Simulation of Wigner Function Transport in Tunneling and Quantum Strucures

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ABSTRACT

The Wigner-function approach to quantum transport in mesoscopic electron devices is presented. The concept of Wigner paths allows the formulation of a Monte Carlo simulation which is quantum mechanically rigorous and yet very simular to the one used in semiclassical transport theory. The effect of a potential profile is separated into a term acting as a classical force in the particle orbits and a scattering integral that contains only quantum effects. Phonon scattering is included in the paths in a way that takes automatically into accounts all quantum effects, such as intracollisional field effect and collisional broadening.

Keywords: Wigner function, quantum transport, Monte Carlo, mesoscopic systems, tunneling.

1 INTRODUCTION

The Wigner function (WF) approach[1]–[4] seems to be most appropriate to deal with quantum electron transport in mesoscopic systems. It explicitely refers to variables defined in an $(\boldsymbol{r},\boldsymbol{p})$ phase space. Furthermore when the phase coherence length of the electrons tends to vanish, the WF reduces to the classical distribution function, while when the electron wavefunction extends to a finite size, the corresponding dynamics of the WF can be interpreted as the motion of representative points in phase space[5]. Such motion is identical to the motion of classical perticles as long as the potential does not change more than quadratically in the region occupied by the wavefunction. Thus in many cases the dynamics of each single electron in terms of the WF can be interpreted as an ensemble of classical particles. Such situations allows to understand why the Boltzmann equation (BE), based on semiclassical approximations, works often so well even for mesoscopic systems, and to identify the special situations where quantum effects are relevant. Wigner paths (WP's) in the above mentioned phase space can be defined that provide a pictorial representation of the quantum evolution of the system of interest and constitute a useful tool for the development of Monte Carlo (MC) simulative algorithms[5]–[7], in strict analogy with the ones used in semiclassical transport theory to solve the BE.

2 WIGNER FUNCTION

For an electron described by the vawefunction $\Psi(\boldsymbol{r},t)$ the WF is defined as the Weyl-Wigner transform of Ψ:

$$f_w(\boldsymbol{r},\boldsymbol{p},t) = \int e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}'}\overline{\Psi(\boldsymbol{r}+\boldsymbol{r}'/2,t)\Psi^*(\boldsymbol{r}-\boldsymbol{r}'/2,t)}\,d\boldsymbol{r}' \qquad (1)$$

where the bar indicates ensemble average (for simplicity, in what follows the bar will be understood).

The normalization has been chosen in such a way that

$$\frac{1}{(2\pi\hbar)^3}\int\int f_w(\boldsymbol{r},\boldsymbol{p})\,d\boldsymbol{p}\,d\boldsymbol{r} = 1\,. \qquad (2)$$

Several properties of the WF makes it analogous to the classical distribution function, even though it must be kept in mind that it cannot be interpreted as a probability density, as it may assume negative values.

It is immediate to verify from the definition (1) that integration over momentum yields the particle density in real space and, similarly, integration over $\boldsymbol{r}$ leads to the particle density in momentum space. Furthermore, the expectation value of any operator which is function of both position and momentum, is obtained by integrating over position and momentum the product of the WF times the Weyl-Wigner transform of the operator itself [6].

3 EFFECT OF A POTENTIAL $V(\boldsymbol{r})$

We shall now consider the dynamical equation of the WF for an electron subject to the hamiltonian:

$$\mathbf{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) = \mathbf{H}_\circ + V(\boldsymbol{r}) \qquad (3)$$

where we assume a single, spherical, and parabolic band with effective mass m, and leave the treatment of the electron-phonon interaction to the next section. $V(\boldsymbol{r})$ is a general potential applied to the electron; it can be due to a structure potential modified by an applied field and, possibly, by the self-consistent field described by Poisson equation.

