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QUANTUM TRANSPORT AND ITS SIMULATION WITH THE WIGNER-FUNCTION APPROACH

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In this paper a review of the research performed in recent years by the group of the authors is presented. The definition and basic properties of the Wigner function are first given. Several forms of its dynamical equation are then derived with the inclusion of potential and phonon scattering. For the case of a potential $V(\boldsymbol{r})$ the effect of the classical force, for any form of $V(\boldsymbol{r})$, is separated from quantum effects due to rapidly varying potentials. An elaboration of the dynamical equation is introduced that leads to Wigner paths formed by free flights and scattering events. These are especially suitable for a Monte Carlo solution of the transport equation for the Wigner function very similar to the semiclassical traditional Monte carlo simulation. The Monte Carlo simulation can be extended also to the momentum and frequency dependent Wigner function based on a two-time Green function. Several numerical results are presented throuhout the paper.

1. Introduction

Semiclassical transport theory of electrons in semiconductors is based on the Boltzmann equation (BE) for the distribution function $f(\boldsymbol{r}, \boldsymbol{p}, t)$. This function is defined as proportional to the density of particles in phase space. Traditionally the validity of the semiclassical approach, and of the BE, is ascribed to the fulfillment of the following conditions:

a) It should be possible to form electron wavepackets of small dimensions in both real and momentum space, such that a defined point $(\boldsymbol{r}, \boldsymbol{p})$ in phase space can be assigned to each electron.

b) Collisions are considered instantaneous and point-like in space; this assumption allows to give a simple form to the collision integral in the BE and also avoids consideration of the intracollisional field effect, the modification of the scattering rates induced by the electric field, and of multiple scattering.

c) Scattering events are rare enough to prevent significative collisional broadening: the average time interval τ between collision is long enough to make negligible the uncertainty in the electron energy $\Delta\varepsilon \sim \hbar/\tau$.

The above assumptions are not independent from each other, and some of them can be released by including refinements in the semiclassical transport theory (e.g. by including multiple collisions in the collision integral).

There are special cases where the semiclassical approach fails dramatically. Some

of these are, e.g., tunneling through barriers, as in the resonant tunneling diode, and coherent interference, as in the Ahronov-Bohm effect. A part from such cases, it is difficult to estimate the validity of the semiclassical approach from a comparison with experimental data, since electron transport theory contains, in general, several unknown parameters, and also the samples used in the experiments are not always perfectly known. Thus, in the last decades, it has become clear that a rigorous quantum approach to electron transport is necessary, not only for the solution of problems where quantum effects are essential but also for testing the semiclassical approximation by comparison with exact quantum results obtained for the very same system.

Several approaches have been attempted: density matrix[1,2,3], path integral[4,5], Green functions[6,7,8,9], Wigner function[10,11,12,13]. All of them are more or less closely related to the Green function concept. The Wigner function (WF) approach will be reviewed in the present paper; it seems the most appropriate to deal with space dependent problems since 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. Such motion is identical to the motion of classical perticles as long as the potential does not change more then 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, based on semiclassical approximations, works often so well, and to identify the special situations where quantum effects are relevant.

The definition of the WF is given in section 2, while its main properties are reviewed in section 3. In section 4 a particular formalism that allows the transformation from the WF to the density matrix and vice versa is presented. It also yiels the evolution of the WF when eigenvalues and eigenfunctions of the hamiltonian are known. The dynamical equation for the WF without electron-phonon interaction, is derived in section 5, while the effect of phonon scattering is included in section 6. In section 7 a Neumann expansion of the integral equation for the WF is performed leading to the definition of paths in the Wigner phase-space, called Wigner paths. Such a Wigner paths concept is used in section 8 to develop a quantum MC algorithm in strict analogy with the traditional MC procedure. In section 9 the formalism developed in the previuos sections is extended to a momentum and frequency dependent WF based on a two-time Green function. Some conclusions are finally summarized in section 10.

2. Elementary Definition of the Wigner Function

The WF was introduced by Wigner in 1932 with the purpose of evaluating quantum corrections for thermodynamic equilibrium in a phase-space formulation [10]. Since then it has been used in several fields of physics[14]

Since about a decade the WF has become popular as a tool to investigate quantum transport[15,13,16,17,18,19,20] as it allows a rigorous description of electron transport in quantum terms using, at the same time, the concept of phase space, so familiar from classical statistical physics. For an electron described by the vawefunction $\Psi(\boldsymbol{r},t)$ the elementary definition of the WF is

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

where the bar indicates ensemble average. For simplicity, in what follows the bar will be understood.

Several forms of normalization are present in the literature. Here it has been chosen in such a way that, if the wavefunction is normalized to 1 in the volume of interest, then

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

Thus, for a homogenuos system of volume V containing N particles

$$\frac{V}{(2\pi)^3}\int [N f_w(\boldsymbol{p})]\,\frac{1}{\hbar^3}d\boldsymbol{p} = N\,. \tag{3}$$

This means that if f_w is multiplied by the total number of particles in the volume of interest, it can be compared with the occupation number of the quantum state $(\boldsymbol{p}/\hbar)$. With this normalization of f_w, numerical results obtained for f_w in a device can be compared with semiclassical distribution function normalized in such a way that Pauli exclusion principle brings a factor $(1-f)$ in the scattering rates.

Several justifications for the definition (1) of the WF can be given. One of them starts from the problem of finding a reasonable numerical function $f(q,p)$ of phase space to associate to the density matrix operator $\rho = |\Psi\rangle\langle\Psi|$, that is the statistical operator to use for the evaluation of average quantities in quantum ensembles. If we assume the criterium that the mean value weighted by f over the phase space of the Fourier functions (that is the Fourier transform of f) must be equal to the corresponding quantum average of the same operator function, we obtain

$$Tr\left[\rho e^{i(\xi\hat{q}+\eta\hat{p})/\hbar}\right] = \frac{1}{2\pi\hbar}\int dq\int dp\, f(q,p)e^{i(\xi q+\eta p)/\hbar}\,. \tag{4}$$

For simplicity, we consider here only one degree of freedom, and the factor in front of the integral has been inserted to be consistent with the above normalization. Furthermore the operators are indicated by means of the conventional simbol, to distinguish them from the corresponding c-numbers on the r.h.s. of the equation. The l.h.s. of the above equation can be transformed, using also the identity $e^{\hat{p}+\hat{q}} = e^{\hat{p}/2}e^{\hat{q}}e^{\hat{p}/2}$ based on Baker-Hausdorff theorem [21], as

$$\begin{aligned} Tr\left[\rho e^{i(\xi\hat{q}+\eta\hat{p})/\hbar}\right] &= \int dq\,\langle q|\Psi\rangle\langle\Psi|e^{i(\xi\hat{q}+\eta\hat{p})/\hbar}|q\rangle \\ &= \int dq\int dq'\,\langle q|\Psi\rangle\langle\Psi|q'\rangle\langle q'|\,e^{i\eta\hat{p}/(2\hbar)}\,e^{i\xi\hat{q}/\hbar}\,e^{i\eta\hat{p}/(2\hbar)}|q\rangle \end{aligned}$$

$$= \int dq \int dq' \, \langle q|\Psi\rangle\langle\Psi|q'\rangle\langle q'+\eta/2| \, e^{i\xi(q-\eta/2)/\hbar} \, |q-\eta/2\rangle$$
$$= \int dq \, \Psi(q)\Psi^*(q-\eta) \, e^{i\xi(q-\eta/2)/\hbar} \, .$$

By substituting into Eq.(4) and inverting the Fourier transform, we obtain

$$f(q,p) = \int d\eta \, e^{-i\eta p/\hbar} \Psi(q'+\eta/2)\Psi^*(q'-\eta/2) \, . \tag{5}$$

This is equivalent to the definition in Eq.(1).

Another possible justification of the definition (1) starts from the definition of the density matrix

$$\rho(\boldsymbol{r}_2, \boldsymbol{r}_1, t) = \Psi(\boldsymbol{r}_2, t)\Psi^*(\boldsymbol{r}_1, t) \, . \tag{6}$$

For $\boldsymbol{r}_1 = \boldsymbol{r}_2$ this expression yields the particle density while, when $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ move away from each other the ensemble average yields nonvanishing values only for distances within the electron coherence lenght. Now if we switch from the variables $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ to the average $\boldsymbol{r}$ and relative $\boldsymbol{r}'$ positions:

$$\boldsymbol{r} = \frac{\boldsymbol{r}_1 + \boldsymbol{r}_2}{2} \, ; \quad \boldsymbol{r}' = \boldsymbol{r}_2 - \boldsymbol{r}_1 \, , \tag{7}$$

then the density matrix $\Psi(\boldsymbol{r}+\boldsymbol{r}'/2, t)\Psi^*(\boldsymbol{r}-\boldsymbol{r}'/2, t)$ yields the density of particle "around $\boldsymbol{r}$", while its Fourier transform with respect to $\boldsymbol{r}'$ gives the density of momentum around the same position. In fact, such Fourier transform coincides with the definition in Eq.(1). Note that $\boldsymbol{r}$ and $\partial/\partial\boldsymbol{r}'$ commute.

A generalization of the above approach is given in Sec. 9 where, starting from the two-time Green functions, a momentum and energy dependent WF is defined.

3. Main Properties of the Wigner Function

Several properties of the WF are worth considering that make 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. In fact the WF may present very fast oscillations that creates severe problems when numerical methods are used.

3.1. *Particle Density in Real and Momentum Space*

It is immediate to verify from the definition (1) that integration over momentum yields the particle density in real space

$$\frac{1}{(2\pi\hbar)^3} \int f_w(\boldsymbol{r}, \boldsymbol{p}) \, d\boldsymbol{p} = |\Psi(\boldsymbol{r})|^2 \, . \tag{8}$$

Similarly, integration over $\boldsymbol{r}$ leads to the particle density in momentum space. In fact

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

$$= \frac{1}{(2\pi\hbar)^3}\int dr_1 \int dr_2 e^{-\frac{i}{\hbar}p\cdot(r_2-r_1)}\Psi(r_2,t)\Psi^*(r_1,t) = |\Phi(p)|^2\,, \qquad (9)$$

where $\Phi(p)$ is the particle wave function in momentum space.

3.2. *Mean Quantities*

If we consider an operator $\mathcal{F}(\hat{r})$ its quantum ensemble average is given by

$$\langle\mathcal{F}\rangle = \int dr\,\mathcal{F}(r)\,|\Psi(r)|^2 = \frac{1}{(2\pi\hbar)^3}\int\int dr\,dp\,f_w(r,p)\,\mathcal{F}(r) \qquad (10)$$

and similarly for a function operator $\mathcal{G}(\hat{p})$

$$\langle\mathcal{G}\rangle = \int dp\,\mathcal{G}(p)\,|\Phi(p)|^2 = \frac{1}{(2\pi\hbar)^3}\int\int dr\,dp\,f_w(r,p)\,\mathcal{G}(p)\,. \qquad (11)$$

The above expressions, obtained by means of Eqs.(8) and (9), are identical to the classical analogous where the function operators are simply substituted by the corresponding c-number functions. More generally, given an operator $\mathcal{A}$, which is a function of both position and momentum, its ensemble quantum average is given, using the r representation, by

$$\begin{aligned}\langle\mathcal{A}\rangle &= Tr\,(\rho\mathcal{A}) = \int dr_1\int dr_2\,\langle r_1|\mathcal{A}|r_2\rangle\langle r_2|\Psi\rangle\langle\Psi|r_1\rangle \\ &= \int dr\int dr'\,\mathcal{A}\left(r-\frac{r'}{2},r+\frac{r'}{2}\right)\Psi\left(r+\frac{r'}{2}\right)\Psi^*\left(r-\frac{r'}{2}\right)\,, \qquad (12)\end{aligned}$$

where the transformation defined in Eq.(7) has been used. In order to recover the WF a $\delta(r'-r'')$ is now inserted in its plane-wave representation:

$$\begin{aligned}\langle\mathcal{A}\rangle &= \int dr\int dr'\int dr''\,\frac{1}{(2\pi\hbar)^3}\int dp\,e^{ip\cdot(r'-r'')/\hbar}\times \\ &\quad \mathcal{A}\left(r-\frac{r'}{2},r+\frac{r'}{2}\right)\Psi\left(r+\frac{r''}{2}\right)\Psi^*\left(r-\frac{r''}{2}\right)\,, \qquad (13)\end{aligned}$$

or

$$\langle\mathcal{A}\rangle = \frac{1}{(2\pi\hbar)^3}\int dr\int dp\,\mathcal{A}_w(r,p)f_w(r,p) \qquad (14)$$

where

$$\mathcal{A}_w(r,p) = \int dr'\,e^{-ip\cdot r'/\hbar}\mathcal{A}\left(r+\frac{r'}{2},r-\frac{r'}{2}\right)\,, \qquad (15)$$

is the Weyl-Wigner transform of the operator $\mathcal{A}$ exactly as the WF in Eq.(1) is the Weyl-Wigner transform of the density matrix operator. Eq.(14) shows the strong analogy between the WF and the classical distribution function.

