A MODEL FOR THE DYNAMICAL TREATMENT OF ELECTRON-PHONON SCATTERING IN QUANTUM CONFINED STRUCTURES

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ABSTRACT

A single electron transport model incorporating the dynamical interaction of an electronic state with lattice phonon states in quantum confined structures is presented. Collisional broadening is incorporated in an algorithm for the numerical solution of the three-dimensional time-dependent Schrödinger equation via the beam propagation method. A double-sided Feynman diagrammatic approach is used to incorporate the decay rate for the diagonal components of the density matrix in a closed two-level system. These decay rates are obtained through a self-consistent solution of the Dyson equation. The damping approximation is used to factor the double-sided Feynman diagram into a product of the wave function and its complex conjugate, thus effectively decoupling these quantities to enable independent numerical solutions. By tracking the off-diagonal density matrix elements in time, quantum coherence effects can be obtained.

I. INTRODUCTION

With the decrease of characteristic device sizes to the ultra-submicron range, much effort has been generated in developing models for quantum mechanical electron transport in semiconductors. A number of different approaches have been proposed (see [1] for a recent overview), but at present no satisfactory treatment of electron-phonon interaction dynamics exists within the context of a tractable numerical model for quantum transport in a realistic device. We present an approach that solves a transient transport problem based on first principles and which includes a dynamical treatment of the electron-phonon interaction for electron transport in quantum confined structures. This approach is general enough to account for collisional broadening, intra-collisional field effects and quantum coherence.

Our technique involves numerically solving the single electron, three-dimensional, time-dependent Schrödinger equation using the beam propagation method (BPM) [2]. The electron-phonon interaction is modeled in the dipole approximation, with alternating absorption and emission (i.e., a two state density matrix) of mono-energetic phonons from a thermal bath. Collisional broadening is incorporated with the aid of double-sided Feynman diagrams [3] in conjunction with a self-consistent solution of the Dyson equation in differential form in the time domain (i.e., renormalization of the free electron propagator for the density matrix).

II. NUMERICAL SCHEME

The time dependent, three-dimensional Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$$

is solved using BPM, in which the wave function $\Psi(\mathbf{r},t)$ is advanced in time by an amount Δt according to

$$\Psi(\mathbf{r},\, t+\Delta t) = PQP\Psi(\mathbf{r},\, t) + O[(\Delta t)^3]$$

where

$$P = \exp\Big(-\frac{iH_o}{\hbar}\frac{\Delta t}{2}\Big) \tag{1}$$

$$Q = \exp\Big[-i/\hbar \int_t^{t+\Delta t} H'(t')\, dt'\Big] \tag{2}$$

$$H_o = -\hbar^2\nabla^2/2m^*$$

$$H' = H_{bias} + H_{c-band} + H_{el-ph}$$

In (1), the operator P applied to $\Psi(\mathbf{r},t)$ is equivalent to solving the unperturbed Schrödinger equation over a time interval $\Delta t/2$. This step in the solution can be obtained using a band-limited Fourier series for $\Psi(\mathbf{r},t)$. This numerical procedure is done efficiently and accurately using the fast Fourier transform (FFT) algorithm. The Q operation is applied, by simple multiplication, causing a change in the phase factor at $\Delta t/2$ due to the influence of the conduction band potential and perturbed Hamiltonian. This is followed by a second P operation to evaluate the wave function Ψ after the full-step propagation time Δt. This routine is then continued over subsequent Δt time steps.

III. TREATMENT OF THE ELECTRON-PHONON INTERACTION

The electron-phonon interaction in the dipole approximation is given by

$$H_{el-ph} = \sum_q V_q(a_q e^{i\vec{q}\cdot\vec{r}} + a_q^+ e^{-i\vec{q}\cdot\vec{r}})\, e^{i\omega_q t}$$

where V_q is the electron-phonon coupling strength, and a_q (a_q^+) is the annihilation (creation) operator of a phonon with mode $\mathbf{q}$. In the present study, only single phonon processes with energy $\hbar\omega_q$ are considered.

Collisional broadening, intra-collisional field effects, and quantum coherence can all be accounted through first principles using a diagrammatic technique for the density matrix. The double-sided Feynman diagram in Fig. 1 illustrates the dominant time ordering of the electron-phonon interactions associated with the density matrix for a closed two-level system. In Fig. 1, the initial state at time t_o corresponds to the ground state, ρ_{11}. From t_o to t, the electron propagates, absorbs a phonon ω_q, propagates further, and then emits a phonon ω_q, returning to the state ρ_{11}. This propagate, interact, propagate, interact, etc., scheme corresponds exactly to the BPM algorithm ($PQPQ...$).