Performing the time derivative of Eq.(1) and using Schrödinger equation, after strightforward calculations[6]

we get:

$$\left(\frac{\partial}{\partial t}+\frac{\boldsymbol{p}}{m}\cdot\nabla\right) f_w\left(\boldsymbol{r},\boldsymbol{p},t\right) = \int d\boldsymbol{p}'\, V_w(\boldsymbol{r},\boldsymbol{p}'-\boldsymbol{p})\, f_w\left(\boldsymbol{r},\boldsymbol{p}',t\right) \qquad (4)$$

where the transfer function V_w is defined by

$$V_w(\boldsymbol{r},\boldsymbol{p}) = \frac{1}{h^3}\int d\boldsymbol{r}'\, e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}'}\frac{1}{i\hbar}\left[V(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2})-V(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2})\right]. \qquad (5)$$

For potentials up to quadratic, the r.h.s. of Eq.(4) can be written has $-\mathbf{F}\cdot\nabla_{\mathbf{p}} f_w$ where $\mathbf{F}=-\nabla V(\boldsymbol{r})$. Therefore, the WF of electrons in presence of potential up to quadratic evolves as an ensemble of classical particles: each point follows a classical path in Wigner phase-space.

We can move a step further in the treatment of the scattering by the potential profile separating the effect of the classical force from quantum effects. To this purpose let us define

$$\tilde{V}_{\pm}(\boldsymbol{r},\boldsymbol{r}') = V\left(\boldsymbol{r}\pm\frac{\boldsymbol{r}'}{2}\right)-\nabla V(\boldsymbol{r})\cdot\left(\pm\frac{\boldsymbol{r}'}{2}\right)$$

With this separation, the dynamical equation for the WF becomes

$$\left(\frac{\partial}{\partial t}+\frac{\boldsymbol{p}}{m}\cdot\nabla+\mathbf{F}\cdot\nabla_{\boldsymbol{p}}\right) f_w\left(\boldsymbol{r},\boldsymbol{p},t\right) = \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{p}'\,\tilde{V}_w(\boldsymbol{r},\boldsymbol{p}-\boldsymbol{p}')f_w(\boldsymbol{r},\boldsymbol{p}'), \qquad (6)$$

where $\mathbf{F}=-\nabla V(\boldsymbol{r})$ is the classical force, and $\tilde{V}_w(\boldsymbol{r},\boldsymbol{p})$ is defined as in Eq.(5) with $\tilde{V}$ in place of V.
The l.h.s. of Eq.(6) is identical to the Liouvillian of the BE, while its r.h.s. describes quantum effects in the form of a collision integral due to a sort of quantum potential. A similar approach was introduces also by Lozovik and Filinov[8].
For the case of an electron interacting with an infinite potential barrier, a new equation has been derived by the authors [5], to be used, in place of Eq.(4), in the region confined by the potential barrier.

4 PHONON INTERACTION

If the system of the electron and phonon gas is considered, a generalized WF can be defined that includes the phonon states in the density matrix $\rho(t)$[9]:

$$f_w\left(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t\right) = \int d\boldsymbol{r}'\, e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}'}\left\langle \boldsymbol{r}+\frac{\boldsymbol{r}'}{2},\{n_q\}\middle|\rho(t)\middle|\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n'_q\}\right\rangle, \qquad (7)$$

where $n_{\mathbf{q}}$ is the occupation number of the phonon mode $\mathbf{q}$. In order to recover the original electron WF, a trace over the phonon states must be performed. As long as only electron variables are considered, a close equation for the WF can be easily obtained. On the contrary, when phonon variables are added, the trace over phonons of the resulting equation does not lead to a close equation for the electron WF, since the trace operation does not commute with the electron-phonon interaction Hamiltonian. The usual hierarchy of equations would be obtained [10]. In the present scheme, the equation is perturbatively solved for the generalized WF and the trace over the phonons is performed not on the equation itself, but on the obtained solution. Let us consider the Hamiltonian of the system as given by

$$\mathbf{H} = \mathbf{H}_0 + V(\boldsymbol{r}) + V_f(\boldsymbol{r}) + \mathbf{H}_p + \mathbf{H}_{ep}\,, \qquad (8)$$

where $V_f(\boldsymbol{r}) = -e\mathbf{E}\cdot\boldsymbol{r}$, being $\mathbf{E}$ a constant and uniform electric field, and