It is easy to show with straightforward calculations from the the definition in Eq.(15) that for any operator $\mathcal{F}(\hat{r})$ which is a function of only the operator $\hat{r}$ or for any operator $\mathcal{G}(\hat{p})$ which is a function of only the operator $\hat{p}$ the Weyl-Wigner

transforms reduce to the equivalent c-number functions coherently with Eqs.(10) and (11).

For an operator which is a function of both $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$ the calculation is somewhat more involved. Let us consider, for example, the simple product of $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$. It can be shown that

$$\begin{aligned} (\hat{\boldsymbol{r}}\hat{\boldsymbol{p}})_w &= \boldsymbol{r}\boldsymbol{p} + \frac{3}{2}i\hbar \\ (\hat{\boldsymbol{p}}\hat{\boldsymbol{r}})_w &= \boldsymbol{r}\boldsymbol{p} - \frac{3}{2}i\hbar\,, \end{aligned} \tag{16}$$

coherently with the fact that neither of these two product operators is hermitian. On the other hand, for the hermitian, simmetrized form, we obtain

$$\frac{1}{2}(\hat{\boldsymbol{r}}\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\hat{\boldsymbol{r}})_w = \boldsymbol{r}\boldsymbol{p} \tag{17}$$

4. The Coefficients $f_{nm}(\boldsymbol{r},\boldsymbol{p})$, Coherent Evolution

Let $\mathcal{H}$ be the time independent hamiltonian that describes the dynamics of the electron. If its eigenvalues ε_n and eigenstates $|\phi_n\rangle$ are known,

$$\mathcal{H}|\phi_n\rangle = \varepsilon_n|\phi_n\rangle\,, \tag{18}$$

then the coherent evolution of the WF can be easily obtained. In fact the time dependent WF can be written as

$$f_w(\boldsymbol{r},\boldsymbol{p},t) = \sum_{n,m}\int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\boldsymbol{r}'/\hbar}\left\langle \boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\middle|\phi_n\right\rangle\left\langle\phi_n\middle|\Psi(t)\right\rangle\left\langle\Psi(t)\middle|\phi_m\right\rangle\left\langle\phi_m\middle|\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right\rangle$$

or

$$f_w(\boldsymbol{r},\boldsymbol{p},t) = \sum_{n,m} f_{n,m}(\boldsymbol{r},\boldsymbol{p})\rho_{n,m}(t)\,, \tag{19}$$

where

$$\rho_{n,m}(t) = \langle\phi_n|\Psi(t)\rangle\langle\Psi(t)|\phi_m\rangle\,, \tag{20}$$

is the density matrix in the basis of the hamiltonian eigenstates, and

$$f_{n,m}(\boldsymbol{r},\boldsymbol{p}) = \int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\boldsymbol{r}'/\hbar}\left\langle \boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\middle|\phi_n\right\rangle\left\langle\phi_m\middle|\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right\rangle\,, \tag{21}$$

are the coefficients[14,20] for the transformation from the density matrix to the WF. They obey the unitarity relations

$$\frac{1}{(2\pi\hbar)^3}\sum_{n,m} f_{n,m}(\boldsymbol{r},\boldsymbol{p})f^*_{n,m}(\boldsymbol{r}',\boldsymbol{p}') = \delta(\boldsymbol{r}-\boldsymbol{r}')\delta(\boldsymbol{p}-\boldsymbol{p}') \tag{22}$$

and

$$\frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{r}\int d\boldsymbol{p}\, f_{n,m}(\boldsymbol{r},\boldsymbol{p})f^*_{n',m'}(\boldsymbol{r},\boldsymbol{p}) = \delta_{n,n'}\delta_{m,m'}\,, \tag{23}$$

as can be verified by strightforward calculations.

Eq.(23) allows to invert the transformation given in (19):

$$\rho_{n,m}(t) = \frac{1}{(2\pi\hbar)^3} \int dr \int dp\, f^*_{n,m}(r,p) f_w(r,p,t)\,. \tag{24}$$

Let us now consider the time evolution of the density matrix

$$\rho_{n,m}(t) = e^{-i(\omega_n - \omega_m)(t-t_o)}\,, \tag{25}$$

where $\omega_n = \varepsilon_n/\hbar$ and t_0 is the time of the initial condition when the WF is supposed to be known. By substituting Eq.(24), evaluated at $t = t_0$, into Eq.(25) and the result into Eq.(19) we finally obtain the free, coherent evolution of the WF:

$$\begin{aligned} f_w(r,p,t) &= \sum_{n,m} f_{n,m}(r,p) e^{-i(\omega_n-\omega_m)(t-t_o)} \\ &\quad \times \frac{1}{(2\pi\hbar)^3} \int dr' \int dp'\, f^*_{n,m}(r',p') f_w(r',p',t_o)\,. \end{aligned} \tag{26}$$

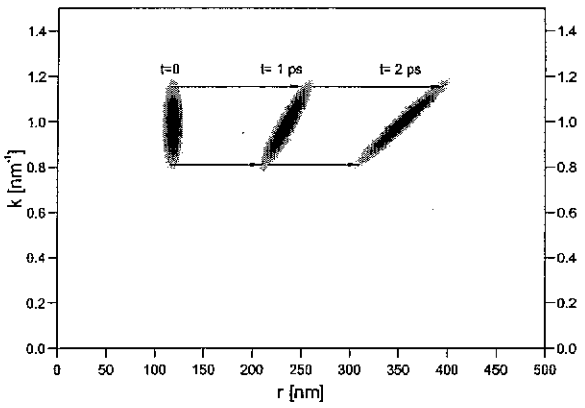

Fig. 1. Free evolution in two-dimensional Wigner phase space of a WF for a wave packet. Each δ-like contribution of the WF follows a classical trajectory.

For the case of free electrons, the eigenfunctions of the hamiltonian are plane waves and the coefficients $f_{n,m}$ assume the form

$$f_{k,k'}(r,p) = \hbar^3 e^{i(k-k')\cdot r} \delta\left(p - \hbar\frac{k+k'}{2}\right)\,. \tag{27}$$

Thus, after some strightforward calculations, the evolution of the WF for free electrons results

$$f_w(\boldsymbol{r}, \boldsymbol{p}, t) = f_w\left(\boldsymbol{r} - \frac{\boldsymbol{p}}{m}(t - t_o), \boldsymbol{p}, t_o\right) . \tag{28}$$

This is the same behavior that we expect for an ensemble of electrons represented by the distribution function f_w: in absence of any force each electron mantains its momentum unaltered, and moves in space with constant velocity $\boldsymbol{p}/m$. Fig.1 shows the above evolution for the case of a wave packet [22].

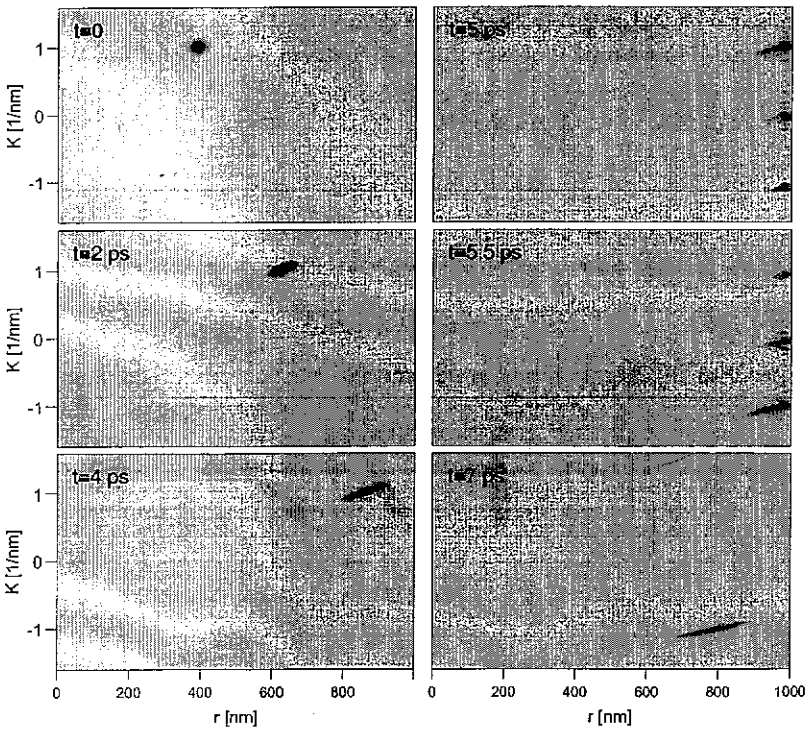

Fig. 2. Time evolution (given at 6 different istants) of the WF of a minimum uncertainity Gaussian wave packet in a quantum well with infinite potential barriers. The WF describes an electron with a Gaussian distribution of the initial wave-vector around the value $k_o = 1$ nm^{-1}.

Such an approach provides a very simple physical interpretation of the broadening of free wave packets: contributions of higher momentum move faster then contributions with lower momentum.

It has been shown numerically, and analytically for a Gaussian wave-packet, that also in the case of a particle hitting an infinite potential barrier, for time long enough after the scattering process, the evolution of the WF coincides with that of a classical distribution function[23] (see Fig.2).

Owing to the linearity of Eq.(26), if the WF at $t = t_o$ is the sum of several contributions, then each of them evolves according to Eq.(26) and the WF at any given time $t > t_o$ will be given by the sum of the single contributions evaluated at the same time. From the discussion above, if the initial WF is considered as the integral of δ-like contributions, each of them, in the absence of external forces, carries its value following a classical path. As we shall see later, the same conclusion is true for electrons subject to a constant or harmonic force. This property of the WF may help to understand why the BE appears to work also beyond its expected limits of validity.

It has been shown [20] that Eq.(26) can be extended to an open system in the case of thermalizing boundaries far from the region with non-constant potential. In such a case, the integral over $\boldsymbol{r}'$ of the initial condition must be evaluated in the internal region and extended with a time integration from t_o to t at the boundaries. Fig.3 shows the WF obtained with the above method for electrons entering from boundaries at local Maxwellian equilibrium, into a region with a potential step.

The problem of bounadaries conditions can be dealt with in a simpler and more general way with the Wigner paths approach discussed below.

5. Dynamical Equation

We shall now consider the dynamical equation of the WF for an electron subject to the hamiltonian $\mathcal{H}$. By differentiating with respect to the time the definition (1) of the WF and using the Schrödinger equation, we obtain

$$i\hbar\frac{\partial f_w}{\partial t} = \int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar} \times \left[\left(\mathcal{H}\Psi\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right)\right)\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right) - \Psi\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right)\left(\mathcal{H}\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right)\right)\right]. \quad (29)$$

Leaving the treatment of the electron-phonon interaction to the next section, we shall consider here the case of a hamiltonian given by

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}), \quad (30)$$

where we assume a single, spherical, and parabolic band with effective mass m. Very little has been done with the WF function beyond this approximation. $V(\boldsymbol{r})$ is a general potential applied to the elctron; it can be due to a structure potential modified by an applied field and, possibly, by the self-consistent process described by the Poisson equation. The different terms in the hamiltonian will be treated separately with a physical interpretation of the resulting dynamical evolution of the WF.

5.1. *Free Electrons*

Let us assume, to begin with, that the dynamics of the electrons is governed by

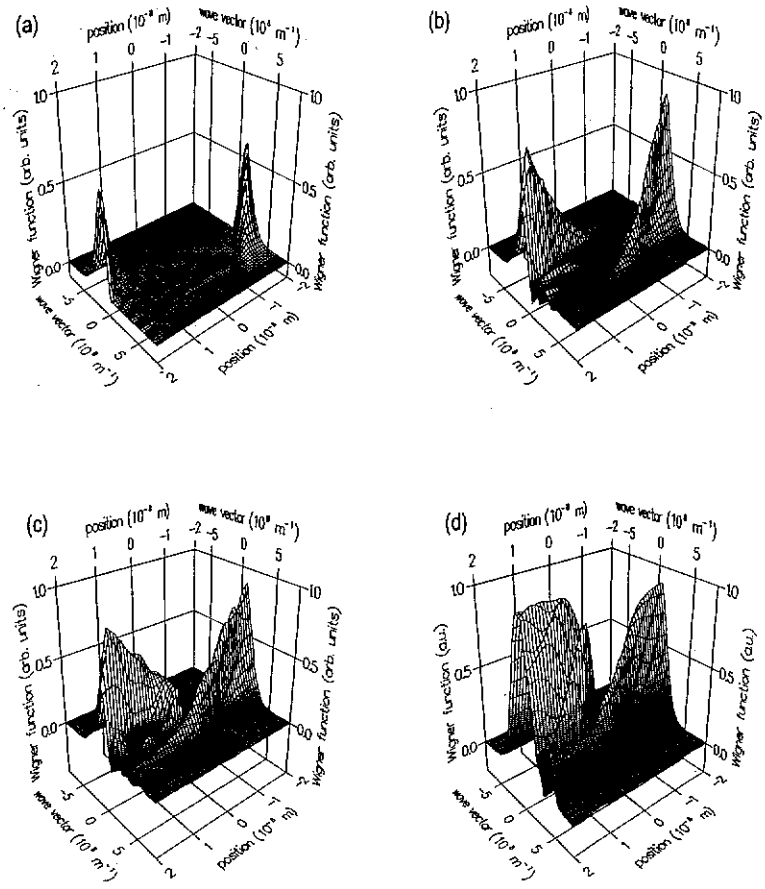

Fig. 3. "Ballistic invasion" of the WF into an empty device with local Maxwellian equilibrium boundary conditions at t=10 fs (a), t=40 fs (b), t=80 fs (c) for electrons entering from the boundaries into a region with a potential step and stationary WF (d), as obtained by means of an equilibrium density matrix diagonal over the scattering states for a 0.1 eV step potential.

