NUMERICAL ASPECTS OF THE QUANTUM TRANSPORT SIMULATION OF FINITE OPEN SYSTEMS

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Abstract

The numerical discretization aspects of the quantum transport simulation of finite open systems are clarified in the framework of the discrete phase-space and lattice Weyl-Wigner formulation (LWWF) of quantum dynamics. For accurate numerical simulation of resonant tunneling devices at zero bias, the symmetry of closure and/or zero-current symmetry has to be imposed to avoid obtaining absurd results, particularly for asymmetric double-barrier structures at zero bias, where previous treatments were inadequate.

1. INTRODUCTION

The lattice Weyl-Wigner formulation of quantum dynamics of Bloch [1,2] electrons has recently been shown as a powerful and convenient analytical tool for deriving the exact many-body quantum transport equation in discrete phase-space [3,4], which is expected to guide future numerical and analytical work on nanoelectronics and quantum-based devices.

The purpose of this paper is to show how LWWF of quantum dynamics of electrons in solids serves to guide the proper numerical implementation of the Wigner distribution-function (WDF) transport equation. Since the WDF transport equation is only an approximation to the exact many-body quantum distribution-function transport equation in solids, the "discretization" of the WDF transport equation must be a direct consequence of the LWWF of quantum transport.

2. DISCRETE PHASE-SPACE MANY-BODY QUANTUM TRANSPORT EQUATION

The equation for the quantum distribution-function, $-iG^<(p,q,E,t)$, is given by [4]

$$\hbar \frac{\partial}{\partial t}(-i)G^<(p,E,q,t) = \left[2/\left[N\frac{h}{2}\right]^2\right]\left\{\sum_{p'q'} K_H^s(p,q;p',q')(-i)G^<(p',q')\right.$$

$$+\sum_{p'q'} K_{\Sigma^<}^s(p,q;p',q')(-i)\,\mathrm{Re}G^r(p',q') - \sum_{p'q'} K_{\Sigma^<}^c(p,q;p',q')(-i)\,\mathrm{Im}G^r(p',q') \qquad (1)$$

$$\left. -\frac{1}{2}\sum_{p'q'} K_\Gamma^c(p,q;p',q')(-i)G^<(p',q')\right\},$$

in the (3 + 1)-dimensional notation for the variables: $p = (\mathbf{p},E)$, $q = (\mathbf{q},t)$. The WDF is defined by the following relation

$$f_w(p,q,t) = \frac{1}{(h/2)}\int dE\,(-i)G^<(p,E,q,t). \qquad (2)$$

The integral kernels are given in terms of the lattice Weyl transforms (LWTs) [3] and have very simple forms, symbolically indicated as follows

$$K_a^{s,c}(p,q;p',q') = \frac{(-i,1)}{2} \sum_{u,v} \exp\left\{\frac{2i}{\hbar}[(q - q') \cdot u + (p - p') \cdot v]\right\} \{a(p+u,q-v) \mp a(p-u,q+v)\}. \quad (3)$$

The exact discretization of the momentum variables will be discussed below.

It is this inherent discrete phase-space nature of the quantum transport equation that must be retained in the numerical calculations. Thus, in the spirit of the WDF approximation we write Eq. (1) as the first term plus the many-body corrections, namely,

$$\frac{\partial}{\partial t} G^<(p,E,q,t) = \frac{-i}{2} \frac{2}{\hbar} \frac{1}{\left[N\frac{h}{2}\right]^2} \sum_{u,v} \exp \frac{2i}{\hbar} [(q - q') \cdot u + (p - p') \cdot v] \quad (4)$$

$$\times \{H(p + u,q - v) - H(p - u,q + v)\} G^<(p',q') + \text{Many-Body terms.}$$

