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Wigner Paths and Boundary Conditions for Electron Transport in Open Systems with Electron-Phonon Interaction

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A Wigner-function approach to the study of quantum transport in open systems in presence of phonon scattering is presented. Two important issues will be discussed in the paper: a) the existence of Wigner paths in phase space with many analogies with the semiclassical description of transport and b) how to deal with boundary conditions for the analysis of real open structures. Theoretical and computational results will be discussed in view of the application of this formalism to the simulation of transport in mesoscopic structures.

1. Introduction

Charge transport in mesoscopic structures must be theoretically studied by means of a quantum theory since typical dimensions involved are comparable with the electron coherence length. The Wigner-function (WF) formalism (see, for example, [1–3]) has been found particularly appropriate since it allows to use, within the rigorous approach of quantum mechanics, familiar functions of position and momentum defined in phase space. This fact produces often a deeper physical insight into the quantum results with respect to other formalisms and leads to an easier interpretation of the semiclassical limit of quantum problems. Furthermore, as it will be discussed in this paper, it provides a suitable description of open systems in terms of initial/boundary conditions assigned inside the region of the device and at the boundary between device and environment. The WF is not always positive over its domain, and its arguments $\boldsymbol{r}$ and $\boldsymbol{p}$ are neither the eingenvalues of the corresponding operators of quantum theory nor the conjugated variables of the semiclassical theory. This must be always kept in mind in order to not push the semiclassical intuition too far within the framework of the quantum problem of interest.

With this warning we shall discuss here how Wigner paths exist in phase space and exhibit many analogies with semiclassical paths. Moreover they can be used to solve the quantum evolution equation for the WF as semiclassical trajectories are used in numerical procedures to solve the Boltzmann transport equation.

The paper is organized as follows: Sect. 2 presents the theoretical approach, in Sect. 3 the application of Wigner paths to boundary conditions will be discussed, Sect. 4 contains a discussion on how Wigner paths can be used for a numerical solution of quantum transport problems. Some results for model structures are given.

2. Wigner Paths

It has been observed in the literature that the evolution equation for the WF in absence of phonon interaction can be deduced from a "particle" dynamics in phase space described by modified Hamilton's equations [4]. These allow to define "Wigner trajectories" that carry a value of the WF which is maintained during the time evolution along the trajectory in phase space. For quantum systems in stationary states Wigner trajectories are the "equi-WF" curves.

A difficulty in the theory of Wigner trajectories is related to the fact that Liouville theorem does not hold for the WF at singularities in the effective potential entering the WF evolution equation. At these points Wigner trajectories can be created or destroyed [4]. Furthermore the quantum force which appears in the effective Hamilton equations depends on the state of the system. Thus many Wigner trajectories are defined for a single initial phase-space point, each of them for any given quantum state of the system. It follows that the concept of Wigner trajectories is in practice of little utility, since it requires the *a priori* knowledge of the WF itself.

An example for the above discussion is shown in Fig. 1, where the WF and Wigner trajectories are shown for the case of an electron inside a one-dimensional potential box. For this case Wigner trajectories are closed curves. Since from the Hamilton's equations the "particle" velocity has the same direction as $\boldsymbol{p}$, trajectories fully contained in the region $p > 0$ or $p < 0$ exhibit singular points correspond-

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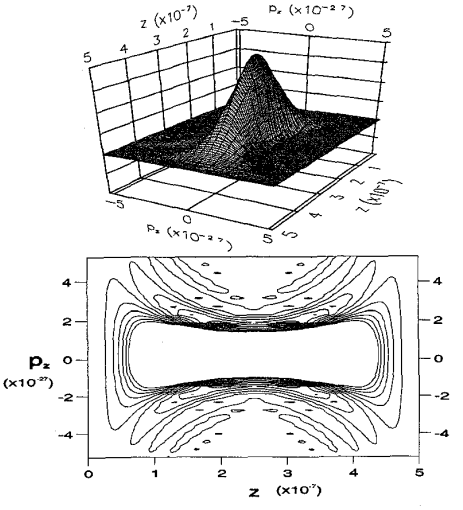

Fig. 1: Wigner function (upper part) and associated trajectories (lower part) for an electron in a one-dimensional potential box occupying the lowest energy state (MKS units).