$$\begin{aligned}\mathbf{H}_0 &= -\frac{\hbar^2}{2m}\nabla^2_{\boldsymbol{r}},\\ \mathbf{H}_p &= \sum_{\boldsymbol{q}}\mathbf{b}^\dagger_{\boldsymbol{q}}\mathbf{b}_{\boldsymbol{q}}\hbar\omega_{\boldsymbol{q}},\\ \mathbf{H}_{ep} &= \sum_{\boldsymbol{q}} i\hbar F(\boldsymbol{q})\left(\mathbf{b}_{\boldsymbol{q}}e^{i\boldsymbol{q}\boldsymbol{r}}-\mathbf{b}^\dagger_{\boldsymbol{q}}e^{-i\boldsymbol{q}\boldsymbol{r}}\right), \end{aligned} \qquad (9)$$

are, respectively, the free electron term (with m electron effective mass), the Hamiltonian for the free phonon system and the electron-phonon interaction term. In the above expressions $\mathbf{b}_{\boldsymbol{q}}$ and $\mathbf{b}^\dagger_{\boldsymbol{q}}$ are the annihilation and creation operators for the phonon mode $\boldsymbol{q}$, $\omega_{\boldsymbol{q}}$ is the frequency of the phonon mode $\boldsymbol{q}$, and $F(\boldsymbol{q})$ is a function depending on the type of phonon scattering analyzed. Using the Hamiltonian given in Eq.(8) in place of the one given in Eq.(3), the r.h.s. of Eq.(6) can be written as the sum of five terms. Developing the calculations (the full derivation is given in Ref.[6]) leads to

$$\begin{aligned}&\left(\frac{\partial}{\partial t}+\frac{\boldsymbol{p}}{m}\cdot\nabla-(e\mathbf{E}+\nabla V(\boldsymbol{r}))\cdot\nabla_{\boldsymbol{p}}\right) f_w\left(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t\right)\\ &= \frac{1}{i\hbar}\left(\varepsilon(\{n_q\})-\varepsilon(\{n'_q\})\right) f_w\left(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t\right)\\ &+ \int d\boldsymbol{p}'\,\tilde{V}_w(\boldsymbol{r},\boldsymbol{p}'-\boldsymbol{p})\, f_w\left(\boldsymbol{r},\boldsymbol{p}',\{n_q\},\{n'_q\},t\right)\\ &+ \left(S_{ph}f_w\right)\left(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t\right). \end{aligned} \qquad (10)$$

where

$$\varepsilon(\{n_q\}) = \sum_{\boldsymbol{q}} n_{\boldsymbol{q}}\hbar\omega_{\boldsymbol{q}} \qquad (11)$$

is the energy of the phonon state $\{n_q\}$, and

$$\begin{aligned}&\left(S_{ph}f_w\right)\left(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t\right)\\ &= \sum_{\boldsymbol{q}'} F(\boldsymbol{q}')\left\{e^{i\boldsymbol{q}'\boldsymbol{r}}\sqrt{n_{\boldsymbol{q}'}+1}\right.\end{aligned}$$

$$\times f_w\left(\boldsymbol{r},\boldsymbol{p}-\frac{\hbar\boldsymbol{q}}{2},\{n_1,\ldots,n_{\boldsymbol{q}'}+1,\ldots\},\{n'_q\},t\right)$$
$$-e^{-i\boldsymbol{q}'\boldsymbol{r}}\sqrt{n_{\boldsymbol{q}'}}$$
$$\times f_w\left(\boldsymbol{r},\boldsymbol{p}+\frac{\hbar\boldsymbol{q}'}{2},\{n_1,\ldots,n_{\boldsymbol{q}'}-1,\ldots\},\{n'_q\},t\right)$$
$$-e^{i\boldsymbol{q}'\boldsymbol{r}}\sqrt{n'_{\boldsymbol{q}'}}$$
$$\times f_w\left(\boldsymbol{r},\boldsymbol{p}+\frac{\hbar\boldsymbol{q}'}{2},\{n_q\},\{n'_1,\ldots,n'_{\boldsymbol{q}'}-1,\ldots\},t\right)$$
$$+e^{-i\boldsymbol{q}'\boldsymbol{r}}\sqrt{n'_{\boldsymbol{q}'}+1}$$
$$\times f_w\left(\boldsymbol{r},\boldsymbol{p}-\frac{\hbar\boldsymbol{q}'}{2},\{n_q\},\{n'_1,\ldots,n'_{\boldsymbol{q}'}+1,\ldots\},t\right)\Bigg\}, \quad (12)$$