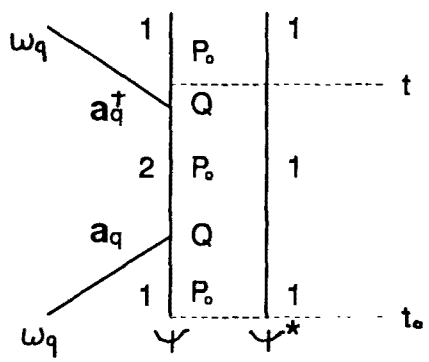

Figure 1

Collisional broadening is naturally accounted for by renormalization of the diagonal components of the density matrix free electron propagator due to the absorption and emission of phonons. This renormalization is accomplished by summing up all the diagrammatic contributions to infinite order for the *exact* propagator for state ρ_{11} as shown in Fig. 2 (For the closed system considered here, $\mathrm{tr}(\rho) = 1$, hence $\rho_{22} = 1 - \rho_{11}$). In k-space, the exact propagator P_T, can be written as

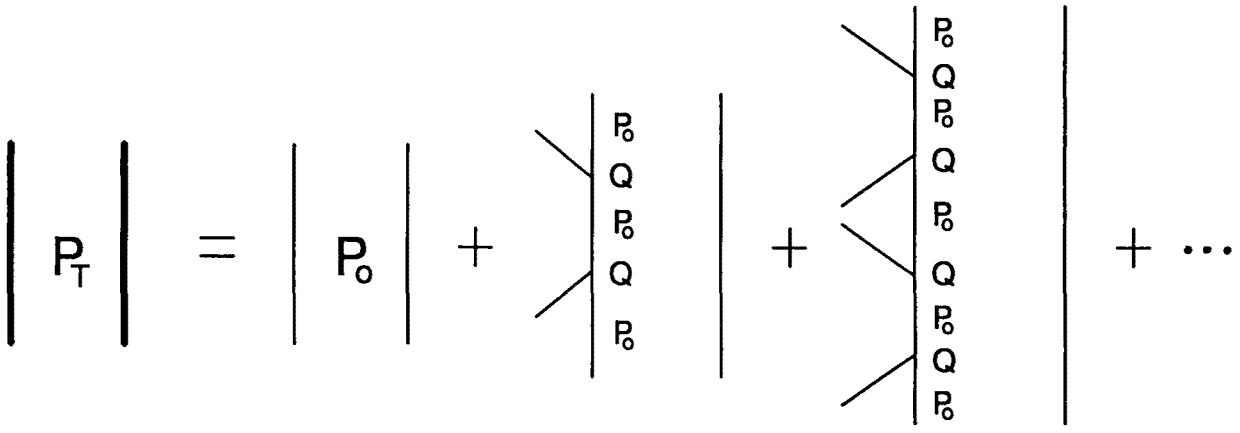

Figure 2

$$\begin{aligned} P_T &= P_o + P_o Q P_o Q P_o + P_o Q P_o Q P_o Q P_o Q P_o + \cdots \\ &= P_o + P_o[Q P_o Q\{P_o + P_o Q P_o Q P_o + \cdots\}] \\ &= P_o + P_o Q P_o Q P_T \end{aligned}$$

Solving for P_T yields the Dyson equation

$$P_T = \frac{P_o}{1 - P_o Q P_o Q} \tag{3}$$

where

$$Q = \frac{V_q}{\hbar}\Delta t$$

$$P_o(\Delta t) = \exp\left[\frac{\mathrm{i}}{\hbar}\frac{\hbar^2 k^2}{2m^*}\Delta t\right]$$

and where both P_o and P_T are propagators for a timestep Δt. The self-energy operator QP_oQ in (3) leads to an exponential decay of the population state ρ_{11}, and in turn results in a broadening of the population lifetime. To incorporate (3) in the BPM routine for solving Schrödinger's equation, requires determining the relation between the propagators for both the density matrix and the wave function. Since we are considering a closed system, the damping approximation [4] can be used to write

$$\rho(\mathbf{k}, \mathbf{k}', t) = \Psi(\mathbf{k}, t)\,\Psi^*(\mathbf{k}', t) \qquad \text{Polarization} \tag{4}$$

$$\rho(\mathbf{k}, \mathbf{k}, t) = \Psi(\mathbf{k}, t)\,\Psi^*(\mathbf{k}, t) \qquad \text{Population} \tag{5}$$

which implies that the propagators for both the density matrix and the wave function are identical. Equations (4) and (5) in general are not valid for higher level systems which require including all possible time orderings of electron-phonon interactions.