In the last equation, $H(p,q)$ is the lattice Weyl transform (LWT) of the effective single-particle Hamiltonian. In the effective-mass approximation, we have

$$H(p,q) = \frac{p^2}{2m*} + V(q), \quad (5)$$

which, when substituted within the curly bracket of Eq. (4), leads to the following equation for the WDF

$$\frac{\partial f_w(p,q,t)}{\partial t} = \frac{-p}{m*} \cdot \nabla_q f_w(p,q,t) - \frac{i}{2} \frac{2\pi}{N\left[\frac{h}{2}\right]} \sum_{p'v} \exp \frac{2i}{\hbar} (p - p') \cdot v \quad (6)$$

$$\times \{V(q - v) - V(q + v)\} f_w(p',q,t) + \text{Scattering Terms.}$$

3. DISCRETIZATION OF THE MOMENTUM VARIABLE

In numerically implementing Eq. (6), extreme caution has to be exercised in the discretization of the momentum variables. The reason for this is that in the LWWF, **p** and **q** are the variables obtained through the transformation,

$$p' = p - u, \qquad q' = q + v, \qquad p'' = p - u, \qquad q'' = q + v, \quad (7)$$

where the primed momentum variables have the usual discretization (in 1-D given by $2\pi/Na$, where a is the lattice constant and N is the total number of lattice points). However, the above transformation have a Jacobian differing from unity. In one-dimensional systems one expects the ratio of the discretization lengths between the old and the new variables to be determined by the Jacobian factor of 4 in

$$dp_x' dp_x'' dq_x' dq_x'' = 4\, dp_x du_x dq_x dv_x. \quad (8)$$

Therefore, if one insists on the physically meaningful discretization of the real space to be given by the crystal lattice, it follows that the discretization of the momentum variables in Eq. (6) is π/Na. This can also be seen from the definition of the LWT for a periodic Hamiltonian,

$$H(p,q) = \sum_v \exp\left[\frac{2i}{\hbar} p \cdot v\right] \langle q - v|\mathcal{H}|q + v\rangle = \sum_v \exp\left[\frac{i}{\hbar} p \cdot 2v\right] e(2v) \quad (9)$$

For the above relation to be invertible, one of the important assumptions in the steps leading to Eq. (6), then it is necessary that $\delta k = \pi/Na$. Note that in a truly discrete case, the LWT of the single-particle Hamiltonian, $H(\mathbf{p},\mathbf{q})$, is not equal to the energy eigenvalue or the energy band. Strictly speaking, it is only in the continuum limit that one can consider $H(\mathbf{p},\mathbf{q})$ to be identical to the energy band of a periodic system.

The following discretization scheme for the momentum variables, which avoids zero momentum and discriminates positive and negative directions (for ease in applying boundary condition), holds for Eq.(6),

$$k_l = (2l - N - 1)\,\frac{\pi}{2Na}, \qquad l = 1, \ldots. N. \tag{10}$$

The zero-momentum value is excluded to eliminate pathological cases and very slow convergence of the numerical transient simulation, thus it is desirable to have an even number for the total number of lattice points N.

4. SYMMETRIZATION IN THE PLACEMENT OF THE ORIGIN

For even number of lattice points, a center of inversion symmetry that lie in one of the lattice points can not be identified. Therefore, in order for the potential term in Eq. (6) to be real, a symmetrization in the placement of the origin at the lattice point has to be performed. A symmetrization of the placement of the origin, at $N/2$ and $(N/2) + 1$, yields a purely imaginary quantity. The result is

$$\sum_{v} \exp\left[\frac{2i}{\hbar}(p - p')\cdot v\right]\{V(q - v) - V(q + v)\}$$

$$= i\ \mathrm{Im}\left\{\sum_{n'=-\left(\frac{N}{2}-1\right)}^{\frac{N}{2}} e^{-i(l-l')\frac{2\pi}{N}n'}\ V(n + n') + \sum_{n'=-\frac{N}{2}}^{\left(\frac{N}{2}-1\right)} e^{-i(l-l')\frac{2\pi}{N}n'}\ V(n + n')\right\}. \tag{11}$$

Therefore, a proper numerical implementation of the WDF transport equation involves taking the fast Fourier transform (FFT) of two distinct sequences of $V(n + n')$ for each value of n, for a given resonant tunneling device (RTD) potential profile.

5. CLOSED AND FINITE OPEN SYSTEM BOUNDARY CONDITIONS

It is the proper treatment of the sequence $V(n + n')$ with respect to the boundary which determines whether one is dealing with an open finite system in contact with a heat bath and exchanging particles with the environment, or whether one has a closed infinite periodic system interacting with a heat bath. In the former case, $V(n + n')$ clearly has to be extended beyond the N lattice points of the device under consideration, i.e., include lattice points of the highly conducting particle reservoirs. In the later case, $V(n + n')$ obeys the Born-von Karman periodic boundary condition, thus simulating an infinite quantum-well superlattice at zero bias.