is the contribution of the electron-phonon interaction. Each term on the r.h.s of Eq.(12) represents a phonon interaction event (vertex) that changes only one set of phonon coordinates, increasing or decreasing the phonon occupation number of mode $\boldsymbol{q}'$ by one unity and changing the electron momentum by $\pm\frac{\hbar\boldsymbol{q}'}{2}$.

Before performing the time integration, it is useful to introduce the so called quantum self-scattering [11]. Let us define

$$\tilde{f}_w(\boldsymbol{r},\boldsymbol{p},t)=e^{\Gamma(t-t_\circ)}f_w(\boldsymbol{r},\boldsymbol{p},t)\,, \quad (13)$$

performing the derivative with respect to time we get

$$\frac{\partial}{\partial t}f_w=-\Gamma e^{-\Gamma(t-t_\circ)}\tilde{f}_w+e^{-\Gamma(t-t_\circ)}\frac{\partial}{\partial t}\tilde{f}_w\,. \quad (14)$$

Substituting Eq.(14) into Eq.(10) and using Eq.(13) leads to

$$\left(\frac{\partial}{\partial t}+\frac{\boldsymbol{p}}{m}\cdot\nabla-\nabla V(\boldsymbol{r})\cdot\nabla_{\boldsymbol{p}}\right)\tilde{f}_w(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t)$$
$$=\frac{1}{i\hbar}\left(\varepsilon(\{n_q\})-\varepsilon(\{n'_q\})\right)\tilde{f}_w(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t)$$
$$+\int d\boldsymbol{p}'\,\tilde{V}_w(\boldsymbol{r},\boldsymbol{p}'-\boldsymbol{p})\,\tilde{f}_w(\boldsymbol{r},\boldsymbol{p}',\{n_q\},\{n'_q\},t)$$
$$+\left(S_{ph}\tilde{f}_w\right)(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t)$$
$$+\Gamma\tilde{f}_w(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t)\,, \quad (15)$$

where the introduction of the exponential factor brings about an additional interaction mechanism, with a constant coupling Γ.

5 INTEGRAL EQUATION

The l.h.s. of Eq.(15) has the same form as the classical BE. Thus path variables can be used in analogy with the Chambers formulation of transport. Then, integrating over time, one obtains

$$\tilde{f}_w(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t)$$
$$=f_w\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t_\circ),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t_\circ),\{n_q\},\{n'_q\},t_\circ\right)$$
$$\times e^{-(i/\hbar)(\varepsilon(\{n_q\})-\varepsilon(\{n'_q\}))(t-t_\circ)}$$
$$+\int_{t_\circ}^{t}dt'\,e^{-(i/\hbar)(\varepsilon(\{n_q\})-\varepsilon(\{n'_q\}))(t-t')}$$
$$\left\{\int d\boldsymbol{p}'\,\tilde{V}_w\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t'),\boldsymbol{p}'-\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t')\right)\right.$$
$$\times\tilde{f}_w\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t'),\boldsymbol{p}',\{n_q\},\{n'_q\},t'\right)$$
$$+\left(S_{ph}\tilde{f}_w\right)\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t'),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t'),\{n_q\},\{n'_q\},t'\right)$$
$$\left.+\Gamma\tilde{f}_w\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t'),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t'),\{n_q\},\{n'_q\},t'\right)\right\} \quad (16)$$

where $\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,s)$ and $\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,s)$ are position and momentum at time s of a classical particle that at time t is in $\boldsymbol{r}$ with momentum $\boldsymbol{p}$. The upper (0) indicates that no scattering occurs between s and t. $t_\circ$ represents the time of the initial condition, when the WF is supposed to be known.

