Complex Potentials, Dissipative Processes, and General Quantum Transport

D. K. Ferry[*], J. R. Barker[**], and R. Akis[*]

[*]Department of Electrical Engineering and Center for Solid State Electronics Research
Arizona State University, Tempe, AZ 85287-5706, ferry@asu.edu
[**]Department of Electronics and Electrical Engineering, University of Glasgow
Rankine Building, Oakfield Avenue, Glasgow G12 8LT, Scotland UK

ABSTRACT

Complex potentials have been used in the past to simulate dissipative processes, but the normal form of a simple constant term of the form $i\hbar/\tau$ serves only to trap/detrap particles and does not properly introduce a process which relaxes a dynamic operator/variable [1]. We have treated a general non-Hermitian Hamiltonian operator, and have developed a modified time-dependent solution of the density matrix equation of motion. An energy-dependent phase-breaking process maintains the wave function while destroying the coherence which leads to the scar itself. In this paper, we discuss the general behavior of these complex potentials, their application to the ballistic quantum dots, and implications for trajectories and histories in the dots. The present formalism will allow the simulation of quantum transport through interfacial regions, rather than having to match boundary conditions, and this is facilitated by a proper inclusion of discontinuities at the interfaces. One can now develop a proper transport theory by using moments of the density matrix, which are valid even in the areas of strong dissipation.

INTRODUCTION

In the simulation of semiconductor devices, decoherence and phase-breaking processes become important in isolating the behavior within one device from that in adjacent devices. For large semi-classical devices, this is routinely accomplished by the use of perturbation treatments of phonon and electron scattering processes. In small devices, where the transport must be treated by fully quantum mechanical approaches, the introduction of the phase-breaking process is much more problematic. As an example, consider a prototypical device as an active region of length L, bounded by two *contact transition* regions in which the electrons must lose their coherence completely so that the actual contacts can be considered in equilibrium. Such a device may resemble the structure of Fig. 1. The source is at the left and the drain at the right, as indicated by the two gray areas, which may be considered to be the "contacts." The areas to the left and right of the traditional active length L, are indicated here as the transition regions. One must properly introduce decoherence effects for the carriers in order to bound the device properties within the active region [2]. Yet the traditional role of assuming this is accomplished by dissipation within the contacts must be re-examined, as the assumption of equilibrium conditions in the contacts means that there must be *transition regions* as shown in the figure, and which *must now be considered part of the active device*. These regions of incoherence, although not understood in detail, provide the crucial properties of *ohmic* contacts in realistic devices.

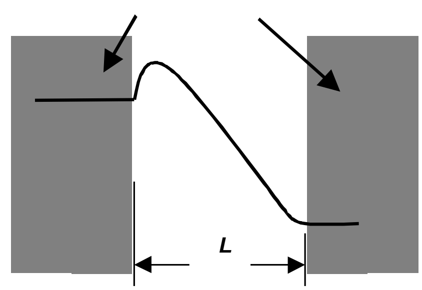

Figure 1: A conceptual device under bias.

The problem of decoherence in quantum mechanics is closely related to the problem of "localization [3]," which in turn is related to the conceptual size which can be associated with the wave function of an individual carrier [4]; that is, into how small a region of space can one concentrate an electron?. Thus, it may be expected that there is no easy, or universally accepted description of the manner in which the dissipation is introduced into small quantum devices, although a number of quantum transport approaches have been discussed for such devices [5]. Consider when the decoherence is introduced by adding an imaginary potential term to the Hamiltonian in the transition regions. The size of this potential is inversely proportional to the phase coherence lifetime τ_ϕ. For rapid decoherence, one needs a large imaginary potential which gives rapid damping of the electron wave function within the contact. *This leads to bound states in the active region.*

