DYNAMICAL TRANSPORT MODEL OF A COUPLED ELECTRON-PHONON SYSTEM IN A QUANTUM WIRE

Julie A. Kenrow and T. Kenneth Gustafson
Department of Electrical Engineering and Computer Sciences
University of California, Berkeley, CA 94720

Abstract

A model has been developed for studying the effect of the electron-polar optical phonon interaction on electron transport in a GaAs/$Al_xGa_{1-x}As$ rectangular quantum wire system. The objective of this work is to investigate electron transport in ultra-submicron devices for which the inverse scattering rate can be on the order of the transit time. We solve the 3D, time-dependent Schrödinger equation non-perturbatively for the time evolution of the wavefunction of the coupled electron-LO and -SO phonon sytem. The time evolution of the mean electron momentum and directed energy are presented as a function of initial directed electron energy and applied voltage between the ends of the wire. Comparisons are made to semi-classical Monte Carlo results which are shown to significantly overestimate the amount of scattering on 100 fs time scales.

I. INTRODUCTION

The emerging capabilities in nanoscale electronic device fabrication have spurred the development of fully quantum mechanical electron transport models in semiconductors. Two important aspects of electron transport in nanoscale devices that necessitate a quantum treatment are confinement in one or more dimensions and ultra-short (i.e., sub-picosecond) transit times. To correctly model electron transport under conditions where transit times are comparable to mean free collision timess ($\sim$ 100 fs), a dynamical treatment of the electron-phonon interaction should be incorporporated. This precludes the common treatment of electron-phonon scattering based upon the use of predetermined Fermi's Golden Rule (FGR) obtained scattering rates. A dynamical treatment requires a quantum mechanical (coherent state) description for both the electron and the lattice phonons. In this paper we develop such a quantum transport model (QTM) for a quantum wire (QWI), which describes the time evolution of an electron wavepacket coupled to the non-equilibrium phonon mode spectrum. As a model problem we consider placing an electron wavepacket in a rectangular, finite length GaAs QWI surrounded by $Al_xGa_{1-x}As$, and model its time evolution as it simultaneously accelerates in response to an applied electric field, and interacts with either the confined LO or interfacial SO phonon modes.

II. QUANTUM TRANSPORT MODEL

We seek the time-dependent wavefunction $\Psi(\vec{r},t)$ of the coupled system, consisting of a single electron, and either the LO or SO polar optical lattice modes with which the electron interacts. The lattice temperature is taken to be 0 K, in order for $\Psi(\vec{r},t)$ to describe a coherent state with a well-defined initial condition. We solve the 3D time-dependent Schrödinger equation in the effective mass approximation,

$$i\hbar\frac{\partial\Psi}{\partial t} = (H_e + H_{ph} + H_{e\text{-}p})\Psi(\vec{r},t) \qquad (1)$$

where

$$H_e = -\frac{\hbar^2\nabla^2}{2m^*} + V(\vec{r}) \tag{2}$$

$$H_{ph} = \sum_q \hbar\omega_q (a_q^\dagger a_q + \tfrac{1}{2}) \ , \tag{3}$$

$V(\vec{r})$ is the potential energy for both the conduction band minimum and an externally applied voltage, and $\hbar\omega$ is the phonon energy. In (1), the interaction Hamiltonians for LO and SO phonons, appropriate for an embedded rectangular QWI, are [1]

$$H_{e\text{-}p}^{LO} = 2i\zeta \cos\left(\frac{\pi x}{\ell_x}\right)\cos\left(\frac{\pi y}{\ell_y}\right)\sum_q \frac{1}{Q}\left[a_q e^{iqz} - a_q^\dagger e^{-iqz}\right] \tag{4}$$

$$H_{e\text{-}p}^{SO} = \sum_q (-e)\,\Phi(q,x,y)\left(\frac{\hbar}{2\omega}\right)^{\frac{1}{2}}\left[a_q e^{iqz} - a_q^\dagger e^{-iqz}\right] \tag{5}$$

where $q \equiv q_z$ is the LO or SO phonon wave number corresponding to the direction of free propagation, along the wire. In this study, since we limit the transport time to 150 fs, we neglect inter-subband transitions, and assume that the electron remains in the transverse (x,y) ground state. Hence, in Eq (4), only the dominant, lowest order transverse LO phonon mode has been retained.