only the first term in Eq.(30). Then, by using Eq.(29) we obtain

$$i\hbar\frac{\partial f_w}{\partial t} = \int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar}\left[\left(-\frac{\hbar^2}{2m}\nabla^2\Psi\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},t\right)\right)\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},t\right)\right.$$
$$\left.-\Psi\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},t\right)\left(-\frac{\hbar^2}{2m}\nabla^2\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},t\right)\right)\right]$$

$$= -\frac{\hbar^2}{2m}\int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar} 2\nabla' \left[\left(\nabla\Psi\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},t\right)\right)\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},t\right) + \Psi\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},t\right)\nabla\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},t\right)\right]$$

where ∇' indicates derivative with respect to $\boldsymbol{r}'$. Integration by parts leads to

$$i\frac{\partial f_w}{\partial t} = -\frac{i}{m}\boldsymbol{p}\int d\boldsymbol{r}'\, e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}'}\,\nabla[\Psi(\boldsymbol{r}+\boldsymbol{r}'/2,t)\,\Psi^*(\boldsymbol{r}-\boldsymbol{r}'/2,t)]\,. \tag{31}$$

Here it has been assumed that, for any $\boldsymbol{r}$, the limits of integration go to infinity, where the wavefunction and its derivative vanish. We report here this simple calculation, already well known in the literature, since we shall see in the following a special situation where this assumption and the resulting equation must be modified. In the present case the above equation reduces to

$$\frac{\partial f_w}{\partial t} + \frac{\boldsymbol{p}}{m}\nabla f_w = 0\,, \tag{32}$$

which is formally identical to the BE for free electrons, in agreement with the evolution seen in Sec. 4.

5.2. *Electrons Subject to a Potential* $V(\boldsymbol{r})$

When the term $V(\boldsymbol{r})$ is inserted in the hamiltonian in Eq.(29) the following expression is obtained

$$i\hbar\frac{\partial f_w}{\partial t}\bigg|_V = \int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar}\left[V\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right)\Psi\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right)\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right) - \Psi\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right)V\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right)\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right)\right]$$

$$= \int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar}\left[V\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right) - V\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right)\right]\Psi\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right)\Psi^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right). \tag{33}$$

Now we have to recover the WF by inserting a δ-function in its plane-wave representation, as it was done in the derivation of Eq.(14). Performing the calculations leads to

$$\frac{\partial f_w}{\partial t}\bigg|_V = \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{p}'\,\mathcal{V}_w(\boldsymbol{r},\boldsymbol{p}-\boldsymbol{p}')f_w(\boldsymbol{r},\boldsymbol{p}')\,, \tag{34}$$

where

$$\mathcal{V}_w(\boldsymbol{r},\boldsymbol{p}) = \frac{1}{i\hbar}\int d\boldsymbol{r}' e^{-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar}\left[V\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right) - V\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right)\right]. \tag{35}$$

This term, summed to the dynamical equation (32) for free electrons, leads to

$$\frac{\partial f_w}{\partial t} + \frac{\boldsymbol{p}}{m}\nabla f_w = \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{p}'\,\mathcal{V}_w(\boldsymbol{r},\boldsymbol{p}-\boldsymbol{p}')f_w(\boldsymbol{r},\boldsymbol{p}')\,. \tag{36}$$

An alternative form[10] for the above equation can be obtained by expanding $V(\boldsymbol{r} \pm \boldsymbol{r}'/2)$ in powers of $\boldsymbol{r}'$:

$$\beta_V(\boldsymbol{r},\boldsymbol{r}') = V\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right) - V\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right) = \sum_{n\,odd} \frac{2}{n!}\nabla^n V(\boldsymbol{r})\cdot\left(\frac{\boldsymbol{r}'}{2}\right)^n . \tag{37}$$

If this expression is inserted into Eq.(33), the dynamical equation for the WF results

$$\frac{\partial f_w}{\partial t} + \frac{\boldsymbol{p}}{m}\nabla f_w = \sum_{n\,odd} \frac{1}{n!}\left(\frac{i\hbar}{2}\right)^{n-1} \nabla^n V(\boldsymbol{r})\cdot\nabla_p^n f_w(\boldsymbol{r},\boldsymbol{p}) . \tag{38}$$

This form is particularly meaningful, being an expansion in powers of $\hbar$. The first term in the expansion ($\hbar^0$) reproduces the classical BE, while further terms carry quantum effects of higher orders in $\hbar$. In particular, it is important to observe that the first quantum correction is of the order of $\hbar^2$ and that, for linear or quadratic potentials (constant or harmonic forces) the BE is rigorously correct. In such cases each δ-like contribution of the WF carries its value in phase space following a classical path, as anticipated in Sec.4.

Note, however, that, in general, the above expansion can be performed only if $V(\boldsymbol{r})$ is analytical in the whole region of interest.

5.3. *Classical Force*

The expansion developed in the previous section suggests a way to separate the effect of the classical force from quantum effects, by isolating the first term of such expansion. To this purpose let us define

$$\begin{aligned} \tilde{V}_{\pm}(\boldsymbol{r},\boldsymbol{r}') &= V\left(\boldsymbol{r}\pm\frac{\boldsymbol{r}'}{2}\right) - \nabla V(\boldsymbol{r})\cdot\left(\pm\frac{\boldsymbol{r}'}{2}\right) \\ \tilde{\beta}_V(\boldsymbol{r},\boldsymbol{r}') &= \tilde{V}_+(\boldsymbol{r},\boldsymbol{r}') - \tilde{V}_-(\boldsymbol{r},\boldsymbol{r}') . \end{aligned}$$

With such definitions the function $\beta_V(\boldsymbol{r},\boldsymbol{r}')$ defined in Eq.(37) takes the form

$$\beta_V(\boldsymbol{r},\boldsymbol{r}') = \tilde{\beta}_V(\boldsymbol{r},\boldsymbol{r}') + \nabla V(\boldsymbol{r})\cdot\boldsymbol{r}' . \tag{39}$$

With this separation, the dynamical equation for the WF becomes

$$\frac{\partial f_w}{\partial t} + \frac{\boldsymbol{p}}{m}\nabla f_w + \mathbf{F}\nabla_p f_w(\boldsymbol{r},\boldsymbol{p}) = \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{p}'\,\tilde{\mathcal{V}}_w(\boldsymbol{r},\boldsymbol{p}-\boldsymbol{p}')f_w(\boldsymbol{r},\boldsymbol{p}') , \tag{40}$$

where $\mathbf{F} = -\nabla V(\boldsymbol{r})$ is the classical force, and $\tilde{\mathcal{V}}_w(\boldsymbol{r},\boldsymbol{p})$ is defined as in Eq.(35) with the expression for $\tilde{\beta}_V$ in place of the function β_V.

The l.h.s. of Eq.(40) 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 Monte Carlo simulation of the Wigner equation with the above splitting between classical force, teken care of in the free flights, and quantum effects as collision

integral, is at present under development by the authors. A similar approach was introduces also by Lozovik and Filinov[24].

5.4. *Infinite Potential Barriers*

When an electron is confined in a limited region of space between high potential barriers, the theory of the WF can be developed either by considering the whole space and the affect of the high potential or by considering only the "inner" region with the request of vanishing wave function at the border. The latter solution is, in general, preferable but requires a revision of the theory, as we shall now see. Let us consider for simplicity a one dimensional case where the electron is confined in the x axis between a and b. A potential $V(x)$ can also be present. Since the Schrödinger equation holds only in the region between a and b, the WF must be defined with proper integration limits:

$$f_w(\boldsymbol{r},\boldsymbol{p}) = \int_{-\xi(x)}^{\xi(x)} dx' e^{-ipx'/\hbar} \Psi\left(x+\frac{x'}{2}\right)\Psi^*\left(x-\frac{x'}{2}\right), \tag{41}$$

where

$$\xi(x) = \begin{cases} 2(x-a) & \text{if } x < (a+b)/2 \\ 2(b-x) & \text{if } x \geq (a+b)/2 \end{cases}$$

The above limits of integration are determined by the conditions

$$a < x + \frac{x'}{2} < b \;\; ; \;\; a < x - \frac{x'}{2} < b \tag{42}$$

and are shown in Fig.4. Let us now take the time derivative of Eq.(41) and use the Schrödinger equation. For the kinetic term, following the same procedure as in Sec.5.1 we get to

$$\begin{aligned} i\hbar\frac{\partial f_w}{\partial t} &= -\frac{\hbar^2}{m}\int_{-\xi(x)}^{\xi(x)} dx' e^{-ipx'/\hbar}\frac{\partial}{\partial x'}\left[\Psi_x\left(x+\frac{x'}{2},t\right)\Psi^*\left(x-\frac{x'}{2},t\right)\right. \\ &\left. +\Psi^*\left(x+\frac{x'}{2},t\right)\Psi_x^*\left(x-\frac{x'}{2},t\right)\right], \end{aligned} \tag{43}$$

where $\Psi_x = \partial\Psi/\partial x$. Integration by part now leads to

$$\begin{aligned} i\hbar\frac{\partial f_w}{\partial t} &= -\frac{\hbar^2}{m}\left\{e^{-ipx'/\hbar}\left[\Psi_x\left(x+\frac{x'}{2},t\right)\Psi^*\left(x-\frac{x'}{2},t\right)\right.\right. \\ &\left.\left. + \Psi_x\left(x+\frac{x'}{2},t\right)\Psi_x^*\left(x-\frac{x'}{2},t\right)\right]\right|_{x'=-\xi(x)}^{x'=\xi(x)} \\ &-i\hbar\frac{p}{m}\int_{-\xi(x)}^{\xi(x)} dx' e^{-ipx'/\hbar}\frac{\partial}{\partial x'}\left[\Psi_x\left(x+\frac{x'}{2},t\right)\Psi^*\left(x-\frac{x'}{2},t\right)\right. \\ &\left. + \Psi^*\left(x+\frac{x'}{2},t\right)\Psi_x^*\left(x-\frac{x'}{2},t\right)\right]. \end{aligned} \tag{44}$$

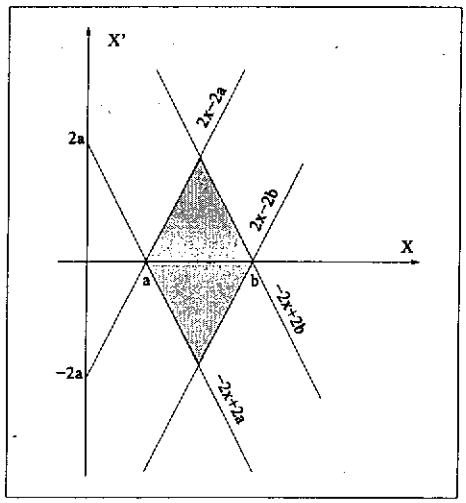

Fig. 4. Domain of integration for the definition of the WF for a particle in a box.

The second term (last two lines) on the r.h.s. leads to the usual term proportional to $\frac{p}{m}\frac{\partial f_w}{\partial t}$. The first two lines of the r.h.s. vanish when f_w is defined on the whole x axis. In our case, however, they do not vanish and lead to a new term in the Wigner equation:

$$\left.\frac{\partial f_w}{\partial t}\right|_B = \frac{i\hbar}{m}\left[e^{-ip\xi/\hbar}P_x(x,\xi,t) - e^{ip\xi/\hbar}P_x(x,-\xi,t)\right], \tag{45}$$

where

$$P(x,x',t) = \Psi\left(x+\frac{x'}{2},t\right)\Psi^*\left(x-\frac{x'}{2},t\right). \tag{46}$$

With the usual insertion of a δ-function in its plane waves representation, it is easy to show that

$$e^{-ip\xi/\hbar}P_x(x,\xi,t) = \frac{1}{2\pi\hbar}\int dp'\, e^{-i(p-p')\xi/\hbar}\frac{\partial}{\partial x}f_w(x,p',t). \tag{47}$$

This expression can be substituted into Eq.(45) to give

$$\left.\frac{\partial f_w}{\partial t}\right|_B = \frac{1}{\pi m}\int dp'\, \sin[(p-p')\xi/\hbar]\,\frac{\partial}{\partial x}f_w(x,p',t). \tag{48}$$

As regards the potential term, following the standard procedure the usual result is obtained, provided that in the definition of $\mathcal{V}_w(x,p)$ corresponding to Eq.(35) the

integral is evaluated in the range $(-\xi,\xi)$. Collecting the above results we may write the Wigner equation for an electron in a box as

$$\frac{\partial f_w}{\partial t} + \frac{p}{m}\frac{\partial f_w}{\partial x} = \frac{1}{(2\pi\hbar)}\int dp'\,\mathcal{V}_w(x,p-p')f_w(x,p',t) + \frac{1}{2\pi\hbar}\int dp'\,\mathcal{B}(x,p-p')\frac{\partial}{\partial x}f_w(x,p',t)\,, \tag{49}$$

where

$$\mathcal{B}(x,p) = \frac{2\hbar}{m}\sin\left[\frac{p}{\hbar}\xi(x)\right]. \tag{50}$$

In this expression $\xi(x)$ is determined by the closest barrier; if the electron is confined only in one direction by a single barrier, $\xi(x)$ will always be determined by that single barrier.