We have treated previously a general non-Hermitian Hamiltonian, and have developed a modified time-dependent solution of the density matrix equation of motion. This leads to decay of an arbitrary operator as [6]

$$\frac{\partial Tr\{A\tilde{\rho}\}}{\partial t}=\frac{i}{\hbar}Tr\{[H_0(t),A]\tilde{\rho}\}\,, \qquad H_0(t)=e^{\hat{H}_1 t/\hbar}\hat{H}_0 e^{-\hat{H}_1 t/\hbar}\;,\; \tilde{\rho}=e^{\hat{H}_1 t/\hbar}\rho \qquad (1)$$

(Although similar in appearance, this is *not* the interaction representation.) Additional force terms arise from the non-commutation of the complex Hamiltonian H_1 and a dynamic operator, such as momentum or energy. Here, we will discuss using this approach to study the quantum transport in ballistic quantum dots, where the latter are defined by split-gate Schottky barriers on a GaAlAs/GaAs heterostructure so that the characteristic dimension d is much less than the mean-free path. The magneto-transport of these dots is known to produce regular oscillatory behavior related to the density of states within the dots, and the wave functions show the presence of scars at particular, repetitive values of the magnetic field [7].

STRUCTURE IN BALLISTIC DOTS

A quantum dot is a confined region of a semiconductor (we deal only with semiconductors here), in which the dynamics is quantized; that is, the motion is essentially constrained in all three dimensions. In closed quantum dots, it has been possible to study the energy level structure, and therefore the oscillating density of states, by careful measurements of the tunneling current in a single-electron tunneling experiment [8]. In open quantum dots, one must carefully study the manner in which the dot states are perturbed by their interaction with the environment states. Experimentally, it is easily possible for the density of states oscillations to be retained in the presence of coupling to the outside world. Indeed, reproducible fluctuations persist across a wide range of magnetic field (but in the small field limit). In addition, the correlation function for the fluctuations is very oscillatory, and is found to be quite universal, although the specific frequency content is very dot dependent. It is quite clear that these magnetoconductance oscillations arise from the fluctuations in the density of states of the dot, which in turn are a result of the quasi-periodic orbits of the carriers inside the quantum dot, and are therefore a reflection of the intrinsic properties of the dots themselves.

Simulations of the quantum transport through a square dot of size 0.3 μm (accounting for edge depletion) also show a very periodic conductance fluctuation, even with an assumed phase breaking time of 0.2 ns [7]. Several "resonances" are seen in the magnetoconductance, and these are accompanied by very heavy scarring of the wave function. An example of the scarring is shown in Fig. 2. However, it is apparent that the wave function does not reach the walls of the dot (where it must vanish), so that the Dirichlet boundary conditions apparently also affect the "real" size of the dot quantum mechanically. The brighter areas in the figure are the regions where the wave function has its relative maxima. *It is important to note that the appearance of the scar has the same periodicity in magnetic field as the oscillations in magnetoconductance that are seen in experiment.*

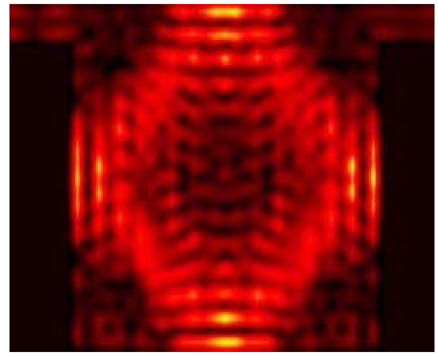

Figure 2: Wave function scar in a 0.3 μm dot.

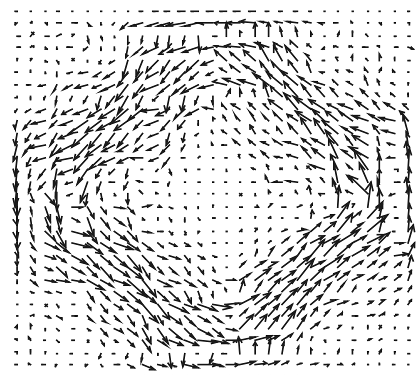

Figure 3: The current in the dot for the scar condition.