We write the solution $\Psi(\vec{r},t)$ as a superposition over the orthogonal basis of LO phonon number states,

$$\Psi(\vec{r},t) = \alpha(\vec{r},t)\,e^{-i\omega(N/2)t}\,|\,0\rangle + \sum_{\ell=1}^{N}\beta_\ell(\vec{r},t)\,e^{-i\omega(1+N/2)t}\,|\,1\rangle_\ell + \sum_{m=1}^{N_2}\gamma_m(\vec{r},t)\,e^{-i\omega(2+N/2)t}\,|\,2\rangle_m \ + \cdots \ , \tag{6}$$

where $|\,i\rangle_j$ represents the ith order phonon number state for the jth unique combination of phonon mode occupancies in the quantum wire, e.g.,

$|\,0\rangle = |0000...0\rangle$ — 0th order (vacuum state)

$|\,1\rangle_1 = |1000...0\rangle,\ |\,1\rangle_2 = |0100...0\rangle,\ ...$ — 1st order

$|\,2\rangle_1 = |1100...0\rangle,\ |\,2\rangle_2 = |1010...0\rangle,\ ...\ ;$ — 2nd order

$|\,2\rangle_{N_2-N+1} = |2000...0\rangle,\ ...,\ |\,2\rangle_{N_2} = |0000...2\rangle$

and where the modes span the spectrum of wavenumbers q. It follows that for a system of N modes, there are N combinations of 1st order number states and $N_2 = N(N+1)/2$ combinations of 2nd order number states. For this study, we retain terms only up through 2nd order in Eq (6). From Eqs (1)-(3), (4) or (5), and (6), the required set of coupled differential equations for the coefficients $\alpha(z,t)$, $\beta_\ell(z,t)$, $\gamma_m(z,t)$ is obtained by directly applying the Hamiltonian operators to $\Psi(\vec{r},t)$ in (6) and then equating coefficients associated with each unique number state. Previously [2], we have reported an approximate 1D solution to this problem for the LO interaction, in which the replacement $\cos(\pi x/\ell_x)\cos(\pi y/\ell_y)\rightarrow 1$ in Eq (4) was made to enable a separable solution

to Eq (1). Results for both the 1D and 3D models are presented here.

III. RESULTS AND DISCUSSION

The initial condition for $\Psi(\vec{r},0)$ is $\beta_\ell(z,0) = \gamma_m(z,0) = 0$ for all ℓ and m (corresponding to the lattice vacuum state at $T = 0$K), and

$$\alpha(\vec{r},0) = \exp[-(z-z_o)^2/2(\Delta z_i)^2 + ik_i z]\,\phi_o(x,y), \tag{7}$$

where $\phi_o(x,y)$ is the 2D ground state eigenfunction for the GaAs/Al_xGa_{1-x}As system ($x = .45$ or 1.0). The effective strength of electron-LO phonon scattering (using the 1D model and $x = .45$) as a function of electron energy is shown in Fig 1a, in which $\langle k_z\rangle_t$ is plotted for several initial directed electron energies, E_i with initial spread $\Delta k_i = 5$ x 10^7 m^{-1}, and no applied field. The initial flatness of the curves in Fig 1a is a result of the time ($\sim 1/\omega_{LO}$) required for conservation of energy. In Fig 1b, plots of $\langle k_z\rangle_t$, calculated from a semiclassical Monte Carlo Model (MCM) are shown. The MCM consists of an ensemble average over 10,000 electrons, with identical initial conditions, propagating along the wire, and interacting with the lattice by means of forward and backward scattering rates obtained from the approximate 1D LO Hamiltonian. The MCM predicts a much faster momentum relaxation since, over 150 fs, virtually all the electrons in the ensemble scatter one or more times, whereas the QTM results predict that a significant fraction of the initial electron wavepacket remains unscattered during this time period.