6. Phonon Interaction

When the case of an electron interacting with phonons is considered, it is convenient to use an extension of the definition of the WF. Let us begin with the definition of the function

$$g(\boldsymbol{r},\{n_q\},t) = e^{i\omega(\{n_q\})t}\Phi(\boldsymbol{r},\{n_q\},t)\,, \tag{51}$$

where

$$\Phi(\boldsymbol{r},\{n_q\},t) = \langle \boldsymbol{r},\{n_q\}|\Psi(t)\rangle\,. \tag{52}$$

Here $|\boldsymbol{r},\{n_q\}\rangle$ is the basis state with the electron in $\boldsymbol{r}$ and the phonon occupation numbers given by the set $\{n_q\}$; thus $\Phi(\boldsymbol{r},\{n_q\},t)$ is the wavefunction of the system in the state $|\Psi(t)\rangle$; the exponential factor in the definition of g cancels the time dependence due to the free phonons dynamics, being

$$\omega(\{n_q\}) = \frac{1}{\hbar}\sum_q n_q\hbar\omega_q\,. \tag{53}$$

The WF is now defined as the trace over the phonons

$$f_w(\boldsymbol{r},\boldsymbol{p},t) = \sum_{\{n_q\}} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q\},t)\,, \tag{54}$$

of

$$f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t) = \int d\boldsymbol{r}'\,e^{-i\boldsymbol{p}\boldsymbol{r}'/\hbar}g\left(r+\frac{r'}{2},\{n_q\},t\right)g^*\left(r-\frac{r'}{2},\{n'_q\},t\right). \tag{55}$$

where, once again, the bar of ensemble average is understood. This definition of the WF is slightly different from the one introduced previously by the authors[20] and will be better justified later, when the ω dependent WF will be discussed, starting from the Green function $G^<$. The hamiltonian of the system now contains, in addition, the free-phonon term $\mathcal{H}_p$ and the electron-phonon interaction $\mathcal{H}_{ep}$

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r) + \mathcal{H}_p + \mathcal{H}_{ep}\,, \tag{56}$$

where

$$\mathcal{H}_p = \sum_q \mathbf{b}_q^\dagger \mathbf{b}_q \hbar\omega_q; \tag{57}$$

and

$$\mathcal{H}_{ep} = \sum_q i\hbar F(\boldsymbol{q}) \left(\mathbf{b}_q e^{i\boldsymbol{q}\boldsymbol{r}} - \mathbf{b}_q^\dagger e^{-i\boldsymbol{q}\boldsymbol{r}}\right), \tag{58}$$

In the above expressions $\mathbf{b}_q$ and $\mathbf{b}_q^\dagger$ are the annihilation and creation operators for the phonon mode $\boldsymbol{q}$ with frequency ω_q and $F(\boldsymbol{q})$ is a real function depending on the type of phonon scattering analyzed.

In order to derive the dynamical equation for the new WF, let us consider that, even though we look for the time dependence of the WF defined in Eq.(54), a closed dynamical equation can be written only for the function $f_w^{(p)}$ since the electron-phonon interaction contains single phonon operators, and, therefore, the dynamical equation involves also terms non diagonal in the phonon state. The trace over the phonons will be performed on the solution and not on the equation. For simplicity in what follows also the function $f_w^{(p)}$ will be called WF, since the context will not allow ambiguity. The time derivative of Eq.(51) yields, after a simple calculation,

$$i\hbar\frac{\partial g}{\partial t} = (\mathcal{H} - \mathcal{H}_p)g\,. \tag{59}$$

When this expression is substituted into the derivative of $f_w^{(p)}$ as defined in Eq.(55), the terms of the hamiltonian depending only on the electron variables lead to the standard Wigner equation (36). As regards the electron-phonon hamiltonian, it gives rise to

$$\frac{\partial}{\partial t} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t)\bigg|_{ep} = \int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar} \sum_{q'} F(\boldsymbol{q}') \times$$

$$\left\{\left[\left(\mathbf{b}_{q'} e^{i\boldsymbol{q}'\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right)} - \mathbf{b}_{q'}^\dagger e^{-i\boldsymbol{q}'\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right)}\right) g\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},\{n_q\}\right)\right] g^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q'\}\right) -\right.$$

$$\left. g\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},\{n_q\}\right)\left[\left(\mathbf{b}_{q'} e^{i\boldsymbol{q}'\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right)} - \mathbf{b}_{q'}^\dagger e^{-i\boldsymbol{q}'\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right)}\right) g\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q'\}\right)\right]^*\right\}. \tag{60}$$

Now we note that

$$\begin{aligned}
\mathbf{b}_{q'} g\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q\},t\right) &= e^{i\omega(\{n_q\})t}\left\langle \boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q\}\middle|\mathbf{b}_{q'}\middle|\Psi(t)\right\rangle \\
&= e^{i\omega(\{n_q\})t}\left\langle \Psi(t)\middle|\mathbf{b}_{q'}^\dagger\middle|\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q\}\right\rangle^* \\
&= e^{-i\omega_{q'}t}\sqrt{n_{q'}+1}\, g\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_1,...,n_{q'}+1,...\},t\right),
\end{aligned} \tag{61}$$

and similarly

$$\mathbf{b}_{q'}^\dagger g\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q\},t\right) = e^{i\omega_{q'}t}\sqrt{n_{q'}}\, g\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_1,...,n_{q'}-1,...\},t\right). \tag{62}$$

If the above results are inserted into Eq. (60) we obtain four terms:

$$\left.\frac{\partial}{\partial t} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t)\right|_{ep} = \sum_{q'} F(\boldsymbol{q}') \times$$
$$\Big\{ e^{i(\boldsymbol{q}'\boldsymbol{r}-\omega_{q'}t)}\sqrt{n_{q'}+1}\, f_w^{(p)}(\boldsymbol{r},\boldsymbol{p}-\hbar\boldsymbol{q}'/2,\{n_1,...,n_{q'}+1,...\},\{n'_q\},t)$$
$$- e^{-i(\boldsymbol{q}'\boldsymbol{r}-\omega_{q'}t)}\sqrt{n_{q'}}\, f_w^{(p)}(\boldsymbol{r},\boldsymbol{p}+\hbar\boldsymbol{q}'/2,\{n_1,...,n_{q'}-1,...\},\{n'_q\},t)$$
$$+ e^{-i(\boldsymbol{q}'\boldsymbol{r}-\omega_{q'}t)}\sqrt{n'_{q'}+1}\, f_w^{(p)}(\boldsymbol{r},\boldsymbol{p}-\hbar\boldsymbol{q}'/2,\{n_q\},\{n'_1,...,n'_{q'}+1,...\},t)$$
$$- e^{i(\boldsymbol{q}'\boldsymbol{r}-\omega_{q'}t)}\sqrt{n'_{q'}}\, f_w^{(p)}(\boldsymbol{r},\boldsymbol{p}+\hbar\boldsymbol{q}'/2,\{n_q\},\{n'_1,...,n'_{q'}-1,...\},t)\Big\} . \quad (63)$$

In conclusion, the dynamical equation for $f_w^{(p)}$ for an electron subject to a constant or harmonic force $\mathbf{F}$, to a potential profile $V(\boldsymbol{r})$ and to the interaction with phonons, reads

$$\frac{\partial}{\partial t} f_w^{(p)} + \frac{\boldsymbol{p}}{m}\nabla f_w^{(p)} + \mathbf{F}\nabla_p f_w^{(p)} = \left.\frac{\partial}{\partial t} f_w^{(p)}\right|_V + \Xi\left(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t\right) \quad (64)$$

where the last two terms on the r.h.s. are given by Eq.(34) and Eq.(63), respectively.

The interaction of electrons with phonons in the Wigner formulation can be treated also in terms of the coefficients $f_{nm}(\boldsymbol{r},\boldsymbol{p})$ described in Sec.4. This approach can be useful when the eigenfunctions of the hamiltonian that includes the potential profile inside the system are known. Some results obtained with this method for the case of a step potential profile and of a double-barrier potential profile[20] in GaAs-based systems are presented in Fig.s 5 and 6, respectively.

Fig.5 shows the electron current as a function of the step-potential height as obtained with the ballistic WF (solid line) and with the WF corrected by the effect of (up to) one electron-phonon scattering process (full circles) switched on 50 fs before the "observation time". Comparison is presented with the outcome of a semiclassical calculation based on the Boltzmann equation in absence (dashed line) and in presence (dotted line) of phonon scattering. The quantum ballistic curve is always lower the the corresponding semiclassical one, and instead of reaching a saturation, it rises up to a maximum and then decreases. This is due to the fact that in the quantum picture increasing the potential step leads, as a consequence of quantum reflection, to a decrease of the transmission coefficent, that is, to a decrease of the current intensity. Finally in both quantum and semiclassical claculations the effect of the electron-phonon interaction is, as expected, a reduction of the current with respect to the ballistic case.

In Fig.6 the currentis displayed as a function of the applied bias for a double barrier potential profile. The solid line is obtained with the ballistic WF while the full circles (with the error bars) are the result of the calculations performed using te WF corrected for effect of (up to) one electron-phonon scattering process. The device consist of two AlGaAs barriers 0.28 eV high and 2.8 nm wide, separated by a GaAs layer of 5 nm. A constant external field has been applied to the structure.

Even considering the uncertainity introduced by problems of numerical accuracy, the effect of the electron-phonon interaction on the characteristic of the $I(V)$ curve is clearly detectable: the peak to valley current ratio is reduced and, in the highest voltage region, the current is encreased. These results can be interpreted in term of the loss of coherence and of the broadening of the resonance states, and are in agreement with those obtained by Frensley[25] and by Ragazzi *et al.*[26] using a semiclassical Boltzmann collision operator.

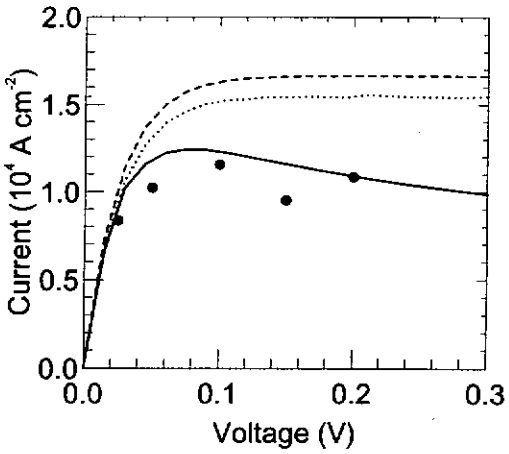

Fig. 5. Electron current across step potential as a function of the step height. In the figure a comparison between quantum and semiclassical calculations with and without e-ph interaction is shown. The following cases are reported: Wigner-ballistic curve (solid line), Wigner curve with one e-ph scattering (full circles), semiclassical ballistic curve (dashed line), semiclassical curve with e-ph scattering (dotted line). A value of the carrier density n at the contacts of $n = 10^{16}$ cm^{-3} has been assumed.

7. Wigner Paths

7.1. *Integral Equation*

The l.h.s. of Eq.(64) 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

$$f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t) \;=\; f_w^{(p)}\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t_o),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t_o),\{n_q\},\{n_q'\},t_o\right)$$

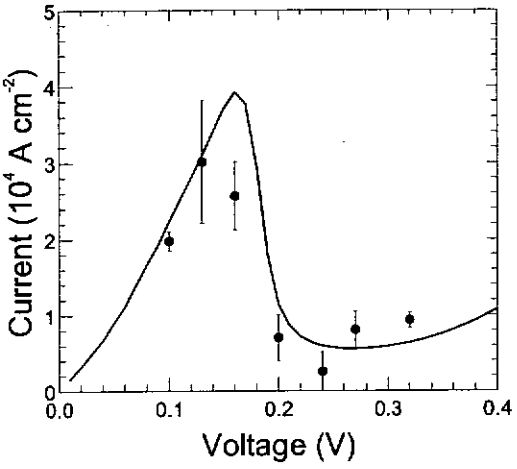

Fig. 6. Electron current as a function of the applied bias for the case of a double-barrier potential profile. A comparison is shown between the results obtained using the ballistic Wigner function (solid line) and the Wigner function corrected by the effect of an electron-phonon scattering process (full circles) switched on 50 fs before the "observation time".

$$+\int_{t_o}^{t} dt' \left\{ \int dp'\, \mathcal{V}_w \left(r^{(0)}(r,p,t\,;\,t'), p' - p^{(0)}(r,p,t\,;\,t') \right) \right.$$
$$\times f_w^{(p)} \left(r^{(0)}(r,p,t\,;\,t'), p', \{n_q\}, \{n_q'\}, t' \right)$$
$$\left. + \Xi \left(r^{(0)}(r,p,t\,;\,t'), p^{(0)}(r,p,t\,;\,t'), \{n_q\}, \{n_q'\}, t' \right) \right\}. \quad (65)$$

Here

$$\begin{cases} r^{(0)}(r,p,t\,;\,s) &= r - \frac{p}{m}(t-s) + \frac{F}{2m}(t-s)^2 \\ p^{(0)}(r,p,t\,;\,s) &= p - F(t-s) \end{cases} \quad (66)$$

are the position and the momentum of the particle at time s if at time t it has position r and momentum p; the upper (0) indicates that no scattering occurs between s and t. t_o represents the time of the initial condition, when the WF is supposed to be known. The integral equation (65) represents the WF at the point (r,p) at time t as sum of three contributions:

(a) A ballistic term, equal to the value of the WF at time t_o in the point on the trajectory of a classical particle which is in (r,p) at time t.

