Contact-Induced Decoherence in Nanodevices

I. Knezevic

Department of Electrical and Computer Engineering,

University of Wisconsin-Madison,

Madison, WI 53706, USA

email: knezevic@engr.wisc.edu

Abstract

The active region of a ballistic nanodevice is an open system, evolving nonunitarily due to the coupling with contacts. In this work, a simple theoretical description of the contact-induced decoherence is presented. The active region–contact interaction Hamiltonian introduced here captures the continuous spectrum of a nanostructure's active region and models carrier injection through the open boundaries. Markovian nonunitary evolution of the active region's many-body density matrix is derived by coarse-graining of the exact non-Markovian short-time dynamics over the energy relaxation time of the bulk-like contacts. On the example of a resonant-tunneling diode, the nonequilibrium steady-state populations of the forward and backward propagating states are obtained at any given bias by using the Markovian evolution, and the resulting I–V curve exhibits all the prominent resonant features.

Keywords: decoherence, quantum transport, open system, contacts, resonant-tunneling diode, Markovian dynamics, nanodevice, nanostructure, ballistic transport

to appear in JCE, special issue: IWCE-12

I. INTRODUCTION

Relaxation towards a steady state in a nanoscale, quasiballistic electronic structure cannot be described by the semiclassical Boltzmann equation [1], because the structure's active region is smaller than the carrier mean free path and efficient scattering no longer governs relaxation. Significant efforts have been aimed at establishing a quantum-transport description of the transient regime in nanostructures, usually by employing the (single-particle) density matrix [2–4], Wigner function [5–8], or (real-time) nonequilibrium Green's function [9, 10] techniques. It is generally accepted that the active region of a nanostructure behaves an open quantum-mechanical system [11, 12], exchanging particles and information with the reservoirs of charge (usually referred to as leads or contacts), in which the carrier density is high and dephasing due to electron-electron interaction happens very rapidly [13].The description and manipulation of the contact-induced coherence loss are presently of great importance in mesoscopic physics [14–17], theory of measurement [18], and quantum information [19].

The purpose of this paper is to provide a simple description of the nonunitary evolution (decoherence) of a ballistic nanostructure's active region due to the injection of carriers from the contacts, starting from first principles (a model active region–contact interaction) and working within the framework of the open systems theory [20]. Carrier injection is traditionally described by either an explicit source term, such as in the Wigner function [8] and Pauli equation [21] transport formalisms, or via a special self-energy term in the ubiquitous nonequilibrium Green's function formalism [22–25]. In this work, the injection of carriers is described through a novel model active region–contact interaction Hamiltonian that accounts for the open boundaries and continuous spectrum of the active region. This new interaction Hamiltonian supplants the resonant-level model [9], commonly used for tunneling structures, but inapplicable away from the resonances or for structures with no resonances at all, such as an *nin* diode or the channel of a MOSFET. With the introduced interaction Hamiltonian, the active region's dynamics in the presence of the contacts is described within the framework of the open system's theory, by tracking the evolution of the active region's many-body reduced density matrix [20]. On timescales coarser than the energy relaxation time of the contacts, a completely positive Markovian evolution for the active region, derived by coarse graining of the exact non-Markovian short-time dynamics

[26, 27], is appropriate. The system used to illustrate the results is a two-barrier tunneling structure, the resonant-tunneling diode (RTD), but the method is applicable to structures without resonances, which is one of its novel features. For a given applied bias, we apply the Markovian evolution to identify the nonequilibrium steady state, in which the occupations of the forward and backward propagating states are found to depend only on the biasing conditions and the resulting single-particle transmission and reflection. The expression for the steady-state current obtained is closely related to the Landauer formula, but captures the strongly nonlocal nature of tunneling. The RTD I–V curve obtained displays all the prominent resonant features. The presented model explicitly provides the ballistic limit of the active region's density matrix away from equilibrium, a starting point onto which scattering can be added perturbatively.

