'\beta'}u^*_{\alpha'\beta'}(\mathbf{r}',\mathbf{k}') \tag{7}$$

is the evolution operator, while $v(\mathbf{k})$ is the component of the carrier group velocity normal to the boundary surface. We clearly see that the value of f^W is obtained from the propagation of the initial condition $f^W(t_0)$ inside the domain Ω plus the propagation of the boundary values f^W_b from the points of the surface at any time t' to the point $\mathbf{r}, \mathbf{k}$ of interest.

Given the above Wigner formulation for open systems, we now introduce a corresponding density-matrix description via the following "inverse" Weyl-Wigner transform:

$$\overline{\rho}_{\alpha\beta} = \int_\Omega d\mathbf{r}\int d\mathbf{k}u^*_{\alpha\beta}(\mathbf{r},\mathbf{k})f^W(\mathbf{r},\mathbf{k}). \tag{8}$$

By applying the above transformation to Eq. (6) and then performing its time derivative, we finally obtain

$$\frac{d}{dt}\overline{\rho}_{\alpha\beta} = \sum_{\alpha'\beta'}\overline{L}_{\alpha\beta,\alpha'\beta'}\overline{\rho}_{\alpha'\beta'} + \overline{S}_{\alpha\beta}, \tag{9}$$

where $\overline{L} = ULU^{-1}$ is the Liouville tensor (3) "dressed" by the transformation

$$U_{\alpha\beta,\alpha'\beta'} = \int_\Omega d\mathbf{r}\int d\mathbf{k}u^*_{\alpha\beta}(\mathbf{r},\mathbf{k})u_{\alpha'\beta'}(\mathbf{r},\mathbf{k}), \tag{10}$$

while

$$\overline{S}_{\alpha\beta} = \sum_{\alpha'\beta'}U_{\alpha\beta,\alpha'\beta'}\int d\mathbf{r}_b\int d\mathbf{k}u^*_{\alpha'\beta'}(\mathbf{r}_b,\mathbf{k}) \times v(\mathbf{k})f^W_b(\mathbf{r}_b,\mathbf{k}) \tag{11}$$

is a source term induced by our spatial boundary conditions.

Equation (9) is the desired generalization to the case of open systems of the conventional SBE in Eq. (2). In addition to the source term in Eq. (11), the presence of spatial boundary conditions induces modifications on the Liouville operator L of the system via the transformation U in Eq. (10).

The generalized SBE (9) can still be regarded as the result of a coherent single-particle dynamics plus incoherent many-body contributions [see Eq. (1)]. Therefore, they can be solved by means of the same MC simulation scheme described in [7]. The method is based on a time-step separation between coherent and incoherent dynamics: The former accounts in a rigorous way for all quantum phenomena induced by the potential profile of the device as well as for the proper boundary conditions. The latter, described within the basis given by the eigenstates α of the

potential profile, accounts for all of the relevant scattering mechanisms by means of a conventional "ensemble" MC simulation [7].

In order to illustrate the power and flexibility of the proposed theoretical approach, we have simulated quantum-transport phenomena in rather different physical systems. Since we are interested in low temperature and low carrier density conditions, only optical-phonon scattering has been considered. We have first carried out the simulation of an electron wave packet entering the double-barrier structure [15] of a GaAs/AlGaAs resonant tunneling diode (RTD). Figure 1 shows the time evolution of the wave packet in the absence of scattering as a function of position (a) and energy (b). It is easy to recognize the well-established resonance scenario typical of any purely coherent dynamics: As the wave packet enters our RTD structure, a part of it is transmitted and a part is reflected [see Fig. 1(a)]. Since scattering is not included in this simulation, the wave-packet central energy is conserved, i.e., no energy relaxation occurs [see Fig. 1(b)]. On the contrary, in the presence of incoherent scattering processes the resonance dynamics of Fig. 1(a) is strongly modified by the scattering itself, as shown in Fig. 2(a). In particular, the presence of phase-breaking scattering processes is found to reduce both the interference peaks and the transmitted wave packet. This is confirmed by the corresponding energy distribution in Fig. 2(b), where we clearly recognize the granular nature of the dissipation process through the formation of an optical-phonon replica. This is the fingerprint of any full microscopic treatment of energy relaxation, in contrast with all previous phenomenological approaches.