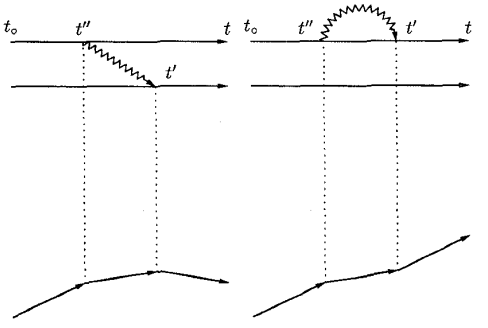

Fig. 2: Example of WP relative to second order real (left) and virtual (right) emission terms of a phonon mode $\boldsymbol{q}$.

ing to the condition $\partial f_W/\partial p = 0$ which act as sinks or sources.

Recently [6] the concept of Wigner paths (WP), based on the linearity of the evolution equation for the WF, has been introduced by the Authors. WPs overcome the theoretical problems discussed above and coincide with the classical trajectories for the cases of constant, linear, or quadratic potentials. When arbitrary potential profiles and/or phonon scattering are introduced, WPs contain "ballistic flights" and "scattering events" in complete analogy with electron paths in semiclassical transport. This topic will be developed in the following.

Free Paths

When the potential $V(\boldsymbol{r})$ in the electron Hamiltonian, corresponding to the force $\boldsymbol{F}(\boldsymbol{r})$, is analytic and contains only terms up to second order in the position, it is well known [7] that the equation which describes the dynamics of the WF has the same form as the collision-free Boltzmann equation:

$$\left(\frac{\partial}{\partial t} + \frac{\boldsymbol{p}}{m}\cdot\nabla_{\mathbf{r}} + \boldsymbol{F}\cdot\nabla_{\mathbf{p}}\right) f_W(\boldsymbol{r},\boldsymbol{p},t) = 0\,. \qquad (1)$$

where m is the electron effective mass. Thus the motion of the WF corresponds to that of a classical distribution function of particles following classical dynamics. Thus, in such a case, WPs coincide with classical trajectories. Owing to the linearity of the dynamical equation, if the WF at the initial time t_0 is regarded as the integral of δ-like contributions, each of these contributions maintains its "δ" character in time and moves as a classical particle.

Potential Scattering

If we now assume that electrons experience, besides the force in Eq. (1), an arbitrary potential profile $V(\boldsymbol{r})$, in absence of phonon interaction, the following evolution equation is obtained [3]:

$$\left(\frac{\partial}{\partial t} + \frac{\boldsymbol{p}}{m}\cdot\nabla_{\mathbf{r}} + \boldsymbol{F}\cdot\nabla_{\mathbf{p}}\right) f_W(\boldsymbol{r},\boldsymbol{p},t) = \\ = \int \mathrm{d}\boldsymbol{p}'\, \mathcal{V}_W(\boldsymbol{r},\boldsymbol{p}'-\boldsymbol{p})\, f_W(\boldsymbol{r},\boldsymbol{p}',t)\,. \qquad (2)$$

The transfer function $\mathcal{V}_W(\boldsymbol{r},\boldsymbol{p})$ is the Weyl-Wigner transform of the potential $V(\boldsymbol{r})$. New path variables can now be introduced in the above equation:

$$\boldsymbol{r}^* = \boldsymbol{r}(t_0) = \boldsymbol{r} - \frac{\boldsymbol{p}}{m}(t-t_0) - \frac{e\boldsymbol{E}}{2m}(t-t_0)^2\,, \\ \boldsymbol{p}^* = \boldsymbol{p}(t_0) = \boldsymbol{p} + e\boldsymbol{E}(t-t_0)\,, \qquad t^* = t\,, \qquad (3)$$