(b) A term collecting, for each time t' and each transferred momentum, contributions from the WF at points of phase space such that, after a scattering by

the potential, are on the "right" classical trajectory that reaches $(\boldsymbol{r},\boldsymbol{p})$ at time t. This term is multiplied by the transfer function $\mathcal{V}_w$ acting as a weighting factor.

(c) A term analogous to (b) due to the four contributions of the electron-phonon interaction.

7.2. *Neumann Expansion*

In more compact form, equation (65) can be written as

$$f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t) = f_\circ + \mathbf{S}_V f + \mathbf{S}_{af} f + \mathbf{S}_{ef} f + \mathbf{S}_{as} f + \mathbf{S}_{es} f \tag{67}$$

where

$$f_\circ = f_w^{(p)}\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t_\circ),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t_\circ),\{n_q\},\{n'_q\},t_\circ\right) \tag{68}$$

$$\mathbf{S}_V f = \int_{t_\circ}^{t} dt' \int d\boldsymbol{p}'\,\mathcal{V}_w\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t'),\boldsymbol{p}'-\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t')\right) \times f_w^{(p)}\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t'),\boldsymbol{p}',\{n_q\},\{n'_q\},t'\right) \tag{69}$$

$$\mathbf{S}_{af} f = \int_{t_\circ}^{t} dt' \sum_{q'} F(\boldsymbol{q}') e^{i\left(\boldsymbol{q}'\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t;t')-\omega_{q'}t'\right)}\sqrt{n_{q'}+1}$$

$$\times f_w^{(p)}\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t'),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t')-\hbar\boldsymbol{q}'/2,\{n_1,...,n_{q'}+1,...\},\{n'_q\},t'\right), \tag{70}$$

and $\mathbf{S}_{ef} f$, $\mathbf{S}_{as} f$, $\mathbf{S}_{es} f$ are defined, similarly to $\mathbf{S}_{af} f$, as the time integration of the three last terms on the r.h.s. of Eq.(63), respectively; a and e indicate an absortpion and an emission event, respectively, while f and s refer to the first and second phonon arguments, as defined in Eq.(55).

Eq.(67) 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:

$$f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t) = f_\circ + \sum_i \mathbf{S}_i f_\circ + \sum_{i,j} \mathbf{S}_i\mathbf{S}_j f_\circ + \sum_{i,j,k} \mathbf{S}_i\mathbf{S}_j\mathbf{S}_k f_\circ + ... \tag{71}$$

where $i,j,k = V, af, ef, as, es$.

As an example $\mathbf{S}_{es}\mathbf{S}_{ef} f_\circ$ corresponds to

$$\Delta_{es,ef} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t) = \int_{t_\circ}^{t} dt_1 \sum_{q'} \mathcal{F}(\boldsymbol{q}') e^{i\left(\boldsymbol{q}'\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;\,t_1)-\omega_{q'}t_1\right)}\sqrt{n'_{q'}}$$

$$\times \int_{t_\circ}^{t_1} dt_2 \sum_{q''} \mathcal{F}(\boldsymbol{q}'') e^{-i\left(\boldsymbol{q}''\boldsymbol{r}^{(1)}_{es}-\omega_{q''}t_2\right)}\sqrt{n_{q''}}$$

$$\times f_w^{(p)}\left(\boldsymbol{r}^{(2)}_{es,ef},\boldsymbol{p}^{(2)}_{es,ef},\{n_1,...,n_{q''}-1,...\},\{n'_1,...,n'_{q'}-1,...\},t_\circ\right). \tag{72}$$

Here

$$\boldsymbol{r}_{es}^{(1)} = \boldsymbol{r}_{es}^{(1)}\left(\boldsymbol{r},\boldsymbol{p},t\,;-\frac{\hbar\boldsymbol{q}'}{2},t_1\,;\,t_2\right) = \boldsymbol{r}-\frac{\boldsymbol{p}}{m}(t-t_1)-\frac{1}{m}\left(\boldsymbol{p}+\frac{\hbar\boldsymbol{q}'}{2}\right)(t_1-t_2)+\frac{\mathbf{F}}{2m}(t-t_2)^2 \tag{73}$$

is the position of the particle at time t_2 if at time t it has position $\boldsymbol{r}$ and momentum $\boldsymbol{p}$ and at time t_1 $(t_2 < t_1 < t)$ it undergoes an emission interaction vertex, a "half-scatering event", decreasing (in forward cronological order) the momentum by a quantity $\hbar\boldsymbol{q}'/2$, and

$$\begin{cases} \boldsymbol{r}_{es,ef}^{(2)} = \boldsymbol{r}_{es,ef}^{(2)}\left(\boldsymbol{r},\boldsymbol{p},t\,;-\frac{\hbar\boldsymbol{q}'}{2},t_1\,;-\frac{\hbar\boldsymbol{q}''}{2},t_2\,;\,t_o\right) \\ \qquad = \boldsymbol{r}-\frac{1}{m}\left(\boldsymbol{p}+\frac{\hbar\boldsymbol{q}'}{2}+\frac{\hbar\boldsymbol{q}''}{2}\right)(t_2-t_o)-\frac{1}{m}\left(\boldsymbol{p}+\frac{\hbar\boldsymbol{q}'}{2}\right)(t_1-t_2) \\ \qquad\quad -\frac{\boldsymbol{p}}{m}(t-t_1)+\frac{\mathbf{F}}{2m}(t-t_o)^2 \\ \\ \boldsymbol{p}_{es,ef}^{(2)} = \boldsymbol{p}_{es,ef}^{(2)}\left(\boldsymbol{r},\boldsymbol{p},t\,;-\frac{\hbar\boldsymbol{q}''}{2},t_1\,;-\frac{\hbar\boldsymbol{q}'}{2},t_2\,;\,t_o\right) = \boldsymbol{p}+\frac{\hbar\boldsymbol{q}'}{2}+\frac{\hbar\boldsymbol{q}''}{2}-\mathbf{F}(t-t_o)\,, \end{cases} \tag{74}$$

are the position and the momentum of the particle at time t_o if at time t it has position $\boldsymbol{r}$ and momentum $\boldsymbol{p}$, and it undergoes two emission vertices, the first at time t_2 and the second at time t_1 $(t_2 < t_1 < t)$, descreasing the momentum of the quantity $\hbar\boldsymbol{q}''/2$ and $\hbar\boldsymbol{q}'/2$ respexctively.

In general multiple-path variables can be defined as

$$\begin{cases} \boldsymbol{r}_{i,\ldots,j}^{(n)} = \boldsymbol{r}_{i,\ldots,j}^{(n)}\left(\boldsymbol{r},\boldsymbol{p},t\,;\,\Delta\boldsymbol{p}_1^i,t_1\,;\,\ldots\,;\,\Delta\boldsymbol{p}_n^j,t_n\,;\,t_o\right) \\ \qquad = \boldsymbol{r}-\frac{1}{m}\left(\boldsymbol{p}+\Delta\boldsymbol{p}_1^i+\ldots+\Delta\boldsymbol{p}_n^j\right)(t_n-t_o)-\ldots \\ \qquad\quad -\frac{1}{m}\left(\boldsymbol{p}+\Delta\boldsymbol{p}_1^i\right)(t_1-t_2)-\frac{\boldsymbol{p}}{m}(t-t_1)+\frac{\mathbf{F}}{2m}(t-t_o)^2 \\ \\ \boldsymbol{p}_{i,\ldots,j}^{(n)} = \boldsymbol{p}_{i,\ldots,j}^{(n)}\left(\boldsymbol{r},\boldsymbol{p},t\,;\,\Delta\boldsymbol{p}_1^i,t_1\,;\,\ldots\,;\,\Delta\boldsymbol{p}_n^j,t_n\,;\,t_o\right) = \boldsymbol{p}+\Delta\boldsymbol{p}_1^i+\ldots+\Delta\boldsymbol{p}_n^j \\ \qquad\qquad\qquad\qquad\qquad\qquad -\mathbf{F}(t-t_o)\,. \end{cases} \tag{75}$$

They represent the position and momentum of the particle at time t_o if at time t it has position $\boldsymbol{r}$ and mometum $\boldsymbol{p}$ after n interaction vertices, the first, at time t_n $(t_o < t_n < \ldots < t_1 < t)$, is due to the mechanism j and induces a variation $\Delta\boldsymbol{p}_n^j$ in the particle momentum, the last, at time t_1, is due to the mechanism i and induces a momentum variation $\Delta\boldsymbol{p}_1^i$ $(i,j = V,af,ef,as,es)$. It should be noticed that, in spite of the cumbersome notation, the physical meaning of the above development is quite simple: these multiple-paths correspond to the semiclassical ones where, in case of electron-phonon interaction, half of the phonon momentum is transferred to the electron at each interaction vertex, while the dynamics between the vertices is a ballistic evolution with the corresponding value of the momentum.

In Sec.(4) it was shown that for free electrons a single δ-like contribution of the WF keeps its value and its δ-character evolving in time along the classical path. In Sec.(5.2) it was shown that this situation extends to the case where a constant or harmonic force is applied to the particle. Eq.(65) 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 transferred momentum, again a δ-contribution of the WF keeps its δ-character.

These considerations allow us to define a Wigner path (WP)[27] as the multiple-path followed by a "simulative particle" carrying a δ contribution 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.

8. Monte Carlo Simulation

8.1. *Paths and Diagrams*

According to the discussion above, the evolution of the WF can be described by means of simulative particles following classical trajectories and experiencing two kinds of scattering:

(a) by potential $V(\boldsymbol{r})$ that changes particle's momentum of any quantity $\Delta\boldsymbol{p}$ with strenght $\mathcal{V}_w(\Delta\boldsymbol{p})$,

(b) by electron-phonon coupling term that increases (decreases) by one the number of phonons in $\boldsymbol{q}$ mode of a single set $\{n_q\}$ and decreases (increases) particle's momentum by $\frac{\hbar\boldsymbol{q}}{2}$.

The series obtained may be solved 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 [28].

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 $f^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t_o) \neq 0$ 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 defined in Eq.(54). As a consequence, only WPs with an even number of vertices involving a specific mode $\boldsymbol{q}$ are present. Under this hypothesis the second order example in Eq.(72) requires $\boldsymbol{q}' = \boldsymbol{q}''$ (see Fig.7) and can be rewritten as

$$\Delta_{es,ef} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q\},t) = \sum_{q'} F^2(\boldsymbol{q}') n_{q'} \int_{t_o}^{t} dt_1 \int_{t_o}^{t_1} dt_2 e^{i[\boldsymbol{q}\boldsymbol{r}_{12}-\omega_{q'}(t_1-t_2)]} \times f_w^{(p)}\left(\boldsymbol{r}_{es,ef}^{(2)},\boldsymbol{p}_{es,ef}^{(2)},\{n_1,...,n_{q'}-1,...\},\{n_1,...,n_{q'}-1,...\},t_o\right), \quad (76)$$

where $\boldsymbol{r}_{12}$ is the vector distance between the two interaction positions:

$$\boldsymbol{r}_{12} = \frac{1}{m}\left(\boldsymbol{p} - \hbar\frac{\boldsymbol{q}}{2}\right)(t_1 - t_2) - \frac{\mathbf{F}}{2m}(t_1 - t_2)^2 \quad (77)$$

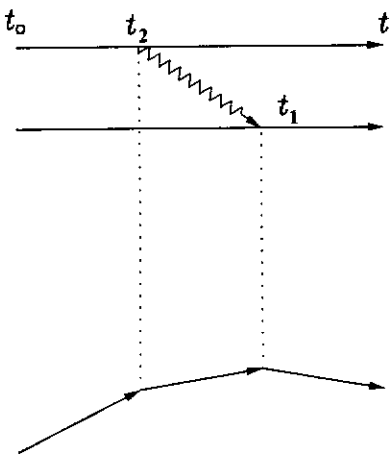

Fig. 7. Example of Wigner paths relative to a second-order contribution to the Neumann expansion of the $f_w^{(p)}$, corresponding to a real emission.

