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Bohm trajectories for the Monte Carlo simulation of quantum-based devices

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A generalization of the classical ensemble Monte Carlo (MC) device simulation technique is proposed to simultaneously deal with quantum-mechanical phase-coherence effects and scattering interactions in quantum-based devices. The proposed method restricts the quantum treatment of transport to the regions of the device where the potential profile significantly changes in distances of the order of the de Broglie wavelength of the carriers (the quantum window). Bohm trajectories associated to time-dependent Gaussian wave packets are used to simulate the electron transport in the quantum window. Outside this window, the classical ensemble MC simulation technique is used. Classical and quantum trajectories are smoothly matched at the boundaries of the quantum window according to a criterium of total-energy conservation. A self-consistent one-dimensional simulator for resonant tunneling diodes has been developed to demonstrate the feasibility of our proposal. © *1998 American Institute of Physics.* [S0003-6951(98)01007-9]

The reliable simulation of devices based on quantum-mechanical (QM) phenomena (such as tunneling) requires the simultaneous consideration of phase-coherence effects and of scattering interactions. Three main different approaches have been proposed to pursue this goal: (i) the solution of the Liouville equation to obtain the Wigner distribution function (WDF);[1–4] (ii) the nonequilibrium Green function theory recently reformulated by Lake *et al.*[5,6] to include band-structure and scattering effects; and (iii) the solution of the effective-mass Schrödinger equation combined with a Monte Carlo (MC) based introduction of scattering.[7–10] In our opinion, the latter approach would be very useful if an adequate description of tunneling in terms of particle trajectories were found. This is the path followed by Salvino and Buot,[9] who used an *ad hoc* model based on the phase tunneling time, and it is also our choice. In this letter, we propose a quantum-MC method based on Bohm trajectories, which provide a consistent description of the QM dynamics.[11,12] Although we have developed a one-dimensional quantum-MC simulator for a resonant tunneling diode (RTD), the proposed technique is appropriate for any vertical-transport-based QM device.

The most widely known causal interpretation of quantum mechanics is the one due to Bohm.[11] Within the Bohm's interpretation, all the particles of a quantum pure-state ensemble follow deterministic trajectories under the combined influence of the classical potential, $V(x,t)$, and a quantum potential, $Q(x,t)$, which is directly related to the wavefunction $\Psi(x,t)$:

$$Q(x,t) = -\frac{\hbar}{2m^*}\frac{1}{|\Psi(x,t)|}\frac{\partial^2|\Psi(x,t)|}{\partial x^2}, \tag{1}$$

m^* being the particle's effective mass. From the point of view of device simulation, the most important property of the Bohm's interpretation is that all the measurable results of standard quantum mechanics are perfectly reproduced by averaging over the Bohm trajectories with correct relative weights.[11]

The tunneling of electrons through one-dimensional potential barriers has been carefully studied within the Bohm's framework.[12,13] Scattering eigenstates have been shown to be unsuitable and time-dependent wave packets are required. In this case, the most convenient procedure to calculate the trajectories is the following:[13] (i) numerical solution of the stationary Schrödinger equation; (ii) choice of the initial wave-packet $\Psi(x,0)$ and projection onto the basis of eigenstates; (iii) calculation of $\Psi(x,t)$ by superposition to obtain the current density $J(x,t)$ and the velocity of the Bohm's particles, $\nu(x,t)$, which is given by

$$\nu(x,t) = \frac{1}{q}\frac{J(x,t)}{|\Psi(x,t)|^2}, \tag{2}$$

q being the absolute value of the electron charge; and (iv) integration of $\nu(x,t)$ to calculate the trajectories $x = x(x_0,t)$ which are uniquely defined for each position x_0 within the initial wave packet. In Fig. 1 we show some representative trajectories in the particular case of a Gaussian wave packet impinging upon a double barrier structure. Since $\nu(x,t)$ is single valued, the trajectories do not cross each other either in phase space or in configuration space, and this has interesting consequences.[13] In particular, the trajectories which are transmitted through the barrier come from the leading front of the wave packet. Those from the rear are reflected, many of them without ever reaching the barrier. By weighting the transmitted trajectories according to the initial probability density $|\Psi(x_0,0)|^2 dx_0$, the standard transmission coefficient is obtained.[12]