where for simplicity the case of a constant force $-e\boldsymbol{E}$ is considered. A successive integration over time, in analogy with what is done in order to obtain the integral form of the Boltzmann transport equation, provides the following integral equation:

$$f_W(\boldsymbol{r},\boldsymbol{p},t) = f_W\left(\boldsymbol{r}(t_0),\boldsymbol{p}(t_0),t_0\right) \qquad (4) \\ + \int_{t_0}^{t} \mathrm{d}t' \int \mathrm{d}\boldsymbol{p}'\, \mathcal{V}_W\left(\boldsymbol{r}(t'),\boldsymbol{p}'-\boldsymbol{p}(t')\right)\, f_W\left(\boldsymbol{r}(t'),\boldsymbol{p}',t'\right).$$

An iterative substitution of the above equation into itself generates the various perturbative terms which constitute the Neumann expansion. Each term of the expansion is the sum (integral) of contributions, each determined by a set of values for the integration variables: the interaction times and the momentum transfers. This set of values defines a WP. The number of "scattering events" included in a WP is equal to the perturbative order in the Neumann expansion.

Between two scattering events the "particle" moves following the dynamics imposed by the external electric field $\boldsymbol{E}$. The WF at a given point of the phase space is

thus obtained as the sum of an infinite number of contributions, each carried by a WP and weighed by the transfer function $\mathcal{V}_W$ evaluated at the interaction vertices.

Phonon Scattering

If phonon scattering is considered, the definition of the WF must be generalized to describe the electron-phonon system as follows [5]:

$$f_W(\boldsymbol{r},\boldsymbol{p},\{n_{\mathbf{q}}\},\{n'_{\mathbf{q}}\},t) = \int \mathrm{d}\boldsymbol{r}' \exp(-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar) \times\langle \boldsymbol{r}+\boldsymbol{r}'/2,\{n_{\mathbf{q}}\}\,|\rho(t)|\,\boldsymbol{r}-\boldsymbol{r}'/2,\{n'_{\mathbf{q}}\}\rangle\,, \quad (5)$$

where ρ is the density operator of the electron-phonon system. For this case a procedure similar to the one discussed in the previous section leads to the following evolution equation for the WF:

$$\begin{aligned}
f_W(\boldsymbol{r},\boldsymbol{p},\{n_{\mathbf{q}}\},\{n'_{\mathbf{q}}\},t) \;=\; & f_W\left(\boldsymbol{r}(t_0),\boldsymbol{p}(t_0),\{n_{\mathbf{q}}\},\{n'_{\mathbf{q}}\},t_0\right)\exp\left(-i\Delta\omega(\{n_{\mathbf{q}}\},\{n'_{\mathbf{q}}\})(t-t_0)\right) \\
& + \int_{t_0}^{t}\mathrm{d}t'\,\exp\left[-i\Delta\omega\left(\{n_{\mathbf{q}}\},\{n'_{\mathbf{q}}\}\right)(t-t')\right]\int \mathrm{d}\boldsymbol{p}'\,\mathcal{V}_W\left(\boldsymbol{r}(t'),\boldsymbol{p}'-\boldsymbol{p}(t')\right) f_W\left(\boldsymbol{r}(t'),\boldsymbol{p}',\{n_{\mathbf{q}}\},\{n'_{\mathbf{q}}\},t'\right) \\
& + \int_{t_0}^{t}\mathrm{d}t'\,\exp\left[-i\Delta\omega\left(\{n_{\mathbf{q}}\},\{n'_{\mathbf{q}}\}\right)(t-t')\right]\sum_{\mathbf{q}'}F(\boldsymbol{q}') \\
& \times\Bigg\{\exp\left(i\boldsymbol{q}'\cdot\boldsymbol{r}(t')\right)\sqrt{n_{\mathbf{q}'}+1}\,f_W\left(\boldsymbol{r}(t'),\boldsymbol{p}(t')-\frac{\hbar\boldsymbol{q}'}{2},\{n_1,\ldots,n_{\mathbf{q}'}+1,\ldots\},\{n'_{\mathbf{q}}\},t'\right) \\
& \quad -\exp\left(-i\boldsymbol{q}'\cdot\boldsymbol{r}(t')\right)\sqrt{n_{\mathbf{q}'}}\,f_W\left(\boldsymbol{r}(t'),\boldsymbol{p}(t')+\frac{\hbar\boldsymbol{q}'}{2},\{n_1,\ldots,n_{\mathbf{q}'}-1,\ldots\},\{n'_{\mathbf{q}}\},t'\right) \\
& \quad -\exp\left(i\boldsymbol{q}'\cdot\boldsymbol{r}(t')\right)\sqrt{n_{\mathbf{q}'}}\,f_W\left(\boldsymbol{r}(t'),\boldsymbol{p}(t')+\frac{\hbar\boldsymbol{q}'}{2},\{n_{\mathbf{q}}\},\{n'_1,\ldots,n'_{\mathbf{q}'}-1,\ldots\},t'\right) \\
& \quad +\exp\left(-i\boldsymbol{q}'\cdot\boldsymbol{r}(t')\right)\sqrt{n'_{\mathbf{q}'}+1}\,f_W\left(\boldsymbol{r}(t'),\boldsymbol{p}(t')-\frac{\hbar\boldsymbol{q}'}{2},\{n_{\mathbf{q}}\},\{n'_1,\ldots,n'_{\mathbf{q}'}+1,\ldots\},t'\right)\Bigg\},
\end{aligned}$$