The above equation represents a specific second-order term of the Neumann expansion, corresponding to a path with two emission vertices, one on the first phonon argument at time t_2, the other on the second phonon argument at time t_1, with $t_o < t_2 < t_1 < t$. The expression for the second-order correction will contain each WP with two interaction vertices, and, due to the diagonality requirement, five "classes" of paths will survive:
(1) paths with two potential scatterings,
(2) paths with a real phonon absorption, containing two phonon absorption vertices of the same $\boldsymbol{q}$;
(3) paths with a real phonon emission, containing two phonon emission vertices of the same $\boldsymbol{q}$;
(4) paths with a virtual phonon emission, containing an emission vertex followed by the absorption vertex of the same mode;
(5) paths with a virtual phonon absortpion, containing an absorption vertex followed by the emission vertex of the same mode.
If the process corresponds to a real transition, the second momentum transfer adds to the first one, so that the total phonon momentum $\hbar\mathbf{q}$ is exchanged with the electron. For virtual transitions at the second vertex of the interaction half of the phonon momentum is given back to the phonon system and the electron recovers its original $\boldsymbol{p}$ value, apart from the effect of the field. The effect of the field between the two vertices gives rise to the intracollisional field effect. The modifications of

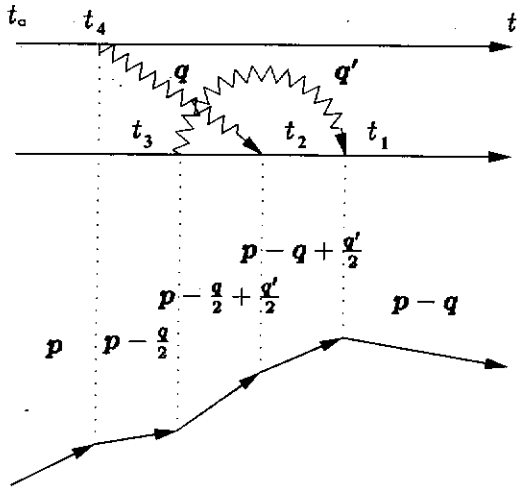

Fig. 8. Example of Wigner paths relative to a fourth-order contribution to the Neumann expansion of the $f_w^{(p)}$.

the electron paths due to virtual transitions are related to polaronic effects. In the classical limit, where the two vertices are considered infinitely close, real transitions become in-scattering events, while virtual transitions become out-scattering events and are related only to the life time of the state $\boldsymbol{p}$.

WP's are defined also for higher-order corrections (see, e.g., Fig.8). When time integrations and sums over $\boldsymbol{q}$ are sampled, each perturbative order contributes to the Wigner correction Δf_w with a sum over paths like those represented in Fig.s 7 and 8.

In a MC procedure for the evaluation of the WF the selection of the possible paths can be performed in many different ways either forward or backward in time. One possibility is shown in the flow-chart of Fig.9, where, for simplicity, only phonon scattering is considered.

8.2. *Multiplicity of the Wigner Paths*

The result of the numerical procedure is obtained by simulating a very large number of paths (according to the desired statistical precision) each weighted by a suitable factor. In the determination of this factor it must be taken into account also that a single WP corresponds to several possible diagrams. To evaluate such multiplicity let us consider first, as an example, the second-order term given in Eq.(76). As stated above, the second-order correction to the $f_w^{(p)}$ will contain each

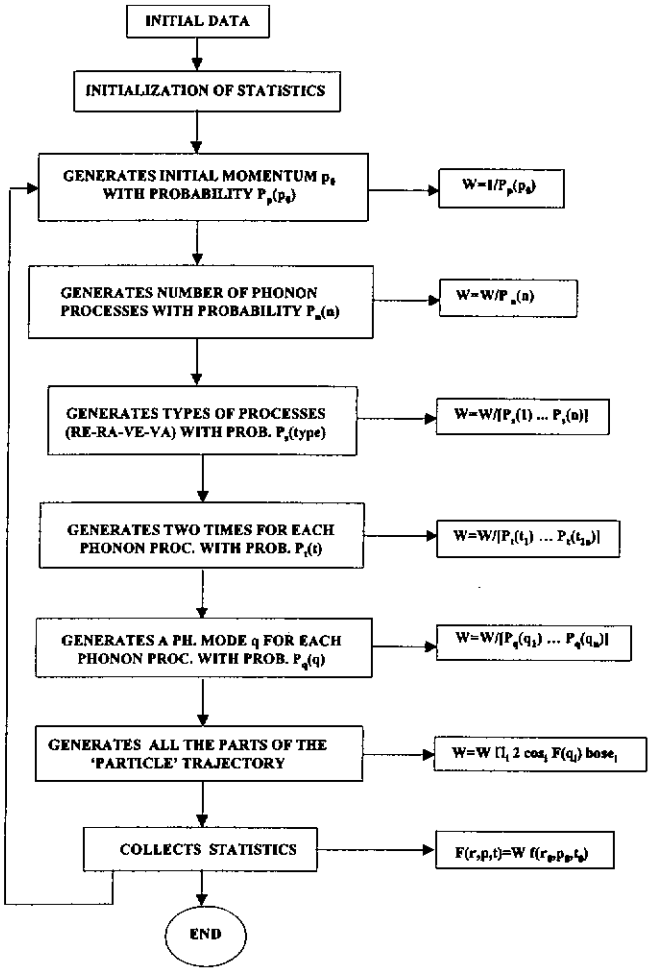

Fig. 9. Flow-chart of a possible quantum MC code. W is the weight of the path.

WP with two interaction vertices, namely $\Delta_{ef,es}$, and its complex conjugate $\Delta_{es,ef}$. As a consequence we get

$$(\Delta_{es,ef} + \Delta_{ef,es})\, f_w^{(p)}(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, \{n_q\}, t) = 2\Re\{\Delta_{es,ef}\}$$
$$= 2\sum_{q'} F^2(q') n_{q'} \int_{t_\circ}^{t} dt_1 \int_{t_\circ}^{t_1} dt_2 \cos[\boldsymbol{q}'\boldsymbol{r}_{12} - \omega_{q'}(t_1 - t_2)]$$
$$\times f_w^{(p)}\left(\boldsymbol{r}_{es,ef}^{(2)}, \boldsymbol{p}_{es,ef}^{(2)}, \{n_1, ..., n_{q'} - 1, ...\}, \{n_1, ..., n_{q'} - 1, ...\}, t_\circ\right), \quad (78)$$

where $\Re$ indicates the real part. The factor 2 that appears on the r.h.s. of the above equation, is the multiplicity of orbit described by Eq.(76) (a real emission) and represented in Fig.7. This consideration can be generalized to terms of any order. To this purpose, let us consider the fourth-order term shown in Fig.8. The diagram contains two scatterings, a real emission ($\overline{RE}$) and a virtual absorption ($\overline{VA}$), where the overbar means that we are considering the specific processes shown in Fig.8. $\overline{RE}$ corresponds to an emission of the momentum $\hbar\boldsymbol{q}/2$ at time t'''' on the first phonon argument, and to the emission of the momentum $\hbar\boldsymbol{q}/2$ at time t'' on the second phonon argument. $\overline{VA}$ is given by an absorption of $\hbar\boldsymbol{q}'/2$ on the second argument at time t''' and by an emission of $\hbar\boldsymbol{q}'/2$ always on the second argument at time t'. Among the infinite number of diagrams that have to be summed to obtain the fourth-order correction, there will always be the ones containing the complex conjugates of $\overline{RE}$ and/or $\overline{VA}$. $\overline{RE}^*$ is given by the emission of $\hbar\boldsymbol{q}/2$ on the second argument at time t'''' followed by the emission of $\hbar\boldsymbol{q}/2$ on the first argument at time t'', while $\overline{VA}^*$ corresponds to the ansorption of $\hbar\boldsymbol{q}'/2$ on the first argument at time t''', and to the emission of $\hbar\boldsymbol{q}'/2$ at time t' again on the first argument. So, in the full expression of the fourth-order correction, the WP in the lower part of Fig.8 collects contributions of the four diagrams:

$$\overline{RE}\cdot\overline{VA} + \overline{RE}^*\cdot\overline{VA} + \overline{RE}\cdot\overline{VA}^* + \overline{RE}^*\cdot\overline{VA}^* = 2\Re\{\overline{RE}\}\cdot 2\Re\{\overline{VA}\}, \quad (79)$$

where $\overline{RE}\cdot\overline{VA}$ is the one represented in the diagram in Fig.8. Then it turns out that also for the case of a fourth-order term (and in general of an n^{th}-order term) each electron-phonon scattering carries a multiplicity 2. In general the weight of each path containing m electron-phonon scatterings must include the cosine of the phonon phase and a multiplicity factor 2^m.

8.3. *Quantum Self-Scattering*

The numerical procedure described above is based on the simulation of a number of WP's, where the larger is the number of paths accounted for, the better is the statistical precision achieved. As a consequence, the simulation times required to obtain reliable results can be very long, thus constituting, so far, the main limitation to an extensive application of the method. However, the efficiency of the numerical algorithm can be improved by including the quantum self-scattering mechanism[30]. This method is based on the introduction of an appropriate immaginary part of

the self-energy $\Gamma = 1/\tau_o$ which plays a role analogous to that of the maximum scattering rate in the traditional MC method. At each perturbative order the exact correction to Γ is evaluated.

Let us define

$$\tilde{f}_w^{(p)}\left(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t\right) = e^{\Gamma(t-t_o)} f_w^{(p)}\left(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t\right), \tag{80}$$

performing the derivative with respect to time we get

$$\frac{\partial}{\partial t} f_w^{(p)} = -\Gamma e^{-\Gamma(t-t_o)} \tilde{f}_w^{(p)} + e^{-\Gamma(t-t_o)} \frac{\partial}{\partial t} \tilde{f}_w^{(p)}. \tag{81}$$

Substituting Eq.(81) into Eq.(64) and using Eq.(80) leads to

$$\frac{\partial}{\partial t}\tilde{f}_w^{(p)} + \frac{\boldsymbol{p}}{m}\nabla \tilde{f}_w^{(p)} + \mathbf{F}\nabla_p \tilde{f}_w^{(p)} = \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{p}' \mathcal{V}_w(\boldsymbol{r},\boldsymbol{p}-\boldsymbol{p}')\tilde{f}_w^{(p)}(\boldsymbol{r},\boldsymbol{p}') + \Xi\left(\tilde{f}_w^{(p)}\right) + \Gamma \tilde{f}_w^{(p)} \tag{82}$$

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

Following the same procedure described above, that is introducing path variables and intagrating over time, we obtain

$$\begin{aligned}
\tilde{f}_w^{(p)}\left(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t\right) &= f_w^{(p)}\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t_o),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t_o),\{n_q\},\{n_q'\},t_o\right) \\
&+ \int_{t_o}^{t} dt' \left\{ \int d\boldsymbol{p}'\, \mathcal{V}_w\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t'),\boldsymbol{p}'-\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t')\right)\right. \\
&\quad \times \tilde{f}_w^{(p)}\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t'),\boldsymbol{p}',\{n_q\},\{n_q'\},t'\right) \\
&\quad + \Gamma \tilde{f}_w^{(p)}\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t'),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t'),\{n_q\},\{n_q'\},t'\right) \\
&\quad \left. + \Xi\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t'),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t'),\{n_q\},\{n_q'\},t'\right)\right\}
\end{aligned} \tag{83}$$

where it has been taken into account that at t_o $\tilde{f}_w^{(p)}$ and $f_w^{(p)}$ coincide, and in the expression of $\Xi\left(\boldsymbol{r}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t'),\boldsymbol{p}^{(0)}(\boldsymbol{r},\boldsymbol{p},t\,;t'),\{n_q\},\{n_q'\},t'\right)$ (see Eq.(63)) $f_w^{(p)}$ is substituted by $\tilde{f}_w^{(p)}$.

As already specified, the above equation is solved iteratively. When the iteration is arrested at the desired order, each $\tilde{f}_w^{(p)}(t)$ on the r.h.s. of Eq.(83) is evaluated at time t_o, and therefore substituted by $f_w^{(p)}(t_o)$. Then solving for $f_w^{(p)}(t)$ corresponds to mulply each interaction term by the damping factor $e^{-\Gamma(t-t_o)}$ related to an electron "mean free time" $\tau_o = 1/\Gamma$. As an example, the second order correction given in Eq.(76) becomes

$$\begin{aligned}
&\Delta_{es,ef} f_w^{(p)}(r,\boldsymbol{p},\{n_q\},\{n_q\},t) = e^{-\Gamma(t-t_o)} \sum_{q'} F^2(\boldsymbol{q}') n_{q'} \int_{t_o}^{t} dt_1 \int_{t_o}^{t_1} dt_2\, e^{i\boldsymbol{q}\boldsymbol{r}_{12}} \\
&\times e^{-i\omega_{q'}(t_1-t_2)} f_w^{(p)}\left(\boldsymbol{r}_{es,ef}^{(2)},\boldsymbol{p}_{es,ef}^{(2)},\{n_1,...,n_{q'}-1,...\},\{n_1,...,n_{q'}-1,...\},t_o\right).
\end{aligned} \tag{84}$$

τ_o, however, is not the correct lifetime, and the corrections are included at each order by the self-scattering processes. In fact, among the interactions at each vertex, Γ must be also considered as a possibility, and, if selected, the electron in the WP continues unperturbed its free flight. In the weighted MC technique, the estimator of the WF obtained with a given WP contains the damping factor $e^{-\Gamma(t-t_o)}$ in the numerator and the probability $P(t_1, ..., t_n)$ of the vertex times in the denominator. If the free-flight durations are selected with the constant rate Γ, the two factors cancel. As a consequence, for long times t, terms with few quantum processes automatically give small contributions because they are generated rarely, while for short times this happens for the terms with many processes. For this reason the introduction of the quantum self-scattering produces an appreciable decrease of the statistical variance of the results, thus allowing to reduce the number of paths simulated with respect to the case where no quantum self-scattering is included.