II. MARKOVIAN EVOLUTION IN THE PRESENCE OF "MEMORYLESS" CONTACTS

In general, the many-body reduced density matrix ρ of the active region has a complicated nonunitary evolution due to the coupling with contacts [20, 28]. Within the contacts, the electron-electron scattering resets the distribution function back to the Fermi-Dirac one within the contacts' energy relaxation time τ, which is of order $10^1 - 10^2$ fs [13], depending on the doping density. Consequently, on timescales coarsened over τ, the contacts appear "memoryless", and therefore a Markovian (exponentially decaying) approximation of the following form is applicable to the evolution of the active region's many-body density matrix ρ [26, 27]:

$$\frac{d\rho}{dt} = (-i\mathcal{L}_{\text{eff}} - \Lambda\tau)\,\rho(t). \tag{1}$$

Here, $\mathcal{L}_{\text{eff}} = \mathcal{L} + [\langle\mathcal{H}_{\text{int}}\rangle, \dots]$ is an effective Liouville superoperator of the active region, containing the noninteracting part $\mathcal{L}$ and a correction due to the contact–active region interaction $\mathcal{H}_{\text{int}}$: $\langle\mathcal{H}_{\text{int}}\rangle = \text{Tr}_C[\rho_C\mathcal{H}_{\text{int}}]$, where ρ_C is the equilibrium (left+right) contact density matrix. Superoperator Λ is essential for the description of coherence loss: certain subspaces of its null-space $\mathcal{N}(\Lambda)$ are decoherence-free [26], and, regardless of τ, the steady state must belong to $\mathcal{N}(\mathcal{L}_{\text{eff}}) \cap \mathcal{N}(\Lambda)$, the intersection of the null-spaces of $\mathcal{L}_{\text{eff}}$ and Λ. Λ is

determined by the interaction Hamiltonian as

$$\Lambda^{\alpha\beta}_{\alpha'\beta'} = \frac{1}{2}\Big\{\langle\mathcal{H}^2_{\rm int}\rangle^{\alpha}_{\alpha'}\,\delta^{\beta'}_{\beta} + \langle\mathcal{H}^2_{\rm int}\rangle^{\beta'}_{\beta'}\,\delta^{\alpha}_{\alpha'} \\ -2\sum_{j,j'}(\mathcal{H}_{\rm int})^{j'\alpha}_{j\alpha'}\,\rho^{j}_{C}\,(\mathcal{H}_{\rm int})^{j\beta'}_{j'\beta} - \big(\langle\mathcal{H}_{\rm int}\rangle^2\big)^{\alpha}_{\alpha'}\,\delta^{\beta'}_{\beta} \\ +2\,\langle\mathcal{H}_{\rm int}\rangle^{\alpha}_{\alpha'}\langle\mathcal{H}_{\rm int}\rangle^{\beta'}_{\beta} - \big(\langle\mathcal{H}_{\rm int}\rangle^2\big)^{\beta'}_{\beta}\,\delta^{\alpha}_{\alpha'}\Big\}. \tag{2}$$

III. EXAMPLE: THE RESONANT-TUNNELING DIODE

For the resonant-tunneling diode, our goal is to obtain the nonequilibrium steady-state ρ from Eq. (1) under any given bias V, and use this information to construct the I–V curve. The GaAs/AlGaAs RTD considered in this example has a well width of 3 nm, barrier thickness of 5 nm, and a barrier height of 0.3 eV. The Fermi level in the contacts is at 0.1 eV, while the equilibrium bound state is at 0.15 eV. The active region of the RTD has naturally open boundaries and continuous single-particle spectrum. For any given energy $\mathcal{E}_k = \hbar^2k^2/2m$ above the bottom of the higher, negatively biased contact (the injector contact), the forward and backward propagating states, Ψ_k and Ψ_{-k}, respectively, can be obtained by solving the single-particle Schrödinger equation for an assumed potential profile. Here, for simplicity, we will assume that the potential drops linearly across the well and barriers (more on achieving a self-consistent solution will be discussed below). Near the injector contact $\Psi_k(x) = e^{ikx} + r_{-k,L}e^{-ikx},\ \Psi_{-k}(x) = t_{-k,L}e^{-ikx}$, while near the collector $\Psi_k(x) = t_{k',R}e^{ik'x},\ \Psi_{-k}(x) = e^{-ik'x} + r_{k',R}e^{ik'x}$. Here, t's and r's are the transmission and reflection amplitudes, and k and k' are the wavevectors in the injector and collector contact, respectively, that correspond to the same energy: $k^2 = k'^2 - 2meV/\hbar^2 = 2m\mathcal{E}_k/\hbar^2$. Associated with Ψ_k (Ψ_{-k}) in the active region are the creation and destruction operators $d^\dagger_k$ and d_k ($d^\dagger_{-k}$ and d_{-k}), so the active region many-body Hamiltonian is $\mathcal{H}_S = \sum_{k>0}\omega_k(d^\dagger_k d_k + d^\dagger_{-k}d_{-k})$. (Spin is disregarded, and $\omega_k = \mathcal{E}_k/\hbar$.)