As a second test bed, we have also simulated electrically injected Bloch oscillations in superlattices (SLs). The system under investigation consists of a biased GaAs/AlGaAs SL [16] surrounded by two semi-infinite GaAs regions. In our simulated experiment an electron wave packet is injected from the left contact (GaAs region) into the SL region [see Fig. 3]. Figures 3 and 4 illustrate the time evolution of the wave packet with and without scattering, respectively. When the wave packet reaches the SL structure most of it gets reflected backwards, while some portion of it tunnels into the Wannier-Stark ladder associated with the SL and starts to oscillate at a frequency of about 3.5 THz. Each time the packet reaches the boundary of the oscillation region a part of it gets transmitted via Zener tunneling. We should notice, however, that such Zener processes do not destroy the Bloch-oscillation dynamics, but simply

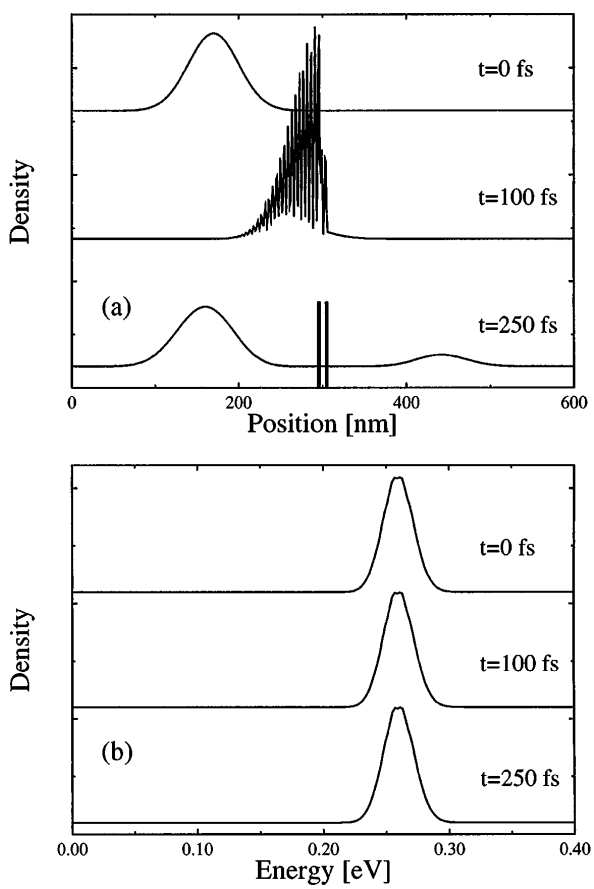

FIG. 1. Carrier density at different times as a function of position (a) and energy (b) corresponding to an electron wave packet injected into a RTD structure in the absence of scattering processes (the two barriers are schematically depicted as black vertical lines).