The effect of LO phonon scattering (using the 1D model and $x = .45$) on $\langle k_z\rangle_t$ has been studied for various electric field strengths with $E_i = 0$ and $\Delta k_i = 5$ x 10^7 m^{-1}, as shown in Fig 2a. For each field strength, the $\langle k_z\rangle_t$ curves increase linearly with time until $\langle k_z\rangle_t = k_{ph} - \Delta k_i = 2.0$ x 10^8 m^{-1}, at which time some of the electron wavenumber components begin to emit LO phonons. The corresponding results predicted by the MCM are shown in Fig 2b. Due to the singular scattering rate at the LO phonon energy of 36.2 meV, all electrons in the ensemble scatter when they reach an energy of 36.2 meV. In contrast, the QTM predicts only partial scattering of the electron wavepacket, so that the unscattered portion of the wavepacket can be accelerated (for the larger field strengths) to energies well in excess of 36.2 meV.

In Fig 3, $\langle k_z\rangle_t$ is plotted for $E_i = 50$ meV, $\Delta k_i = 5$ x 10^7 m^{-1}, and no applied field, for both $x = .45$ and 1.0, using either the 3D electron-LO or -SO Hamiltonians

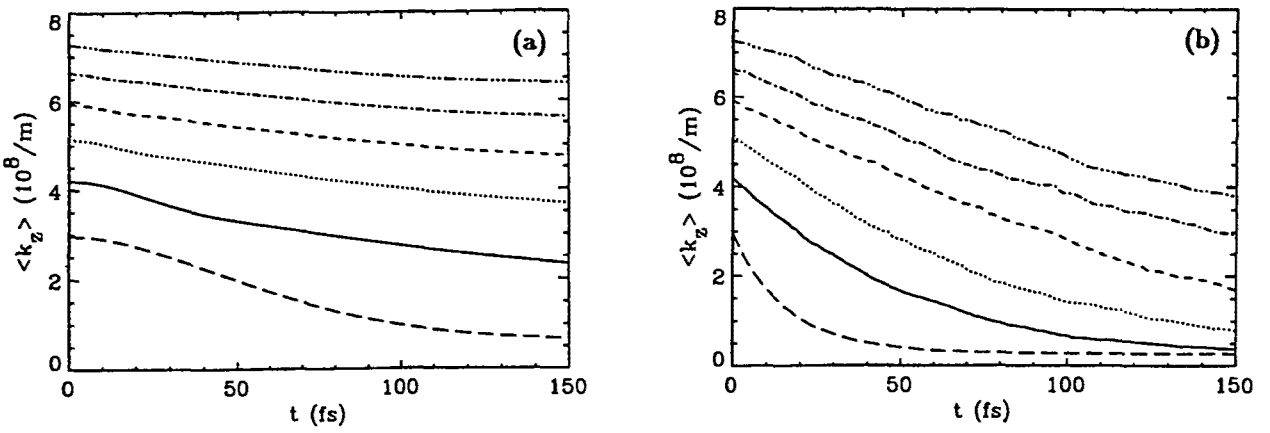

Fig. 1. $\langle k_z\rangle_t$ vs. t (a) QTM and (b) MCM for $E_i = 0.05$, 0.1, 0.15, 0.20, 0.25, 0.30 eV.

[Eqs (4)-(5)]. In agreement with published scattering rates for GaAs/AlAs quantum wires [1], the electron-LO interaction is more effective than the electron-SO interaction at dissipating the directed electron momentum. In addition to a greater interation strength for H_{LO} versus H_{SO}, the electron-LO interaction is more effective at randomizing the scattered wavevectors. This can be seen in Fig 3b, in which the electron probability density is plotted along the k_z axis at 150 fs for the cases from Fig 3a corresponding to $x = 1.0$, for each type of interaction. A large unscattered component is evident for the H_{SO} curve, and it can be seen that the forward- and back-scattered wavevector components (centered about $k_z = 0$) are much more nearly equal in magnitude for the H_{LO} curve compared to the H_{SO} curve, also in agreement with scattering rate predictions [3].