In order to account for the open boundaries and continuous spectrum of the RTD active region, a novel model interaction Hamiltonian is introduced to supplant the resonant-level model [10] that is inapplicable away from the resonant conditions or for nanostructures without resonances. The coupling between the forward propagating states in the active

region and the two contacts is modeled as

$$\mathcal{H}_{\rm int}^{\rm fwd} = \sum_{k>0} \Delta_k \Big\{ \left(c_{k,L} + \mathcal{R}_k c_{-k,L}\right) d_k^\dagger + h.c. \\ + \mathcal{T}_k c_{k',R}^\dagger d_k + h.c. \Big\}. \quad (3)$$

$c_{k,L}^\dagger$ ($c_{k,L}$) and $c_{k',R}^\dagger$ ($c_{k',R}$) create (destroy) an electron with a wavevector k in the left and k' in the right contact, respectively, while $\mathcal{R}_k$ and $\mathcal{T}_k$ are the reflection and transmission coefficient at a given energy, satisfying $\mathcal{R}_k + \mathcal{T}_k = 1$. The model interaction captures injection from the contacts: namely, the coupling coefficient Δ_k in (3) is the rate of injection of carriers with momentum $\hbar k$ from the left contact into the active region, i.e., it is proportional to the current injected into the state Ψ_k by the hopping of one electron: $\Delta_k = \hbar k/m \|\Psi_k\|^2$, where $\|\Psi_k\|^2 = \int_0^W dx |\Psi_k(x)|^2 dx$ is the norm squared of Ψ_k over the active region of width W. Similarly, the coefficient multiplying $c_{-k,L} d_k^\dagger$ is the rate of reflection, proportional to the reflected current and thus equal to $\mathcal{R}_k \Delta_k$, while the coefficient multiplying $c_{k'}^\dagger d_k$ is the rate of transmission, equal to $\mathcal{T}_k \Delta_k$. The Hamiltonian for the backward propagating states can be written in an analogous fashion. Furthermore, we will assume that bias is swept slowly (so that between two bias points the system is allowed to relax) and in small increments (so that the transmission and reflection coefficients and the barrier profile do not change much between two bias points, and can be regarded constant during each transient). For the Markovian map (1) to be valid, we should have $\|\mathcal{L}_{\rm eff}\| \gg \|\Lambda\|\tau$, which basically yields $\Delta_k^2 \tau \ll \omega_k$. By approximating $\|\Psi_k\|^2 \approx W$, we obtain $2\hbar\tau/m \ll W^2$, which will be satisfied for $\tau \approx$10 fs (appropriate for contact doping of about 10^{20}cm^{-3}), in GaAs-based structures whose active region is longer than a few nanometers.

Both $\mathcal{L}$ and Λ in (1) are sums of independent contributions over individual modes [e.g., $\Lambda = \sum \Lambda_k$] that attack only single-particle states with a given k. Consequently, we are dealing with a multitude of two-level problems [26], one for each state Ψ_k, where the two levels are a particle being in Ψ_k ("+") and the particle being absent from Ψ_k ("-"). Each such 2-level problem is cast on its own 4-dimensional Liouville space, with $\rho_k = \left(\rho_k^{++}, \rho_k^{+-}, \rho_k^{-+}, \rho_k^{--}\right)^{\rm T}$ being the reduced density matrix that describes the occupation of Ψ_k. $\rho_k^{++} = f_k(t)$ and $\rho_k^{--} = 1 - f_k(t)$, where f_k is the distribution function for the active region states. According to (1),

$$\frac{d\rho_k}{dt} = \left(-i\mathcal{L}_k - \Lambda_k \tau\right) \rho_k, \quad (4)$$

where

$$\mathcal{L}_k = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 2\omega_k & 0 & 0 \\ 0 & 0 & -2\omega_k & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{5a}$$

$$\Lambda_k = \begin{bmatrix} A_k & 0 & 0 & -B_k \\ 0 & C_k & 0 & 0 \\ 0 & 0 & C_k & 0 \\ -A_k & 0 & 0 & B_k \end{bmatrix}. \tag{5b}$$