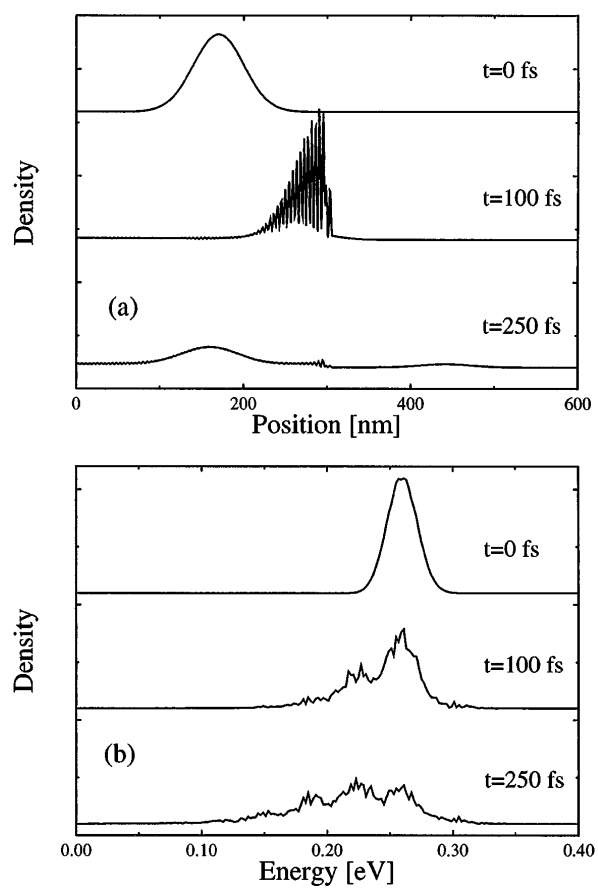

FIG. 2. Same as in Fig. 1, but in the presence of scattering processes (see text).

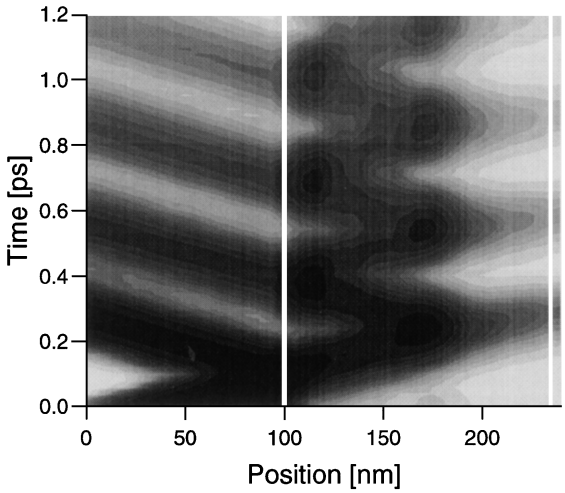

FIG. 3. Contour plot of the charge density corresponding to a wave packet electrically injected into a finite SL region (marked with vertical white lines) in the absence of scattering processes.

reduce the charge density within the SL region. Indeed, in the scattering-free case [see Fig. 3], the Bloch oscillations are found to persist on a picosecond time scale. In contrast, once scattering mechanisms are considered [see Fig. 4], the phonon-induced dephasing drastically reduces their lifetime.

In conclusion, we have proposed a generalization to open systems of the well-known SBE. This approach allows for a proper description of the strong coupling between phase coherence and relaxation. Indeed, our simulated experiments clearly show the failure of any purely coherent or incoherent approach in describing typical quantum-transport phenomena in semiconductor nanostructures. Contrary to all previous quantum-transport investigations, the proposed theoretical scheme allows one to fully recover—and benefit from—the unquestionable advantages of the semiclassical MC simulation, thus opening the way to the theoretical modeling of realistic quantum devices.

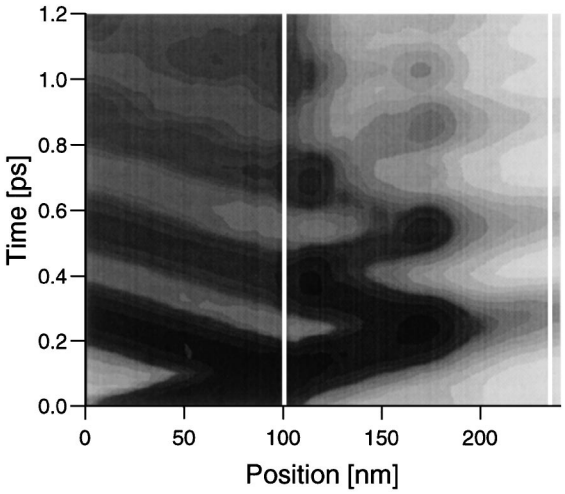

FIG. 4. Same as in Fig. 3, but in the presence of scattering processes (see text).

We are grateful to Carlo Jacoboni, Tilmann Kuhn, and Massimo Fischetti for stimulating and fruitful discussions. This work was supported in part by the EC Commission through the TMR Network "ULTRAFAST".

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