Transient Response of a Tunneling Device Obtained from the Wigner Function

William R. Frensley
Central Research Laboratories, Texas Instruments Incorporated, Dallas, Texas 75265
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A model of an open quantum system is presented in which irreversibility is introduced via boundary conditions on the Wigner function. The model is applied to the quantum-well resonant-tunneling diode. The calculations reproduce the negative-resistance characteristic of the device, and indicate that the tunneling current approaches steady state within a few hundred femtoseconds of a sudden change in applied voltage.

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The progress of semiconductor fabrication technology, particularly the heteroepitaxial technology, has permitted the fabrication of structures[1] and devices[2,3] whose behavior is dominated by quantum interference effects. A key property of such devices (which determines their switching speed) is the transient response to changes in the externally applied voltage. The proper way to calculate the transient response is to integrate that equation which describes the time evolution of the statistical distribution function of the device in question. Such calculations have been attempted recently and have shown an unpleasant tendency to develop unstable solutions.[4,5] The persistence of difficulties of this sort can be a symptom of a conceptual flaw in the formulation of the problem. In the present case, this has been identified as a failure to treat properly the inherent irreversibility of an open system like an electron device.

An electron device is necessarily an open system; it is useless unless connected to an electrical circuit and able to exhange electrons with that circuit. Moreover, "openness" in this sense is a form of interaction with the environment that appears to have received little attention in the context of quantum statistical mechanics. There has been much work on the theory of damping in optical systems.[6] As the particles in the case are massless bosons, and therefore are not conserved, the distinction between "damping" and "openness" is not significant. There is also a large body of work on the damping of particle motion by the interaction with a heat bath[7] (in the context of Brownian motion, but also applicable to Ohmic conduction). In this case the particles are conserved but there is energy dissipation. In the present case we are concerned with the gain and loss of electrons by a system, and because the relevant interactions strictly conserve these particles, this gain and loss occurs as a current through the boundaries of the system. (The boundary of the system can be either a physical interface, such as the surface of a semiconductor crystal to which metallic contacts have been applied, or a more idealized partitioning of the domain for the convenience of the analysis.) An obvious way to try to deal with this sort of open system is to describe the coupling to the external environment as a boundary condition on the system.

The boundary conditions representing such openness are properly applied to the single-particle distribution function of the system, as represented either by the density matrix in real space or by the Wigner function.[8] The Liouville (super)operator will generate the time evolution of the distribution function. The problems encountered in the modeling of open systems can be traced to the eigenvalue spectrum of the Liouville operator. For a closed system with no damping, the Liouville operator is of course Hermitian and its eigenvalues are purely real. If the boundary conditions are modified so as to permit particles to pass through the boundary, the Hermiticity is violated, and at least some eigenvalues will acquire nonzero imaginary parts. If the open-system boundary conditions are time reversible, then these imaginary parts will occur in conjugate pairs, leading to unstable (growing) exponential components as well as stable (decaying) components. The unstable components can persist even in the presence of moderate damping.[9] The way to avoid such difficulties is to formulate the boundary conditions so that they are time irreversible.

A physically appealing set of irreversible boundary conditions follows from our regarding the contacts as ideal particle reservoirs with properties analogous to those of a black body. We assume that the distribution of particles entering the system from the reservoir is equal to the equilibrium distribution of the reservoir, and that particles in the system that impinge upon the boundary are absorbed without reflection by the reservoir. This model of the contacts is implicitly assumed in the scattering approach to the modeling of quantum devices,[10] and in Monte Carlo models of classical transport.[11] It also contains an implicit Markoff assumption, in the sense that all information about the state of a particle is lost when it passes into a reservoir.

In order to apply boundary conditions of this sort, we must be able to distinguish the sense of the velocity of the particles at the position of the boundary, and this suggests that the Wigner distribution is the appropriate representation for the statistical state. In the Wigner representation the Liouville equation is[8]

$$\partial f(x,k)/\partial t = -(\hbar k/m)\partial f/\partial x - \int dk' V(x,k-k')f(x,k') \equiv (L/i\hbar)f, \tag{1}$$

where f is the Wigner function, L is the Liouville operator, and the kernel of the potential operator is given by

$$V(x,k) = (2/\hbar)\int_0^\infty dy \sin(ky)[v(x+\tfrac{1}{2}y) - v(x-\tfrac{1}{2}y)]. \tag{2}$$

If the boundaries of the system are at $x=0$ and $x=l$, the boundary conditions described above will fix $f(0,k)$ for $k>0$ and $f(l,k)$ for $k<0$ to be equal to the equilibrium-distribution characteristic of the respective reservoir.