Intra-collisional field effects are automatically accounted for in this formalism since the interaction term Q in (3) includes the exact Hamiltonion for the applied (or self-consistent) electric field. Quantum coherence effects are easily obtained by tracking the phase of the off-diagonal density matrix elements with time.

IV. NUMERICAL EXAMPLE

To illustrate the numerical solution of Schrödinger's equation using BPM, we have solved for the time evolution of an initial three-dimensional gaussian wave packet, in the electron quantum wire coupler of Fig. 3. The wave packet was injected in the left guide at t=0 with a directed energy of 0.14 eV in the z-direction. The device dimensions were chosen with $L_z = 400\,\text{nm}$, $s = 4\,\text{nm}$, and $w = h = 5\,\text{nm}$. The number of computational grid spacings was taken as $N_x = N_y = 32$, and $N_z = 128$, while the time step Δt was 0.1 fs. For this example, there was no applied bias and electron-phonon scattering was not included. Figure 4 shows the probability amplitude at t=0 and 60 fs. In a future paper, electron-phonon scattering will be incorporated in the numerical model following the procedure outlined here.

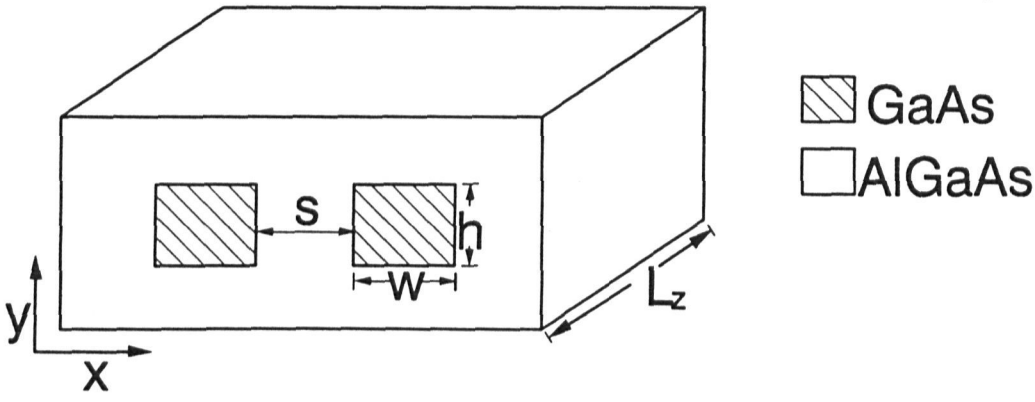

Figure 3

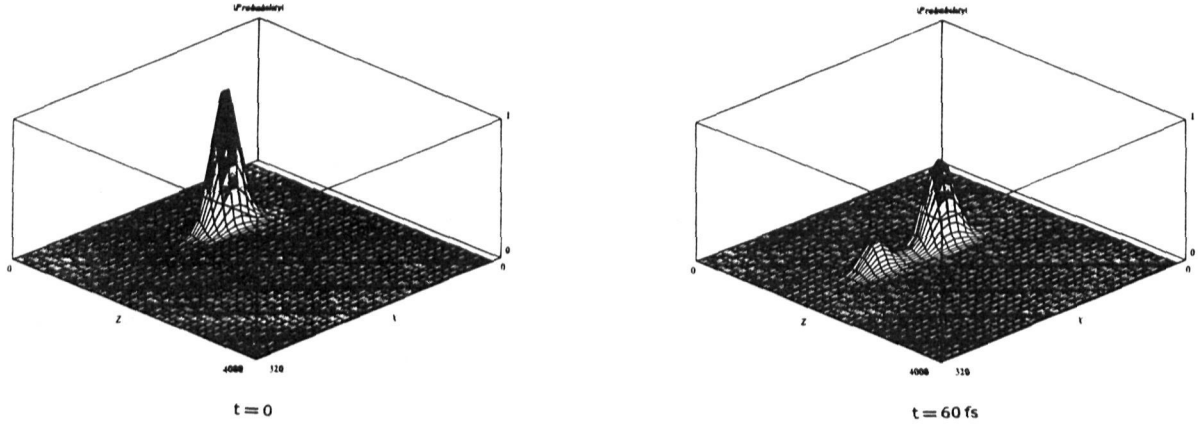

Figure 4. Dimensions are in angstroms.

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