Here $A_k = \Delta_k^2\{(1+\mathcal{R}_k^2)(1-f_k^L) + \mathcal{T}_k^2(1-f_{k'}^R)\}$, $B_k = \Delta_k^2\{(1+\mathcal{R}_k^2)f_k^L + \mathcal{T}_k^2 f_{k'}^R\}$, and $C_k = \Delta_k^2\left(1+\mathcal{R}_k^2+\mathcal{T}_k^2\right)/2$, while f_k^L and $f_{k'}^R$ are the equilibrium distribution functions in the left and right contact, respectively. Clearly, $\rho_k^{+-} = \rho_k^{-+} = 0$ in the steady state. From the two equations for ρ_k^{++} and ρ_k^{--} we obtain $\frac{df_k(t)}{dt} = -\tau A_k f_k(t) + \tau B_k[1-f_k(t)] = -\tau(A_k + B_k)f_k(t) + \tau B_k$ (for $-k$, by analogy). Finally, the distribution functions in the steady state are

$$f_k^\infty = \frac{f_k^L(1+\mathcal{R}_k^2) + f_{k'}^R\mathcal{T}_k^2}{1+\mathcal{R}_k^2+\mathcal{T}_k^2}, \tag{6a}$$

$$f_{-k}^\infty = \frac{f_{k'}^R(1+\mathcal{R}_k^2) + f_k^L\mathcal{T}_k^2}{1+\mathcal{R}_k^2+\mathcal{T}_k^2}. \tag{6b}$$

In equilibrium, $f_k^\infty = f_{-k}^\infty = f_k^L = f_k^R$, but away from equilibrium, $f_k^\infty \to f_k^L$ and $f_{-k}^\infty \to f_{k'}^R$ only if the transmission is low; a transmitting nanostructure feels the distribution functions in both contacts. The discontinuity of the distribution functions across each open boundary is a price to pay to conserve the flux across it, the same as in the heuristic treatment of carrier injection in the density matrix, Wigner function, and Pauli equation formalisms (see the discussion on p. 4907 of Ref. [**?**]).

The current (per spin orientation) involves a sum over all forward and backward propagating states, and is given by

$$I^\infty = \frac{eW}{h}\int_0^\infty d\mathcal{E}_k \left(\frac{f_k^\infty}{\|\Psi_k\|^2} - \frac{f_{-k}^\infty}{\|\Psi_{-k}\|^2}\right)\mathcal{T}_k. \tag{7}$$

(This expression is effectively independent of W, as $\|\Psi_{\pm k}\|^2$ scale with W.) Figure 1 shows the I–V curve of the RTD, as calculated according to the expression (7) and the Landauer

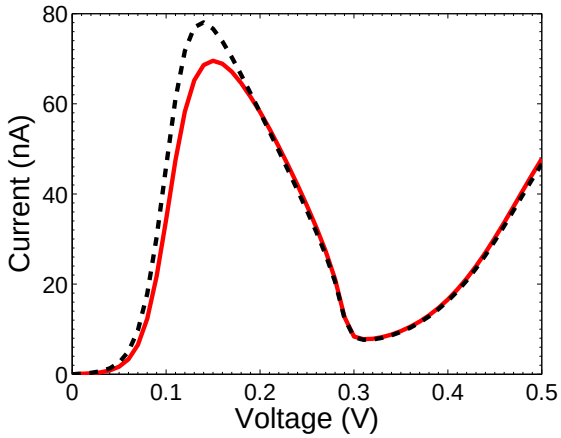

FIG. 1: I–V curve according to the expression (7) (solid curve) and the Landauer formula (dashed curve) at 77 K.

formula for the current per spin orientation $I^{\infty}_{\rm Lan} = \frac{e}{h}\int_0^{\infty} d\mathcal{E}_k \ \left[f^L_k - f^R_{k'}\right]\mathcal{T}_k$. As stated before, for simplicity, the voltage is assumed to drop linearly across the well and barriers. In general, Eqs. (6) need to be coupled with a Poisson and a Schrödinger solver to obtain a realistic potential profile and charge distribution: f's are used to calculate the charge distribution, which is fed into the Poisson solver that yields the potential profile, which is in turn needed to solve the single-particle Schrödinger equation and obtain $\mathcal{R}_k$'s and $\mathcal{T}_k$'s needed to recalculate f's (6). Both curves in Fig. 1 describe ballistic transport, so they do not cross like the curves with and without inelastic scattering do [8]. However, the Landauer formula predicts a lower peak voltage and higher peak current than (7). The difference comes from the fact that (7) captures the pronounced nonlocal nature of tunneling: f^{∞}_k and f^{∞}_{-k} coincide with the contact distributions f^L_k and $f^R_{k'}$, respectively, only if the transmission is low; otherwise, a transmitting nanostructure feels the Fermi distributions in both contacts.