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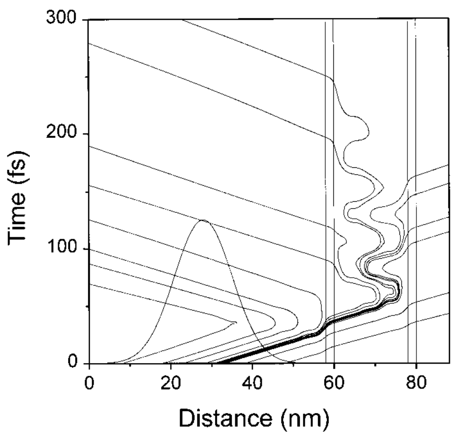

FIG. 1. Bohm trajectories associated to an initial Gaussian wave packet with a central energy of 0.16 eV and a spatial dispersion of 10 nm, impinging upon a GaAs/AlGaAs double barrier structure with 2 nm wide barriers of 0.3 eV and a 18 nm wide well. The position of the barriers and the initial Gaussian wave packet are also shown.

Since Bohm trajectories are causal, some magnitudes such as the tunneling times,[12,13] which are not well defined within the standard QM theory, are natural within the Bohm's picture. Although these nonstandard magnitudes should be regarded with diffidence, we must emphasize that the charge and current densities are perfectly reproduced by the Bohm trajectories:

$$|\Psi(x,t)|^2=\int_{-\infty}^{\infty} dx_0 |\Psi(x_0,0)|^2 \delta(x-x(x_0,t)), \tag{3}$$

$$J(x,t)=q\int_{-\infty}^{\infty} dx_0 |\Psi(x_0,0)|^2 \nu(x,t)\, \delta(x-x(x_0,t)). \tag{4}$$

In this regard, our proposal is a simulation tool which obtains standard QM results, though by means of Bohm trajectories, i.e., the Bohm's theory is used as an equivalent mathematical reformulation of quantum mechanics, rather than as an alternative physical interpretation.

Our simulator defines a QM window (QW) and restricts the QM treatment to this window. Outside the QW, the classical MC technique is used taking into account impurity and phonon-scattering mechanisms. When an electron reaches the boundary of the QW, a Gaussian wave packet is associated to it:

$$\Psi_k(x,0)=\frac{1}{(\pi\sigma_x^2)^{1/4}} \exp\left(-\frac{(x-x_B)^2}{2\sigma_x^2}+ikx\right), \tag{5}$$

x_B being a fixed position centered in the emitter side of the QW, k the central momentum, and σ_x the spatial standard deviation. The selection of the wave-packet parameters is of critical importance. The central position x_B is chosen to be far enough into the emitter side of the diode, where the potential is flat enough to allow an analytical projection onto the eigenstates.[14] Since the transmission probability depends on the width of the wave packet, the selection of σ_x also requires a physical criterion. The narrower is the wave packet (small σ_x), the smoother and wider are the found transmission resonances and the smaller is the peak-to-valley current. A reasonable criterion is the choice of wide enough wave packets ($\sigma_x \geqslant 25$ nm) so that the corresponding transmission coefficient is roughly that of the eigenstate associated to the central momentum k (i.e., narrow in k space as compared with the features of the local density of states). In our MC simulator we have considered bias-independent wave-packet parameters and, in particular, $\sigma_x=25$ nm. Inside the QW, each electron follows a randomly selected Bohm trajectory and the charge and current densities inside the QW are computed using the methods of the classical MC technique. The coupling to classical trajectories and the selection of k are based on the conservation of the total electron energy. To implement these matching criteria, we require the following condition at both interfaces of the QW:

$$\frac{\hbar^2 k_c^2}{2m^*}+V(x)=\frac{1}{2}\, m^* \nu^2(x,t)+V(x)+Q(x,t), \tag{6}$$

where k_c is the x component of the momentum of the classical particle. This equation requires the previous choice of the trajectory, i.e, of the initial position x_0, which is selected by generating a random number distributed according to $|\Psi_k(x_0,0)|^2 dx_0$. Notice that this distribution does not depend on k. For a Gaussian wave packet such as of Eq. (5), the velocity and quantum potential at $t=0$ are given by

$$Q(x_0,0)=\frac{\hbar^2}{2m^*\sigma_x^2}\left(1-\frac{(x_0-x_B)^2}{\sigma_x^2}\right); \quad \nu(x_0,0)=\frac{\hbar k}{m^*}. \tag{7}$$