where $F(\boldsymbol{q})$ is a function that describes the electron coupling with phonon mode $\boldsymbol{q}$, and $\hbar\Delta\omega\left(\{n_{\mathbf{q}}\},\{n'_{\mathbf{q}}\}\right)$ is the energy difference between the two indicated phonon states. The above equation shows that the contribution of a single vertex to the WF at the point $(\boldsymbol{r},\boldsymbol{p})$ at time t is obtained through a path that connects $\boldsymbol{r}$ with the position $\boldsymbol{r}-\boldsymbol{p}(t-t')/m$. Furthermore, at the interaction time the momentum of the representative point is changed by half of the phonon momentum $\hbar\boldsymbol{q}$. Again, substituting iteratively the above equation into itself we obtain the Neumann series with terms at arbitrary perturbative orders. The lowest perturbative correction which has a classical analogue is associated to the second-order term and corresponds to one scattering event. As an example, typical paths associated with this term are represented in the diagrams contained in Fig. 2. They correspond to the semiclassical paths where $\hbar\boldsymbol{q}/2$ is transferred to the electron at each vertex, while the dynamics between two vertices is a ballistic evolution with the corresponding momentum. If the process corresponds to a real transition, the second momentum transfer adds to the first one, so that the total phonon momentum $\hbar\boldsymbol{q}$ is transferred to 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 at the beginning of the interaction. The solution is anyway influenced by the virtual transitions, which are associated with out-scattering and polaronic effects. In the general case, when electrons, under the action of an external field $\boldsymbol{E}$, move across a potential profile in presence of phonon scattering, the formulation presented above still holds and WPs include scattering vertices due to both phonons and the potential $V(\boldsymbol{r})$.

3. Boundary Conditions

The mathematical procedure described in the previous sections contains a formal integration over time of the differential equation obtained after the substitution of the path variables introduced in Eq. (3). Let us now assume that the WF is known at time t_0 inside a closed region of phase space and at any time $t > t_0$ on its boundary. In such a case, instead of performing the time integration from t_0 to t, we can perform this integration from $\bar{t}$ to t, where $\bar{t} = t_0$ in case the "ballistic path" that terminates in $\boldsymbol{r}$ at time t starts at t_0 inside the domain of interest; in case the "ballistic path" crosses the boundary at a time $t_b > t_0$, then $\bar{t} = t_b$. With this integration procedure and its iterative expansion it can be seen that the WF in $\boldsymbol{r}$ at t is given by *a)* all paths that start inside the region of interest at time t_0 and end in $\boldsymbol{r}$ at time t after an arbitrary number of scattering events without exiting this region, and *b)* all paths that enter the region of interest at any time after t_0 and again suffer any number of interactions inside. This picture is again strictly analogous to the corresponding semiclassical transport picture.