IV. CONCLUSION

A simple theoretical description of the contact-induced decoherence in nanostructures was provided within the framework of the open systems theory. The model active region – contact interaction ensures proper carrier injection from the contacts. The steady-state density matrix of the active region was calculated by relying on the Markovian map derived

through coarse graining of the exact short time dynamics over the energy relaxation time of the bulk-like contacts. On the example of the RTD, an I–V curve that displays the prominent resonant features was obtained based on the nonequilibrium steady-state density matrix obtained for any given bias. The presented model provides the ballistic limit of the active region's nonequilibrium density matrix, and can further be built on to include the electron-electron interaction (both within the active region and between the active region and the contacts), as well as inelastic scattering due to optical phonons.

Acknowledgment

This work has been supported by the NSF, award ECCS-0547415.

---

[1] C. Jacoboni and L. Reggiani, Rev. Mod. Phys. **65**, 645 (1983).

[2] R. Brunetti, C. Jacoboni, and F. Rossi, Phys. Rev. B **39**, 10781 (1989).

[3] E. Ciancio, R. C. Iotti, and F. Rossi, Phys. Rev. B **69**, 165319 (2004).

[4] G. Platero and R. Aguado, Phys. Rep. **395**, 1 (2004).

[5] N. C. Kluksdahl, A. M. Kriman, D. K. Ferry, and C. Ringhofer, Phys. Rev. B **39**, 7720 (1989).

[6] L. Shifren, C. Ringhofer, and D. K. Ferry, IEEE Trans. Electron Devices **50**, 769 (2003).

[7] C. Jacoboni, R. Brunetti, and S. Monastra, Phys. Rev. B **68**, 125205 (2003).

[8] M. Nedjalkov, H. Kosina, S. Selberherr, C. Ringhofer, and D. K. Ferry, Phys. Rev. B **70**, 115319 (2004).

[9] N. S. Wingreen, A.-P. Jauho, and Y. Meir, Phys. Rev. B **48**, 8487 (1993).

[10] A.-P. Jauho, N. S. Wingreen, and Y. Meir, Phys. Rev. B **50**, 5528 (1994).

[11] W. Pötz, J. Appl. Phys. **66**, 2458 (1989).

[12] W. R. Frensley, Rev. Mod. Phys. **62**, 745 (1990).

[13] M. A. Osman and D. K. Ferry, Phys. Rev. B **36**, 6018 (1987).

[14] H. L. Grubin and D. K. Ferry, Semicond. Sci. Tech. **13 (8A), Suppl. S**, A44 (1998).

[15] D. K. Ferry, R. Akis, J. P. Bird, M. Elhassan, I. Knezevic, C. Prasad, and A. Shailos, J. Vac. Sci. Technol. B **21**, 1891 (2003).

[16] I. Knezevic and D. K. Ferry, Superlatt. Microstruct. **34**, 367 (2003).

[17] R. Gebauer and R. Car, Phys. Rev. Lett. **93**, 160404 (2004).

[18] W. H. Zurek, Rev. Mod. Phys. **75**, 715 (2003).

[19] L.-A. Wu, D. A. Lidar, and M. Friesen, Phys. Rev. Lett. **93**, 030501 (2004).

[20] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).

[21] M. V. Fischetti, J. Appl. Phys. **83**, 270 (1998).

[22] R. Lake, G. Klimeck, R. C. Bowen, and D. Jovanovic, Phys. Rev. B **81**, 7845 (1997).

[23] S. Datta and M. P. Anantram, Phys. Rev. B **45**, 13761 (1992).

[24] A. Svizhenko, J. Appl. Phys. **91**, 2324 (2002).

[25] D. Mamaluy, D. Vasileska, M. Sabathil, T. Zibold, and P. Vogl, Phys. Rev. B **71**, 245321 (2005).

[26] I. Knezevic, J. Comput. Theor. Nanosci. **4**, 749 (2007).

[27] I. Knezevic, submitted for publication .

[28] I. Knezevic and D. K. Ferry, Phys. Rev. A **69**, 012104 (2004).