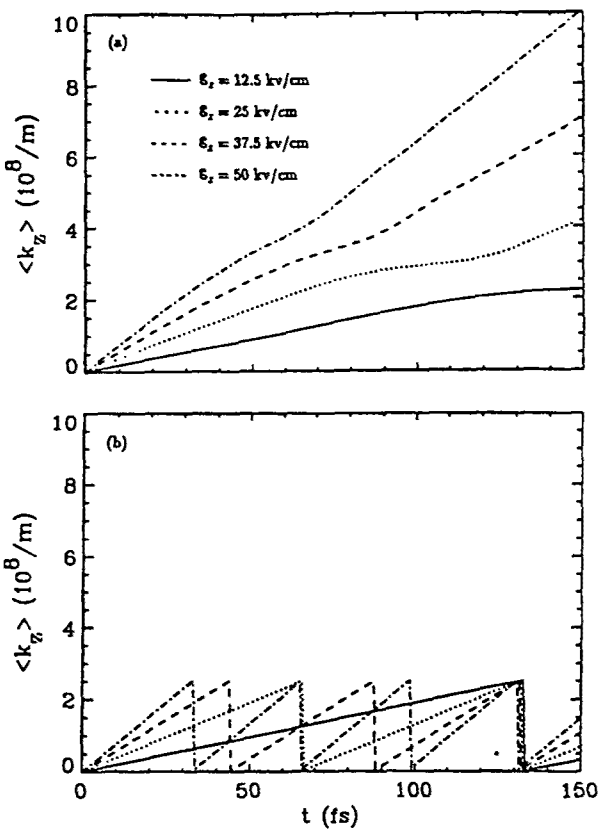

Fig. 2. $\langle k_z \rangle_t$ vs. t for $E_i = 0.0$ eV and various applied fields (a) QTM and (b) MCM.

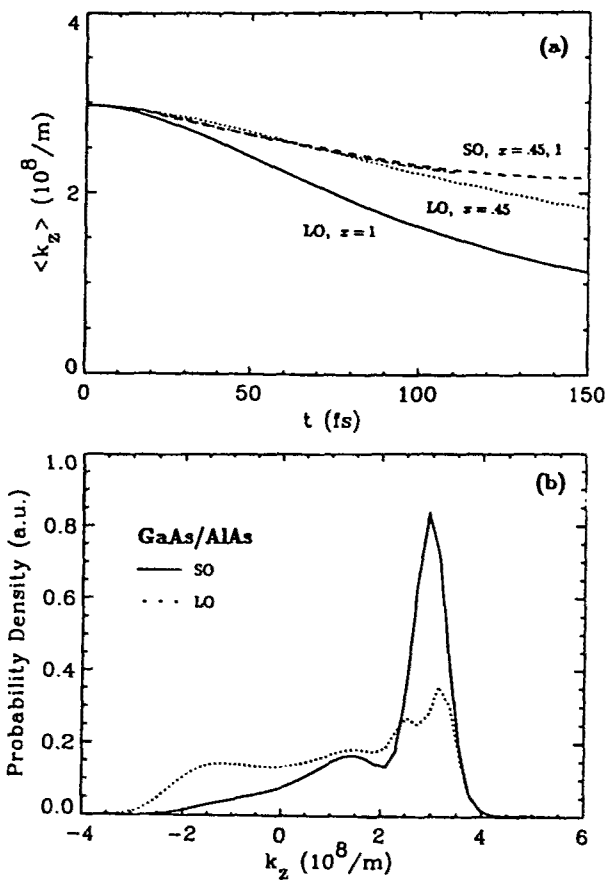

Fig. 3. (a) $\langle k_z \rangle_t$ vs. t for $E_i = 0.05$ eV. (b) Electron probability density $\rho_e(k_z, t)$ at 150 fs.

References

[1] K. W. Kim, M. A. Stroscio, A. Bhatt, R. Mickevicius, and V. V. Mitin, *J. Appl. Phys.* 70, 319 (1991).

[2] J. A. Kenrow and T. K. Gustafson, submitted for publication to *Phys. Rev. B.*

[3] R. Mickevicius, V. V. Mitin, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, *J. Phys.: Condens. Matter* 4, 4959 (1992).