It must be noted that the WF of the electron-phonon system must be known at the boundary of the system of interest. For example, if electrons are interacting with phonons while entering the region of interest, this information must be contained in the boundary condition for

the WF. If the boundary is located at a metallic contact, there we know that electron-electron interaction is very effective in destroying the phase correlation of the electron wave function that constitutes the difference between the WF and the semiclassical distribution function. In such a case the dynamics near the contact is difficult to account for. These problems are not new. They have all been faced (and only partially solved) in semiclassical transport theory.

4. Monte Carlo Procedure

The theory of WPs presented in the previous sections suggests to extend in a very natural way to the case of quantum transport the Weighed Monte Carlo procedure developed for semiclassical transport. In principle it provides a rigorous solution of electron-transport problems inside any device accounting for coherent electron dynamics and any interaction with the phonon gas, with potential profiles or scattering centers. The similarity with semiclassical transport also suggests the guiding criteria to extend the method to the problems investigated with traditional Monte Carlo procedures such as, e.g., electron-electron interaction and hot-phonon effects. Several considerations must be made at this point.

a) WPs carry phase information that result in positive and negative contributions to the WF. A large cancellation of these terms requires a very large statistics compared to the semiclassical case. However the situation is not as bad as in pure path-integral approaches since, in the present case, all free paths that lead to the semiclassical trajectory between two scattering events are already accounted for.

b) Energy conservation, as far as it is maintained in quantum theory, is guaranteed only by these cancellations.

c) The transfer function $\mathcal{V}_W$ is well defined only if $V(\boldsymbol{r})$ has a single value at infinity. If two boundaries are kept at different potentials, this fact can be taken into account by a constant field acting on the free flights of the WPs.

A Monte Carlo algorithm is now being implemented by the Authors on the lines indicated above. An intermediate procedure has already been implemented with a somewhat different approach that makes use of scattering states. It treats the boundary conditions as previously shown, it evaluates the integrals over time numerically and the integral over the phonon modes through a Monte Carlo sampling. Results have been obtained at present up to the second perturbative order in the Neumann expansion, corresponding to one phonon emission or absorption. As an example, the $I(V)$ characteristic of electrons moving across a double-barrier potential profile in presence of a constant external electric field are shown in Fig. 3. Thermalizing contacts have been assumed as boundary condition. The results obtained for this case are consistent with data obtained for the same system from simpler quantum approaches [8].

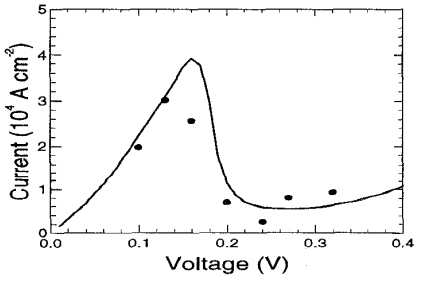

Fig. 3: Electron current as a function of the applied bias for the case of a double-barrier potential profile. A comparison is shown between the results obtained using the ballistic WF (solid line) and the WF corrected by the effect of an electron-phonon scattering process (full circles) switched on 50 fs before the "observation time".

5. Conclusions

We have presented a general theoretical scheme for the solution of quantum electron transport in the framework of the WF approach which is based on the concept of Wigner path. The solution of a given problem can be interpreted as a sum of contributions, each carried by a Wigner path. A single Wigner path includes free flights and scattering vertices, in strict analogy with what happens for a semiclassical trajectory. Within this framework we have shown that, for open systems, the theory naturally suggests the use of suitable boundary conditions to account for the interaction between the system of interest and the environment.

A new Monte Carlo procedure is here proposed, based on the generation of Wigner paths, with many analogies with the semiclassical procedure, based on the generation of classical trajectories. The method, in a preliminary implementation, has been applied to calculate the current-voltage characteristics associated with electron quantum transport across model systems in presence of single phonon-scattering processes.

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