These boundary conditions assure that the solutions to the Liouville equation are stable by assuring that the real parts of the eigenvalues of $L/i\hbar$ are all negative. This is most easily demonstrated by evaluation of the expectation value of $L/i\hbar$ for an arbitrary distribution function, for homogeneous boundary conditions (because the eigenvalues are really a property of the homogeneous operator). The contribution from the potential operator vanishes by antisymmetry, and the gradient term can be integrated to give

$$\langle f,(L/i\hbar)f\rangle = \int dx \int dk\, f(L/i\hbar)f = (\hbar/2m)\int dk\, k[f^2(0,k) - f^2(l,k)]$$

$$= (\hbar/2m)\left[\int_{-\infty}^0 kf_s^2(0,k)dk + \int_0^\infty kf_r^2(0,k)dk - \int_{-\infty}^0 kf_r^2(l,k)dk - \int_0^\infty kf_s^2(l,k)dk\right].$$

The subscripts r and s indicate that the distributions are properties of the reservoir and the system, respectively. For the homogeneous problem, the f_r are zero, and the remaining terms are negative, thus demonstrating that the eigenvalues of $L/i\hbar$ are negative. This is the key to our obtaining meaningful results for the transient behavior of an open system. The boundary conditions presented here should be applicable to the analysis of open systems in other contexts, in addition to the present application to electron devices.

This formulation has been applied to the study of a semiconductor device of current interest, the resonant-tunneling diode.[2,3] This device consists of a single quantum well bounded by tunneling barriers, as shown in Fig. 1. As a bias voltage is applied to the device, the resonant state in the well is pulled down in energy with respect to the more negative electrode, and the tunneling current through this state depends on the density of occupied states in the electrode. When the resonant state is pulled below the conduction-band edge of the electrode, the tunneling current decreases. The device thus shows negative differential resistance, which is attributable to quantum interference.

The Wigner function for the resonant-tunneling diode was evaluated numerically. A finite-difference approximation was used, with 80 mesh points in x and 60 points in k. A mesh spacing of 0.565 nm was used in the x direction to make the assumed layer thicknesses commensurate with the atomic layer spacing of the (Al,Ga)As system. The finite-difference approximation reduces the integrodifferential Liouville equation (1) to a large system of linear differential equations in time, with the boundary conditions supplying inhomogeneous terms. In steady state, these differential equations reduce to algebraic equations, which were solved by Gaussian elimination.

The steady-state calculation was performed for a range of bias voltages, and the current density was evaluated from the resulting Wigner function. The current-voltage characteristic from this calculation is shown in Fig. 2, along with the curve derived from a conventional scattering calculation. The Wigner-function

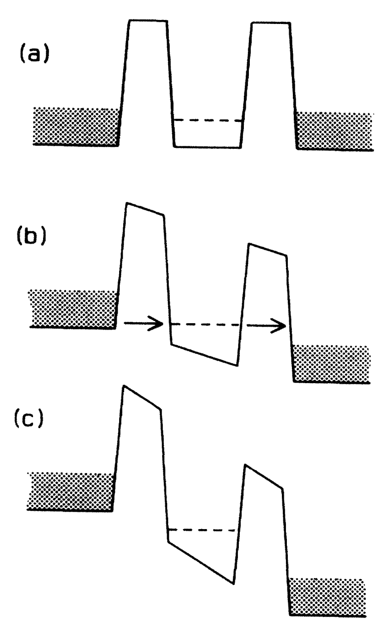

FIG. 1. Potential diagram for a resonant-tunneling diode. The barriers are thin layers of a wider-gap semiconductor, typically (Al,Ga)As, and the quantum well and the regions outside the barriers are GaAs. A size-quantized state is confined in the well; its energy is indicated by the dashed line. (a) The structure in equilibrium. (b) When a voltage is applied, electrons can resonantly tunnel out of occupied states (shaded region) through the confined state. (c) As the voltage is increased, the resonant state is pulled below the occupied levels and the tunneling current decreases, leading to a negative-resistance characteristic.

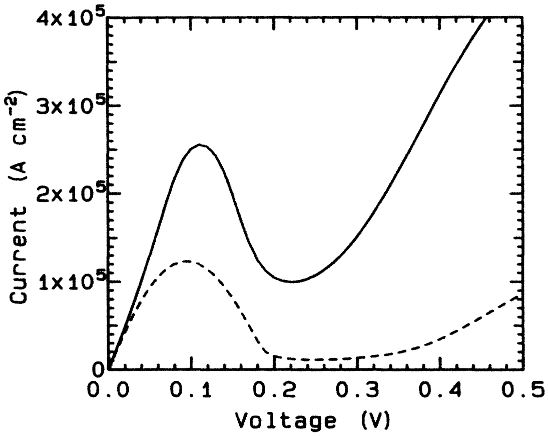

FIG. 2. Current vs voltage for a resonant-tunneling diode consisting of 2.8-nm layers of $Al_{0.3}Ga_{0.7}As$ bounding a 4.5-nm GaAs well, at a temperature of 300 K. The boundaries were assumed to be located 22.6 nm from the center of the quantum well. The current derived from a calculation of the Wigner function (solid line) is compared to that derived from a more conventional scattering calculation (dashed line).