8.4. *Phonon Average*

A crucial point that deserves further analysis is how to perform the average over the phonon variables[31]. We assume an initial condition for $f_w^{(p)}$ which is the product of an electron distribution function and of the equilibrium phonon distribution function; furthermore, the interaction hamiltonian is linear in the creation and annihilation operators of modes $\boldsymbol{q}$.

In the numerical procedure WP's are generated that start from an initial state $(\boldsymbol{p}_{in}, \{n_{q\,in}\}, t_o)$ and ends on the state $(\boldsymbol{p}, \{n_q\}, t)$. Each path contains a sequence of phonon wave-vectors $\boldsymbol{q}$ which are absorbed or emitted. As long as we are not interested in hot-phonon effects the electron always interacts with an equilibrium bath and we can assume that each phonon mode is chosen only once in a given sequence of processes.

If a phonon $\boldsymbol{q}$ is absorbed in a real transition and the corresponding occupation number at time t is n_q, the occupation number of the initial state must be $(n_q + 1)$, and the matrix element of the interaction hamiltonian contains the factor $\sqrt{n_q + 1}$. In order to finish the process the hamiltonian must act on the other argument of $f_w^{(p)}$ in the same way, thus bringing the moltiplicative factor $(n_q + 1)$ to the numerical estimator. In the case of virtual absorption one argument is first changed from $(\boldsymbol{p}, n_q)$ to $(\boldsymbol{p}' = \boldsymbol{p} + \hbar\boldsymbol{q}/2, n_q - 1)$ with an absortpion, and then from $(\boldsymbol{p}', n_q - 1)$ back to $(\boldsymbol{p}, n_q)$ at a successive time through an emission of the same mode. The net result after the completion of the process is the presence of a multiplicative factor n_q in the numerical estimator. Analogous considerations show that for the case of real or virtual emissions the multiplicative factor is n_q or $n_q + 1$, respectively.

For each generated multiple WP of order $2n$ (here n indicates the number of electron-phonon scatterings in the path) an estimator is evaluated that, once averaged over the possible initial phonon states, gives rise to a contribution of the

form

$$\Delta f_w^{(p)(2n)} \propto \sum_{\{n_q\}_{in}} f_w^{(p)}\left(\boldsymbol{r}_{\rm in}^{(2n)}, \boldsymbol{p}_{\rm in}^{(2n)}, \{n_q\}_{\rm in}, \{n_q\}_{\rm in}, t_o\right) P_{eq}\left(\{n_q\}_{\rm in}\right) \prod_q N_q\,, \quad (85)$$

where $\{n_q\}_{\rm in}$ are the occupation numbers of the modes $\boldsymbol{q}$ in the initial state, $P_{eq}\left(\{n_q\}\right)$ is the probability od finding each mode $\boldsymbol{q}$ occupaied by n_q phonons at equilibrium, and N_q is a multiplicative factor that takes the values n_q or n_q+1, as seen above, for the phonon modes $\boldsymbol{q}$ involved in the generated sequence, and 1 for all the other phonon modes not involved in the process. Now we know that $P\left(\{n_q\}_{\rm in}\right)$ is given by the product $\prod_q P_{eq}(n_q)$. If a phonon $\boldsymbol{q}$ is not chosen, then the sum over all possible occupation numbers n_q of $P_{eq}(n_{q\,\rm in})$ must be equal to unity,

$$\sum_{n_q} P_{eq}(n_{q\,\rm in}) = 1\,, \quad (86)$$

and this factor does not contribute to the product in Eq. (85). If instead we consider a $\boldsymbol{q}$ chosen in the random generation, we have two possible cases. In the case of absorption,

$$\sum_{n_q}(n_q+1)P_{eq}(n_q+1) = n_q|_{\rm Bose} \qquad \text{(real absorption)} \quad (87)$$

$$\sum_{n_q} n_q\, P_{eq}(n_q) = n_q|_{\rm Bose} \qquad \text{(virtual absorption)} \quad (88)$$

where $n_q|_{Bose}$ is the equilibrium occupation number given by the Bose distribution. In the case of emission,

$$\sum_{n_q} n_q\, P_{eq}(n_q-1) = n_q|_{\rm Bose}+1 \qquad \text{(real emission)} \quad (89)$$

$$\sum_{n_q}(n_q+1)\, P_{eq}(n_q) = n_q|_{\rm Bose}+1 \qquad \text{(virtual emission)}\,. \quad (90)$$

In both cases we use the Bose distribution for the evaluation of the term without introducing any approximation on the electron-phonon coupling but for the assumption thatthe phonon gas is constantly kept in equilibrium conditions. In full analogy with the semiclassical treatment the recipe consists in using $n_q|_{\rm Bose}$ in the case of absorptions, and $n_q|_{\rm Bose}+1$ in the case of emissions.

8.5. *Some Numerical Results*

An important application of the method of the WP's is the comparison between classical and quantum scattering. Results obtained for different contributions to the scattering terms of the Wigner and Boltzmann transport equations have been compared[29]. As an example the term in the Neumann expansion in the Boltzmann equation describing two in-scattering phonon-emission events and the corresponding terms of the Neumann expansion of the Wigner equation (four-vertices terms

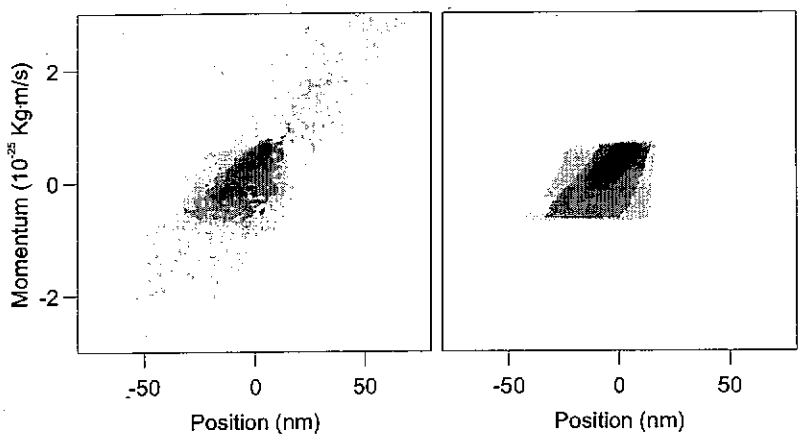

Fig. 10. Comparison between the quantum Wigner contribution (left) and the semiclassical contribution (right) to the distribution coming from two real phonon emissions of an electron starting from a given (z, p_z) phase-space point.

associated with two real emissions) have been considered. Fig.10 (right) shows the result for the semiclassical calculation at time $t = 100$ fs after the initial condition. The semiclassical electrons start from a well defined initial state (z, p_z). Fig.10 (left) shows the result for the quantum calculation assuming the same initial condition for a δ-like WF, or "simulative particle". Integration is performed over the possible interaction times and phonon modes $\mathbf{q}$. It is seen that the interference present in the calculation of the quantum term, at the considered time (100 fs), already reproduces to a good extent the classical energy/momentum conserving structure seen in the corresponding classical term. However a broadening of the distribution over a larger portion of the phase space is present in the quantum case since within 100 fs transitions that do not strictly conserve energy may be effective. This effect is more evident in Fig.11 (left) that shows the quantum distribution as a function of energy after the two real emissions (continuous line). Since in this case no field is applied, in the classical picture the distribution in Fig.11 would be a delta function at the energy indicated on the figure by the arrow. Contributions coming from separate (dashed line) and from multiple (dotted line) scatterings,corresponding to crossed graphs, have been independently evaluated by means of Monte Carlo generations of the corresponding WP's. It is seen that the large energy broadening present at the considered time in the term associated with separate scatterings is reduced by the contribution coming from multiple collisions. Furthermore, this last contribution shifts the energy value of the peak towards the classical conservation energy. This

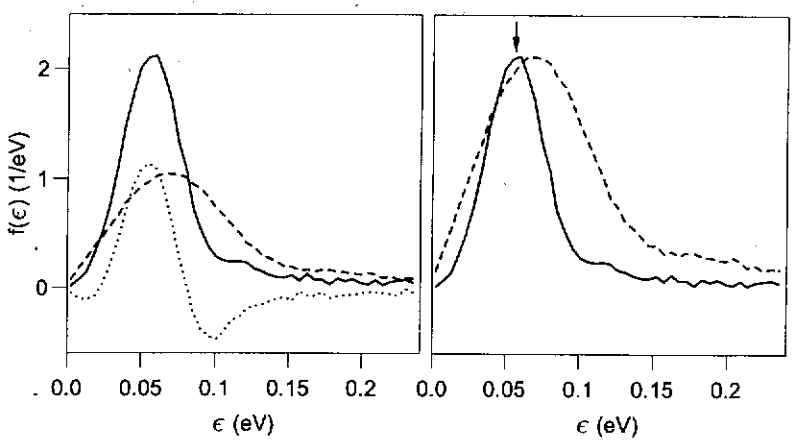

Fig. 11. Contribution to the energy distribution of the scattering term associated with two real phonon emissions. Left: total contribution (solid line), separate-scattering contribution (dashed line), multiple-scattering contribution (dotted line). Right: comparison between the total contribution (solid line) and the separate-scattering contribution (dashed line) renormalized to the same maximum value. The arrow indicates the energy-conservation value predicted by the semiclassical theory.

effect can be better seen in the right part of Fig.11, where the total distribution and the one for separate scatterings are plotted together, normalized to the same maximum value. We can conclude that the quantum correction including multiple scatterings is closer to the semiclassical result based on the assumption of completed collisions with respect to the quantum case where only separate scatterings are considered.

Preliminary calculations performed with the density-matrix aproach for the homogeneous case confirm that the inclusion of only separate collisions in the quantum approach deteriorates the agreement between quantum and semiclassical predictions.

9. p and ω Dependent Wigner Function from the $G^<$ Green Function

The WF introduced by Wigner in elementary terms in 1932, has been generalized in more recent times as a Fourier Transform of the $G^<$ Green function[6]. In this case a two-time correlation function is considered and the Fourier transform with respect to the time difference leads to a dependence of the WF on energy that appears as a new variable independent from momentum.

In this section we show how this new definition can be extended to the case of

an electron interacting with phonons; how it reduces to the more traditional WF in the limit of two equal times, and, above all, how the simulative approach described in the previous section can be naturally extended to determine the momentum and energy dependent WF.