In Fig. 3, we plot the current streamlines corresponding to the scar of Fig. 2. It is clear that this is a high angular momentum state, with the current following the peaks of the wave function in the scarred state. One may also see that there is little contribution from the corners of the structure, which may explain why rounding of these corners has little effect on the conductance itself [9]. We return to this point later.

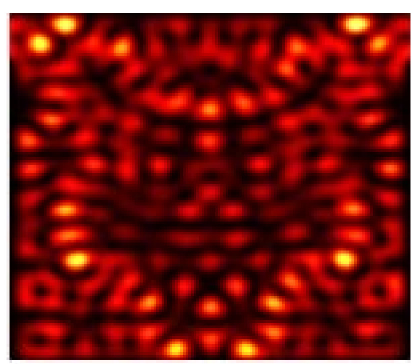

Figure 4: Wave function amplitude for a 7.7 mT shift in magnetic field.

In Figs. 4 and 5, we plot the equivalent wave function and current, respectively, for a shift of the magnetic field of 7.7 mT (to 0.265 T from 0.2727 T). Here, the scar is broken up, but one can still see relative peaks in the wave function, and the current clearly shows remnants of the circulating current. However, the corners are now filled with more circulating components, with a high vorticity. It seems clear that the circulating components in the corners still do not contribute to the conductance.

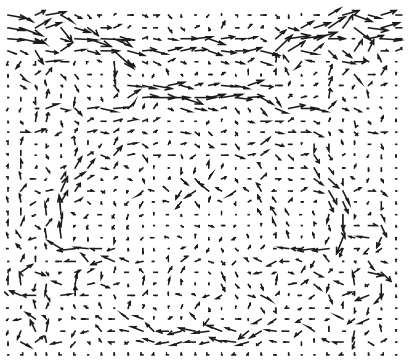

Figure 5: Current streamlines for Fig. 4.

ENERGY DEPENDENT DISSIPATION

In eqn. (1), several different possible forms of dissipation are possible, which correspond to the actual relaxation of real physical properties. Here, we want to discuss an energy relaxation (or phase breaking as it is often referred to in the mesoscopic community). For this, we introduce a component of the Hamiltonian described by

$$i\alpha p^2 / 2m^* \quad . \tag{2}$$

This is a complex Hamiltonian, which is a function of the momentum operator. Here, we use a value of α which gives an average energy relaxation time of 3.5 ps. In Fig. 6, we plot the wave function of the quantum dot at the magnetic field at which the scarred wave function of Fig. 2 occurs. It is clear that the scar is broken up, which eases the relaxation process. However, even with this very large damping there is residual evidence of the presence of the scar which clearly shows its stable nature. The method by which this relaxation occurs is more clear when we plot the current streamlines, which are shown in Fig. 7. The normal circulating current, for the case of Fig. 3, is broken into eddies which facilitates the relaxation process. (The Fermi energy is 14.7 meV in all cases.)

A careful examination of the streamlines of Fig. 7 reveals the presence of significant vortex activity, with directions both aligned with the magnetic field and counter to it. While the present simulations are not self-consistent, and use hard wall boundary conditions, fully self-consistent solutions have been done without the heavy energy relaxation term, and yield essentially equivalent results [10,11]. However, these self-consistent calculations were performed using a linear density approximation for exchange and correlation, which may not be adequate.

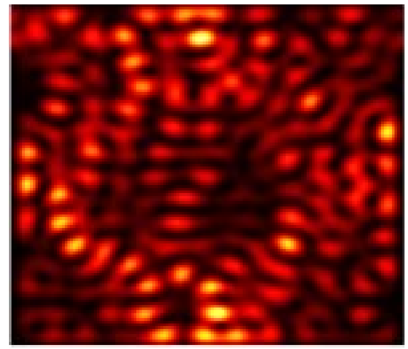

Figure 6: Magnitude of the wave function for a large energy relaxation process present.