Substitution into Eq. (6) after having generated x_0, allows the determination of k. Discontinuity of the particle position is avoided by allowing the electron to travel classically from the boundary of the QW to the corresponding x_0. Electrons incident from the collector are classically reflected before entering in the QW (i.e., for the moment, only tunneling from emitter to collector is considered). Scattering has not been implemented in the QW and this is the main limitation of our approach in the present stage of development. In particular, this has forced us to consider a Thomas–Fermi approximation for the calculation of the electronic charge in the emitter accumulation layer to avoid unphysical depletion of charge in this region and nonrealistic self-consistent potential profiles.[15]

To show the feasibility of our proposal, we have simulated the current–voltage ($I-V$) characteristic of a typical GaAs/AlGaAs RTD (barrier width of 3 nm, barrier height of 0.3 eV, and well width of 5.1 nm) at 77 K. The ionized impurity density in the emitter and collector GaAs electrodes is 1.51×10^{17} cm^{-3} (i.e., a realistic doping of 5×10^{18} cm^{-3}). A one-valley model with a single effective mass (that of GaAs Γ point) has been considered for the whole structure. Figure 2 shows the self-consistent potential and the electron concentration profiles, together with the current calculated at each position of the RTD, for an applied bias of 0.39 V (near the resonant maximum of the $I-V$ characteristic). The validity of our matching procedure is supported by the fact that the self-consistent potential does not show spurious effects at the boundaries of the QW and because current continuity is preserved in the whole device. The current is noisier in the collector because it is carried by a reduced number of high-energy electrons, while in the emitter the whole low-energy distribution is shifted towards small values of positive momenta. The largest current spike

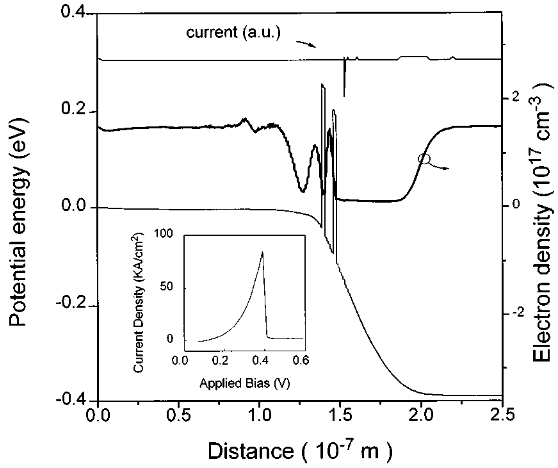

FIG. 2. Results obtained with our QM Monte Carlo simulator for a 3.0/5.1/3.0 nm GaAs/AlGaAs double barrier RTD (barrier height of 0.3 eV) at 77 K. Simulated electron concentration and self-consistent potential profile at a resonant bias near the peak of the $I-V$ curve ($V_{appl}=0.39$ V). The horizontal solid line represents the current density (in arbitrary units) along the whole device computed as the product of the average electron charge density per average velocity (i.e., current continuity is demonstrated). The inset represents the simulated $I-V$ curve.

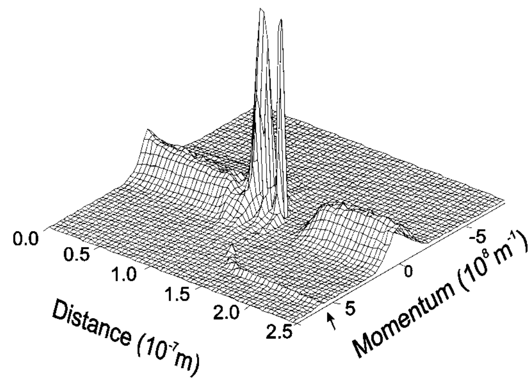

FIG. 3. Phase space distribution function along the device of Fig. 2 at the applied bias of 0.39 V. Notice the tunneling ridge (indicated by an arrow), which is originated in the QW by resonant Bohm trajectories and which becomes progressively thermalized in the collector by scattering mechanisms.