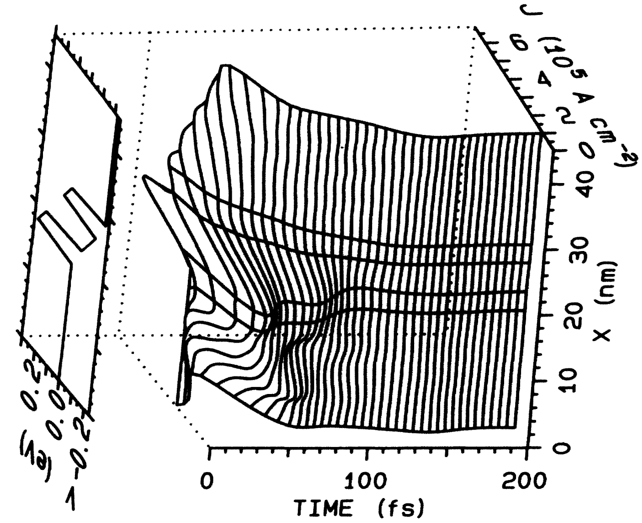

FIG. 3. Transient response of the resonant-tunneling diode of Fig. 2. Current density is plotted as a function of time and position within the device. The potential profile illustrates the device structure. At $t=0$, the voltage was suddenly switched from 0.11 V (corresponding to the peak current) to 0.22 V (corresponding to the valley current). After an initial peak, the current density approaches the lower steady-state value in 100–200 fs.

calculation predicts a higher current density and lower peak-to-valley current ratio than the scattering calculation. The voltages at which the peak and valley occur agree very well. The Wigner-function calculation more nearly resembles the experimental results at 300 K, but at lower temperatures it seriously underestimates the peak-to-valley ratio. Moreover, the presently neglected phonon-scattering processes, which account for most of the temperature dependence, will tend to reduce the peak-to-valley ratio. Thus, at present, the scattering theory is more likely to fit the experimental data[12] when such processes are taken into account. The difference between the Wigner and scattering calculations is probably due to the difference in the boundary conditions. The current-voltage curves calculated from the Wigner function depend weakly on the assumed position of the boundaries.

The transient response of the resonant-tunneling diode model was investigated by numerical integration of the discretized Liouville equation, with a steady-state Wigner function as an initial value. A calculation in which the initial bias of 0.11 V (corresponding to the peak in the current) was suddenly switched to 0.22 V (corresponding to the bottom of the valley) at $t=0$ is illustrated in Fig. 3. The response is complex, as might be expected, but shows some features that are readily interpreted. The current density initially increases throughout the structure, so that the device displays a positive resistance over a short time. The destructive interference which underlies the negative resistance takes some tens of femtoseconds to manifest itself. The current has settled quite near to its steady-state value after 200 fs. Of course the response of real devices will be limited by the time required to charge the device capacitance through the parasitic series resistance of the contacts. Such effects were deliberately omitted from the present model in order to observe the intrinsic response of the tunneling process itself.

The boundary conditions which I have used to model the open system might appear to violate the uncertainty principle. They certainly do not lead to any mathematical inconsistency; the problem is well posed. The only possible logical inconsistency is that the evaluation of the potential operator (2) requires information on the potential outside of the system, that is, within the reservoirs. This does not appear to be a significant problem, and I have simply assumed that the potential is extended with a constant value equal to that at the system-reservoir boundary.

It would be desirable to have more detailed microscopic models of the coupling between a device and its contacts, while still treating the contact as a reservoir. Techniques such as those used to integrate out the heat-bath variables in studies of dissipative systems[6,7] might be applied to integrate out the reservoir variables. The boundary conditions used here are perhaps a crude model, but they illustrate the essential physics of the system-reservoir interaction.

There is no dissipation due to random scattering within the device in the present model. Energy dissipation occurs through the loss of energetic electrons to the reservoirs. Local scattering approximations,[13] such as a Boltzmann collision operator, could be incorporated into the model without significantly increasing the computational effort. This has not yet been done.

In summary, a model of an open quantum system has been presented. Irreversibility is introduced into the model through boundary conditions on the Wigner function which couple the system to particle reservoirs. The model was applied to the resonant-tunneling diode and the irreversibility permited a calculation of the approach to steady state of the tunneling current after a change in the applied voltage. This transient response is a feature of tunneling devices which has not been addressed by the conventional models based upon scattering theory.[14]

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