At zero bias, it is very important to incorporate the existing symmetry of equilibrium (zero-current state) for both the open and closed system, otherwise one could get absurd nonzero-current results caused by numerical inaccuracies. The present work is partly motivated by the absurd results at zero bias, particularly for asymmetric RTD, obtained by the method of both Jensen and Buot [5] and that of Frensley [6], which have proven to give extremely good results for the current at nonzero biases. By

incorporating the existing symmetry at zero bias in the present work, the current is numerically equal to zero for both symmetric and asymmetric RTD.

The WDF transport simulation at zero bias is expected to show the difference in the energy-level structure of the quantum well for the finite open system, consisting of a single RTD structure, compared to that of an infinite periodic system of quantum-well superlattice (real energy bands in the quantum well and virtual energy bands in the highly conducting intervening leads).

Using the numerical technique described in this paper, we have simulated both systems, consisting of asymmetric double-barrier structure, at zero bias for $T = 77$ K, results are shown in Figs. 1-2. The Fermi level was calculated using the neutrality of electrons, holes and ionized donors for a doping level of $2 \times 10^{18}/cm^3$ at 77 K. Indeed, the quantum-well superlattice shows electron occupation of the energy bands in the quantum well, whereas the sharper ground-state energy level of a single quantum well do not contain any visible electrons. This results serve to validate the high-accuracy of the present numerical technique for simulating the WDF transport equation. The simulation of the intrinsic bistability of an asymmetric RTD will be given in a separate paper.

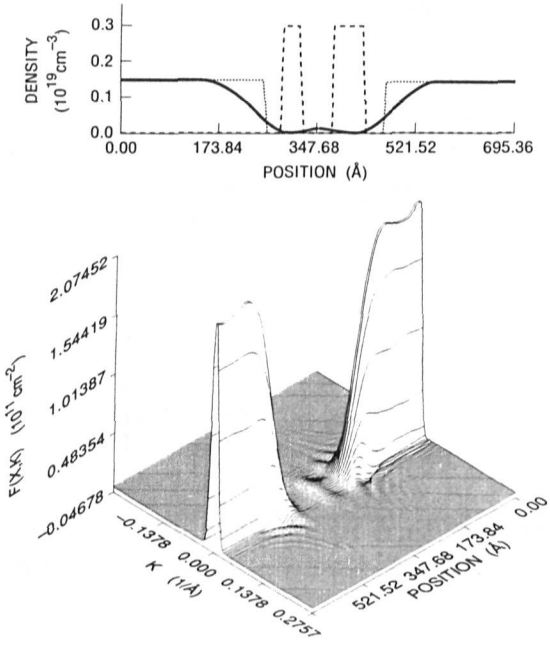

Fig. 1 — WDF at zero bias for an asymmetric barrier-well-barrier structure of 40Å-51Å-62Å, obtained by applying the periodic boundary condition, simulating an infinite quantum-well superlattice.

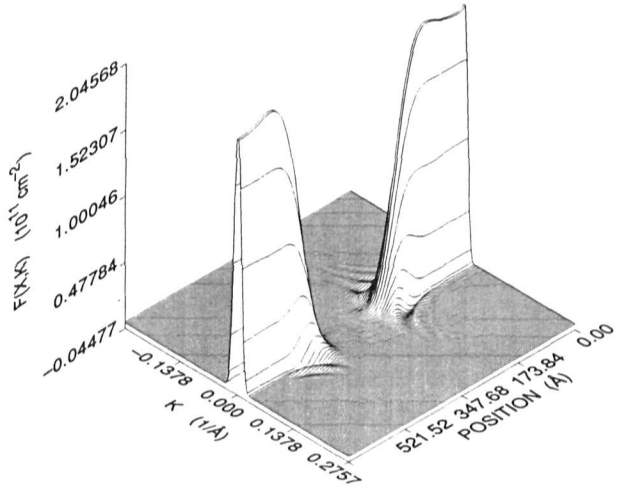

Fig. 2 — WDF of the same structure used in Fig. 1, using the finite open system boundary condition, simulating a single quantum well.

Acknowledgements: The author has benefited from helpful discussions with Dr. Kevin L. Jensen. The work is supported by the Office of Naval Research.

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