obtained at the boundary of the QW is not physically significant, being a spurious effect caused by the numerical calculation of $Q(x,t)$ as required by Eq. (6). The electron concentration profile shows an oscillatory behavior before the barriers and an accumulation in the quantum well. The obtained $I-V$ characteristic (inset of Fig. 2) shows the main qualitative features of those of actual devices. However, as in previous works,[7,9] the current almost vanishes after the resonant peak (it increases again at higher bias when electrons are injected through or over the top of the barrier) as a consequence of having ignored scattering in the QW (i.e., injection from the one-side bound states of the accumulation layer is neglected). In this regard, we must stress that previous tools did not consider scattering either and that they used *ad hoc* models for the QM dynamics.[7–9] As shown in Fig. 3, the MC simulator provides the momentum distribution of particles as a function of position along the device. These results qualitatively resemble those obtained within the WDF approach,[3] showing QM oscillations in the prebarrier region, accumulation of charge in the quantum well at the resonance bias, and a tunneling ridge (also at resonance) which progressively vanishes due to thermalization of carriers in the collector. However, contrarily to the WDF, our particle distribution is always positive by construction.

The presented results explicitly demonstrate the feasibility of using Bohm trajectories to extend the classical MC technique to tunneling devices. In addition to the potential profile and the current at the terminals of the device, the proposed quantum-MC technique provides local information of the momentum and energy distributions (the quantum potential must be accounted for, if the standard QM results are to be reproduced[12,16]), which can eventually contribute to improve the understanding and design of the devices. Our approach has the additional advantage of reaching the nanoelectronic range without abandoning the intuitive picture of carrier trajectories for the simulation of electron devices. Immediate future developments will include the consideration of scattering between Bohm trajectories inside the QW and the analysis of Bohm trajectories associated with one-side bound states in the emitter accumulation layer.

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[1] W. R. Frensley, Rev. Mod. Phys. **62**, 745 (1990).
[2] B. A. Biegle and J. D. Plummer, IEEE Trans. Electron Devices **44**, 733 (1997).
[3] K. L. Jensen and F. A. Buot, IEEE Trans. Electron Devices **38**, 2337 (1991).
[4] F. Rossi, P. Poli, and C. Jacoboni, Semicond. Sci. Technol. **7**, 1017 (1992).
[5] R. Lake, G. Klimeck, R. C. Bowen, and D. Jovanovic, J. Appl. Phys. **81**, 7845 (1997).
[6] R. C. Bowen, G. Klimeck, R. Lake, W. R. Frensley, and T. Moise, J. Appl. Phys. **81**, 3207 (1997).
[7] T. Baba, M. Al-Mudares, and J. R. Barker, Jpn. J. Appl. Phys., Part 2 **28**, L1682 (1989).
[8] K. K. Gullapalli, D. R. Miller, and D. P. Neikirk, IEEE IEDM'91 Digest of Technical Papers, 511 (1991).
[9] R. E. Salvino and F. A. Buot, J. Appl. Phys. **72**, 5975 (1992).
[10] S. Ragazzi, A. Di Carlo, P. Lugli, and F. Rossi, Phys. Status Solidi B **204**, 339 (1997).
[11] P. R. Holland, *The Quantum Theory of Motion* (Cambridge University Press, Cambridge, 1993).
[12] C. R. Leaves and G. C. Aers, in *Scanning Tunneling Microscopy III*, edited by R. Wiesendanger and H. J. Güntherodt (Springer, Berlin, 1993), p. 105.
[13] X. Oriols, F. Martín, and J. Suñé, Phys. Rev. A **54**, 54 (1996).
[14] R. S. Dumont and T. L. Marchioro II, Phys. Rev. A **47**, 85 (1993).
[15] W. R. Frensley, Solid-State Electron. **32**, 1235 (1989).
[16] J. R. Barker, Semicond. Sci. Technol. **9**, 911 (1994).