Let us start from the definition

$$G^<(\boldsymbol{r}_1,t_1;\boldsymbol{r}_2,t_2)=\frac{i}{\hbar}\langle\Psi^\dagger(\boldsymbol{r}_2,t_2)\Psi(\boldsymbol{r}_1,t_1)\rangle=\frac{i}{\hbar}\langle\Phi_H|\Psi^\dagger(\boldsymbol{r}_2,t_2)\Psi(\boldsymbol{r}_1,t_1)|\Phi_H\rangle \quad (91)$$

where Ψ and $\Psi^\dagger$ are the electron annihilation and creation field operators, $\langle\rangle$ indicates quantum average, and Φ_H is the state of the system in the Heisenberg picture. As in the rest of this paper, in the last term of Eq.(91) the bar of ensemble average is uderstood. Moving to the Schrödinger picture we obtain

$$\begin{aligned}&G^<(\boldsymbol{r}_1,t_1;\boldsymbol{r}_2,t_2)\\&=\frac{i}{\hbar}\langle\Phi(t_2)|U(t_2,t_\circ)U^\dagger(t_2,t_\circ)\Psi^\dagger(\boldsymbol{r}_2)U(t_2,t_\circ)U^\dagger(t_1,t_\circ)\Psi(\boldsymbol{r}_1)U(t_1,t_\circ)U^\dagger(t_1,t_\circ)|\Phi(t_1)\rangle\\&=\frac{i}{\hbar}\langle\Phi(t_2)|\Psi^\dagger(\boldsymbol{r}_2)U(t_2,t_1)\Psi(\boldsymbol{r}_1)|\Phi(t_1)\rangle\,,\end{aligned} \quad (92)$$

where $U(t,t_\circ)$ is the evolution operator. Now we assume that our system is formed by a single electron interacting with the phonons and define the wavefunction

$$\Phi(\boldsymbol{r},\{n_q\},t)=\langle\boldsymbol{r},\{n_q\}|\Phi(t)\rangle\,. \quad (93)$$

In second quantization, the state vector is given by

$$|\Phi(t)\rangle=\int d\boldsymbol{r}\sum_{\{n_q\}}\Phi(\boldsymbol{r},\{n_q\},t)\Psi^\dagger(\boldsymbol{r})|\{n_q\},0\rangle \quad (94)$$

where $|\{n_q\},0\rangle$ is the state with $\{n_q\}$ phonons and no electron. If this expression is inserted into Eq.(92), we obtain

$$\begin{aligned}&G^<(\boldsymbol{r}_1,t_1;\boldsymbol{r}_2,t_2)=\frac{i}{\hbar}\int d\boldsymbol{r}\sum_{\{n_q\}}\int d\boldsymbol{r}'\sum_{\{n'_q\}}\\&\langle\{n_q\},0|\Psi(\boldsymbol{r})\Phi^*(\boldsymbol{r},\{n_q\},t_2)\Psi^\dagger(\boldsymbol{r}_2)U(t_2,t_1)\Psi(\boldsymbol{r}_1)\Phi(\boldsymbol{r}',\{n'_q\},t_1)\Psi^\dagger(\boldsymbol{r}')|\{n'_q\},0\rangle\end{aligned} \quad (95)$$

Now using

$$[\Psi(\boldsymbol{r}),\Psi^\dagger(\boldsymbol{r}')]_+=\delta(\boldsymbol{r}-\boldsymbol{r}')\,.$$

we obtain

$$\Psi(\boldsymbol{r}_1)\Psi^\dagger(\boldsymbol{r}')|0\rangle=\delta(\boldsymbol{r}_1-\boldsymbol{r}')|0\rangle$$

and

$$\langle0|\Psi(\boldsymbol{r})\Psi^\dagger(\boldsymbol{r}_2)=\langle0|\delta(\boldsymbol{r}-\boldsymbol{r}_2)$$

then Eq.(92) rewrites

$$G^<(\boldsymbol{r}_1,t_1;\boldsymbol{r}_2,t_2) = \frac{i}{\hbar}\int d\boldsymbol{r}\sum_{\{n_q\}}\int d\boldsymbol{r}'\sum_{\{n_q'\}}$$
$$\times\langle\{n_q\},0|\delta(\boldsymbol{r}-\boldsymbol{r}_2)\Phi^*(\boldsymbol{r},\{n_q\},t_2)U(t_2,t_1)\Phi(\boldsymbol{r}',\{n_q'\},t_1)\delta(\boldsymbol{r}_1-\boldsymbol{r}')|\{n_q'\},0\rangle$$
$$= \frac{i}{\hbar}\sum_{\{n_q'\}}\sum_{\{n_q'\}}\Phi^*(\boldsymbol{r}_2,\{n_q\},t_2)\Phi(\boldsymbol{r}_1,\{n_q'\},t_1)\langle\{n_q\},0|U(t_2,t_1)|\{n_q'\},0\rangle\,. \quad (96)$$

In order to continue, it is now necessary to make some assumptions on the evolution operator and therefore on the hamiltonian that describes the dynamics of the system. Here the hamiltonian is given by Eq.(56). If the evolution operator is developed in series of powers of the hamiltonian, it will contain the sum of the number 1 plus terms given by products of field operator that, except for $\mathcal{H}_p$ have on the right electron annihilation operators. Applied to the vacuum state, these latter give zero. Thus, the expression for $G^<$ becomes

$$G^<(\boldsymbol{r}_1,t_1;\boldsymbol{r}_2,t_2) = \frac{i}{\hbar}\sum_{\{n_q\}}\sum_{\{n_q'\}}\Phi^*(\boldsymbol{r}_2,\{n_q\},t_2)\Phi(\boldsymbol{r}_1,\{n_q'\},t_1)\langle\{n_q\},0|e^{-i\mathcal{H}_p(t_2-t_1)/\hbar}|\{n_q'\},0\rangle$$
$$= \frac{i}{\hbar}\sum_{\{n_q\}}\sum_{\{n_q'\}}\Phi^*(\boldsymbol{r}_2,\{n_q\},t_2)\Phi(\boldsymbol{r}_1,\{n_q'\},t_1)e^{-i\omega(\{n_q\})(t_2-t_1)}\langle\{n_q\},0|\{n_q'\},0\rangle$$
$$= \frac{i}{\hbar}\sum_{\{n_q\}}e^{-i\omega(\{n_q\})(t_2-t_1)}\Phi^*(\boldsymbol{r}_2,\{n_q\},t_2)\Phi(\boldsymbol{r}_1,\{n_q\},t_1)\,.$$

Then, using the definition given in Eq.(51)

$$G^<(\boldsymbol{r}_1,t_1;\boldsymbol{r}_2,t_2) = \frac{i}{\hbar}\sum_{\{n_q\}}g^*(\boldsymbol{r}_2,\{n_q\},t_2)g(\boldsymbol{r}_1,\{n_q\},t_1)\,. \quad (97)$$

Now we put

$$t = \frac{t_1+t_2}{2}, \quad \tau = t_2 - t_1$$

and

$$\boldsymbol{r} = \frac{\boldsymbol{r}_1+\boldsymbol{r}_2}{2}, \quad \boldsymbol{r}' = \boldsymbol{r}_2-\boldsymbol{r}_1$$

and perform the Fourier transform

$$G^<(\boldsymbol{r},\boldsymbol{p},t,\omega) = \frac{i}{\hbar}\sum_{\{n_q\}}\int d\boldsymbol{r}'\,e^{i\boldsymbol{p}\boldsymbol{r}'/\hbar}$$
$$\times\int d\tau\,e^{-i\omega\tau}g^*\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},\{n_q\},t+\frac{\tau}{2}\right)g\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q\},t-\frac{\tau}{2}\right). \quad (98)$$

We then obtain the Wigner function as

$$f_w(\boldsymbol{r},\boldsymbol{p},t,\omega) = -i\hbar G^< = \sum_{\{n_q\}}\int d\boldsymbol{r}'\,e^{-i\boldsymbol{p}\boldsymbol{r}'/\hbar}$$
$$\times\int d\tau\,e^{-i\omega\tau}g\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},\{n_q\},t+\frac{\tau}{2}\right)g^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q\},t-\frac{\tau}{2}\right). \quad (99)$$

We generalize now to non diagonal elemets with respect to phonon states

$$f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t,\omega) = \int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\boldsymbol{r}'/\hbar} \times \int d\tau\, e^{-i\omega\tau} g\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},\{n_q\},t+\frac{\tau}{2}\right) g^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q'\},t-\frac{\tau}{2}\right). \quad (100)$$

With this definition the Wigner function is defined as the trace over the phonon states

$$f_w(\boldsymbol{r},\boldsymbol{p},t,\omega) = \sum_{\{n_q\}} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q\},t,\omega)\,. \quad (101)$$

In order to derive the dynamical equation for the WF defined in Eq.(100) we follow the same procedure already developed in Sec.(6), obtaining

$$\frac{\partial}{\partial t} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t,\omega) = \int d\boldsymbol{r}'\, e^{-i\boldsymbol{p}\boldsymbol{r}'/\hbar} \int d\tau\, e^{-i\omega\tau} \times \frac{1}{i\hbar}\left\{\left[(\mathcal{H}-\mathcal{H}_p)\, g\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},\{n_q\},t+\frac{\tau}{2}\right)\right] g^*\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q'\},t-\frac{\tau}{2}\right) - g\left(\boldsymbol{r}+\frac{\boldsymbol{r}'}{2},\{n_q\},t+\frac{\tau}{2}\right)\left[(\mathcal{H}-\mathcal{H}_p)\, g\left(\boldsymbol{r}-\frac{\boldsymbol{r}'}{2},\{n_q'\},t-\frac{\tau}{2}\right)\right]^*\right\}, \quad (102)$$

where, as for the case of Sec.6, the free-phonon hamiltonian has been eliminated. Now the evaluation of the effects of each term of the hamiltonian on the dynamics proceeds in complete analogy with the derivations developed in Sec.s 5 and 6.

For the kinetic term we get

$$\left.\frac{\partial}{\partial t} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t,\omega)\right|_{\circ} + \frac{\boldsymbol{p}}{m}\nabla f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t,\omega) = 0 \quad (103)$$

formally identical to Eq.(32).

When the term $V(\boldsymbol{r})$ is considered, the following expression is derived

$$\left.\frac{\partial}{\partial t} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t,\omega)\right|_{V} = \int d\boldsymbol{p}'\mathcal{V}_w(\boldsymbol{r},\boldsymbol{p}-\boldsymbol{p}') f_w^{(p)}(\boldsymbol{r},\boldsymbol{p}',\{n_q\},\{n_q'\},t,\omega)\,, \quad (104)$$

again formally identical to Eq.(34), where $\mathcal{V}_w$ is given by Eq.(35). As for the case of Sec.5.3, the introduction of a constant or elastic force $\mathbf{F}$ leads to

$$\left.\frac{\partial}{\partial t} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t,\omega)\right|_{F} = -\mathbf{F}\nabla_p f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t,\omega)\,. \quad (105)$$

The electron-phonon interaction gives rise to the term

$$\left.\frac{\partial}{\partial t} f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n_q'\},t,\omega)\right|_{ep} = \sum_{q'} F(\boldsymbol{q}') \times \left\{ e^{i(\boldsymbol{q}'\boldsymbol{r}-\omega_{q'}t)}\sqrt{n_{q'}+1}\, f_w^{(p)}(\boldsymbol{r},\boldsymbol{p}-\hbar\boldsymbol{q}'/2,\{n_1,...,n_{q'}+1,...\},\{n_q'\},t,\omega-\omega_{q'}/2)\right.$$

$$
\begin{aligned}
&- e^{-i(\boldsymbol{q}'\boldsymbol{r}-\omega_{q'}t)}\sqrt{n_{q'}}\, f_w^{(p)}(\boldsymbol{r},\boldsymbol{p}+\hbar\boldsymbol{q}'/2,\{n_1,...,n_{q'}-1,...\},\{n'_q\},t,\omega+\omega_{q'}/2)\\
&+ e^{-i(\boldsymbol{q}'\boldsymbol{r}-\omega_{q'}t)}\sqrt{n'_{q'}+1}\, f_w^{(p)}(\boldsymbol{r},\boldsymbol{p}-\hbar\boldsymbol{q}'/2,\{n_q\},\{n'_1,...,n'_{q'}+1,...\},t,\omega-\omega_{q'}/2)\\
&- e^{i(\boldsymbol{q}'\boldsymbol{r}-\omega_{q'}t)}\sqrt{n'_{q'}}\, f_w^{(p)}(\boldsymbol{r},\boldsymbol{p}+\hbar\boldsymbol{q}'/2,\{n_q\},\{n'_1,...,n'_{q'}-1,...\},t,\omega+\omega_{q'}/2)\Big\} \quad (106)
\end{aligned}
$$

which is the equivalent to Eq.(63). In this case at each interaction vertex half of the phonon frequency is exchanged with the electron (as well as half of the phonon momentum as in the case of equal time WF).

In conclusion, a dynamical equation formally identical to Eq.(64) is derived for $f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t,\omega)$ where the last two terms on the r.h.s. are given by Eq.s(104) and (106), respectively.

As a consequence of such formal analogy, the concept of WP described above is still applicable and allows to extend the MC procedure based on the generation of WP already used to evaluate the single-time WF to the calculation of $f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t,\omega)$. The only requirement to be added in the sequence of random choices and operations which define a particular path is that at each electron-phonon interaction vertex half of the phonon frequency (besides half of the phonon momentum) is either added or substracted to the electron energy according to the selected integrand in the r.h.s. of Eq.(106). Since energy is not exactly conserved in the scattering process, momentum and energy are now independent variables. A MC algorithm simulating the time evolution of $f_w^{(p)}(\boldsymbol{r},\boldsymbol{p},\{n_q\},\{n'_q\},t,\omega)$ in the presence of electron-phonon scattering is at present under development by the authors[32].

10. Conclusions

In this paper we have reviewed the Wigner approach to quantum electron transport in semiconductors. We have shown that a multiple-path formalism can be developed in strict analogy with the semiclassical formalism. The main differences in the quantum approach are:

a) The effect of the potential includes quantum features (as, for example, tunneling) and reduces to the classical limit only for linear or parabolic potantials. In treating the potential we have shown how to separate quantum effects from the classical force.

b) A single phonon scattering process it is described by two vertices in the WP (at each vertex half of the phono momentum is exchanged with the electron) and automatically includes intracollisional field effects and collisional broadening.

Based on the above analogy, MC algorithms can be developed similar to a traditional semiclassical MC, even though rigorous from the quantum mechanical viewpoint. Multiple-paths allow to Monte Carlo simulate open systems with given boundary conditions, in principle also when electrons enter from the contacts while are already interacting with the phonon bayh. Finally, the connection with the $G^<$ function leads to a WF dependent on $\boldsymbol{p}$ and ω separately, and such WF can be simulated by

means of a MC program (in this case at each interaction vertex half of the phonon frequency besides half of the phonon momentum is exchanged with the electron).

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