6 WIGNER PATHS AND MONTE CARLO SIMULATION

Eq.(16) may be iteratively substituted into itself giving a Neumann expansion that describes the evolution of the WF as a sum of contributions containing increasing powers of the interaction coupling, evaluated at successive times t_i. Recalling that, from the definition, $\tilde{f}_w(\boldsymbol{r},\boldsymbol{p},t_\circ)=f_w(\boldsymbol{r},\boldsymbol{p},t_\circ)$, the inclusion of the quantum self-scattering implies that between one scattering and the next one a factor $e^{-\Gamma(t_i-t_j)}$ has to be added.

In previous works [5]–[7] the authors have shown that for free electrons and for potential up to quadratic, a single δ-like contribution of the WF keeps its value and its δ-character evolving in time along the classical path. Eq.(16) and its iterative expansion show that, taking into account phonon scattering, for each single scattering time t' and a single phonon mode $\boldsymbol{q}'$ a δ-contribution still remains δ-like. With the potential, for a scattering time t' and a given transferred momentum, again a δ-contribution of the WF keeps its δ-character.

These considerations allow us to define WP's [12] followed by a "simulative particles" carrying δ contributions of the WF through the Wigner phase space. While along a free path a single δ-like contribution of the WF mantains its value, at each interaction vertex it acquires a new weighting factor accounting for the effect of the interaction. Thus the Neumann series obtained by Eq.(16) may be evaluated by a Monte Carlo technique, sampling the integrals over the scattering times and the momentum transferred by potential or phonons, in complete analogy to the "Weighted Monte Carlo" solution of Boltzmann equation in its integral form [13].

We are interested in the evaluation of a WF that is diagonal over phonon occupation numbers at the final time. If the requirement of diagonality is imposed also at the initial time by taking $f^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t_\circ) \neq 0$ only if $\{n_q\} = \{n'_q\}$, then only terms containing a sequence of creation and annihilation operators that changes in the same way the two sets of phonon occupation numbers contribute to the evaluation of the WF. As a consequence, only WP's with an even number of vertices involving a specific mode $\boldsymbol{q}$ are present.

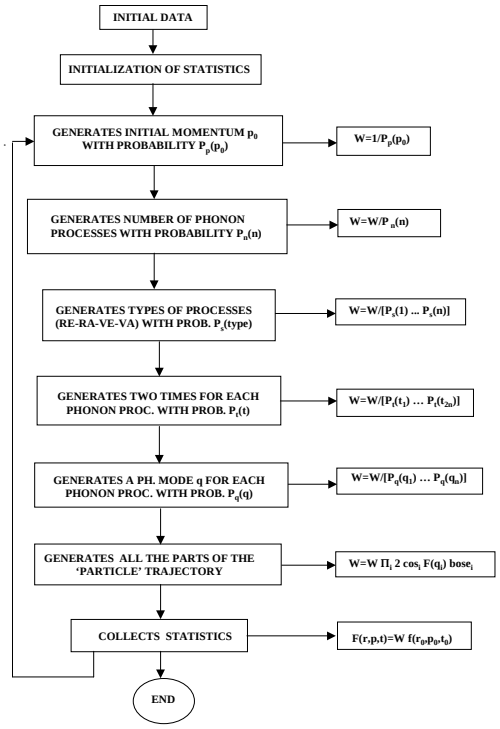

Figure 1. *Flow-chart of a possible quantum MC code. W is the weight of the path.*

The way of selecting the WP's is completely free [14]. As a consequence a number of different algorithms can be devised according to the specific problem to be faced. Fig.1 describes a specific one, among those we have developed, where for simplicity only scattering with phonons (real emission RE, real absorption RA, virtual emission VE and virtual absorption VA) is included. It should be noticed that each Wigner path corresponds to several possible sampling of the integrands. This introduces the multiplicity factors 2 in front of the cosine weights reported in the diagram in Fig.1.

The WP's method can also be extended to the case of a two-time WF. In fact, a dynamical equation formally identical to Eq.(10) has been derived by the authors for a general WF dependent on momentum and energy separately [5]. The MC algorithm simulating the time evolution of the WF in the presence of electron-phonon scattering can be extended to evaluate $f_w(\boldsymbol{r},\boldsymbol{p},\omega,t)$.

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