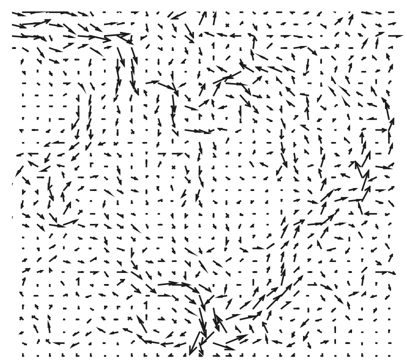

Figure 7: Current streamlines for the case of Fig. 6.

One problem,which we have addressed earlier [2], is to properly incorporate the single-valuedness of the wave function. The *velocity* is normally described from $\mathbf{v} = \nabla S / m$, where S is the action in the phase of the wave function, and the periodic nature of S leads to the well-known EBK quantization

$$\oint \mathbf{v} \cdot d\mathbf{r} = lh / m \quad , \tag{3}$$

where l is an integer. In classical hydrodynamics, the integral on the left is known as the velocity circulation, and is related through Stoke's theorem to the vorticity of the motion. There is a conservation theorem that makes the vorticity constant, *except at boundaries, in shocks, or in scattering processes.* The latter of course is occuring here. Nevertheless, systems in which quantization occurs cannot be treated as irrotational systems, irrespective of the presence of any magnetic field. When the magnetic field is present, however, the additional presence of the vortices in the current streamlines, clearly present in Figs. 5 and 7, means that there will be an additional component of the exchange and correlation energy that has its source in the vector potential [12, 13]. Such an effect can be expected to strongly impact the self-consistent potential in quantum dots with such strong vortex effects as we see here.

CONCLUSIONS

We have discussed a new formulation of incorporation of dissipation in quantum transport simulations, and have demonstrated its efficacy with studies of the scarring in ballistic quantum dots. We find that introduction of an energy relaxation process leads to breakup of current paths into vortices in which dissipation is more easily accomplished within the dot.

This work has been supported in part by the Office of Naval Research and the Defense Research Projects Agency. The authors would like to express their appreciation for helpful discussions with D. Vasileska, J. P. Bird, and H. L. Grubin.

REFERENCES

[1] See, e.g., G. A. Baraff, Phys. Rev. B **58**, 13799 (1998).

[2] D. K. Ferry and J. R. Barker, VLSI Design **8**, 165 (1998).

[3] D. Giulini *et al*., “Decoherence and the Appearance of a Classical World in Quantum Theory,” Springer, 1996.

[4] D. K. Ferry and H. L. Grubin, *in* Proc. 6th International Workshop on Computational Electronics, Osaka, IEEE Press—98EX116, 84-87, 1998.

[5] D. K. Ferry and H. L. Grubin, in *Solid State Physics*, Vol. 49, Ed. by H. Ehrenreich and F. Spaepen, Academic Press, 283-448, 1995.

[6] D. K. Ferry and J. R. Barker, Appl. Phys. Lett **74**, 582 (1999).

[7] R. Akis, D. K. Ferry, and J. P. Bird, Phys. Rev. B **54**, 17705 (1996).

[8] P. L. McEuen, E. B. Foxman, U. Meirav, M. A. Kastner, Y. Meir, N. S. Wingreen, and S. J. Wind, Phys. Rev. Lett. **66**, 1926, (1991).

[9] R. Akis, D. K. Ferry, and J. P. Bird, Jpn. J. Appl. Phys. **36**, 3981 (1997).

[10] R. Akis, D. Vasileska, D. K. Ferry, J. P. Bird, Y. Okubo, Y. Ochiai, K. Ishibashi, Y. Aoyagi, and T. Sugano, Physica B **249**, 368 (1998).

[11] R. Akis, D. Vasileska, D. K. Ferry, and J. P. Bird, J. Physics: Cond. Matt., *in press*.

[12] G. Vignale and M. Rasolt, Phys. Rev. B **37**, 10685 (1988).

[13] O. Steffens, M. Suhrke, and U. Rössler, Europhys. Lett. **44**, 222 (1998).