Quantum transport of electrons in open nanostructures with the Wigner-function formalism

P. Bordone, M. Pascoli, R. Brunetti, A. Bertoni, and C. Jacoboni
Istituto Nazionale per la Fisica della Materia, Dipartimento di Fisica, Università di Modena, Via Campi 213/A, 41100 Modena, Italy

A. Abramo
DIEGM, Università di Udine, Viale delle Scienze 208, 33100 Udine, Italy

(Received 13 July 1998)

A theoretical Wigner-function approach to the study of quantum transport in open systems in presence of phonon scattering is presented. It is shown here that in order to solve the Wigner equation in its integral form the knowledge of the Wigner function at all points of the phase space at an initial time t_0 can be substituted by the knowledge of the same function inside the region of interest at t_0 and on its boundary at all times t' less then the observation time t. The theory has been applied to calculate the current associated with electron quantum transport across given potential profiles and in presence of phonon scattering.
[S0163-1829(99)12703-6]

I. INTRODUCTION

Electron transport in mesoscopic systems has been widely investigated in recent years.[1–4] The increasing interest on this subject is mainly related to the fundamental problems of basic physics involved, as well as to possible applications in the field of device modeling.

Since the dimensions of mesoscopic systems are comparable with typical electron coherence lengths, a correct analysis of transport phenomena in such systems requires a detailed quantum-mechanical treatment. The Wigner-function (WF) formalism[5–7] has been found particularly appropriate for the theoretical analysis of quantum transport since it combines the rigorous approach of quantum mechanics with more familiar functions defined in phase space. However, while ballistic coherent transport has been extensively investigated in the recent literature using the WF, dissipative scattering by phonons has been included in the theory only by means of phenomenological approaches (e.g., the relaxation-time approximation[6,7]). Recently an approach to the problem of quantum transport in presence of phonon scattering has been proposed by the authors of the present paper in the framework of the WF.[8–11] However, the problem of a rigorous description of an open system of independent electrons interacting with phonons has been left unsolved. Nevertheless, any real electronic device is an open system that can be thought of as a bounded region exchanging particles with at least two external reservoirs. Thus, the extension of the theory mentioned above is of great relevance in view of its possible applications.

In order to solve the Wigner equation for an open system by means of a suitable numerical procedure[8,12] the main difficulty is related to the fact that the initial condition for the WF (i.e., knowledge of the WF at all points of the phase space at a given initial time t_0) does not provide a suitable description of an open system, for which the WF must be supposed known on the boundary between the system of interest and the rest of the universe at any time, in addition to the knowledge of the same function inside the region of interest at the initial time.

In this paper, the above initial/boundary conditions at the basis of the existence of Wigner paths[11] are proved to be equivalent to the initial condition over an infinite domain to the purpose of solving the Wigner equation for an open system. Numerical calculations for some model physical systems will be shown in the limit of single-collision electron propagation.

The general framework of the WF approach used in the present paper is summarized in Sec. II. In Sec. III, the theoretical development related to the boundary-condition treatment for an open system is presented. In Sec. IV, the iterative expansion of the integral equation for the WF is analyzed. Numerical results are shown and discussed in Sec. V. Conclusions and perspectives are summarized in Sec. VI.

II. THEORETICAL APPROACH

A three-dimensional system of independent electrons interacting with phonons is considered. For simplicity translational invariance along two directions (x,y) is assumed here, even though this assumption is not essential to the basic theory. The Hamiltonian $\mathbf{H}$ of the system is

$$\mathbf{H}=\mathbf{H}_0+\mathbf{H}_{e\text{-}p}=\frac{-\hbar^2\nabla^2}{2m}+\mathbf{V}(r)+\sum_{\boldsymbol{q}}\ \mathbf{b}_{\boldsymbol{q}}^{\dagger}\mathbf{b}_{\boldsymbol{q}}\hbar\omega_{\boldsymbol{q}}+\mathbf{H}_{e\text{-}p}\,, \tag{2.1}$$

where m is the electron effective mass and $\mathbf{V}(r)$ is the electron potential profile (including the applied voltage), $\mathbf{b}_{\boldsymbol{q}}$ and $\mathbf{b}_{\boldsymbol{q}}^{\dagger}$ are the annihilation and creation operators of the phonon mode $\boldsymbol{q}$ with frequency $\omega_{\boldsymbol{q}}$. The electron-phonon interaction Hamiltonian $\mathbf{H}_{e\text{-}p}$ is given by

$$\mathbf{H}_{e\text{-}p}=\sum_{\boldsymbol{q}}\ i\hbar F(\boldsymbol{q})(\mathbf{b}_{\boldsymbol{q}}e^{i\boldsymbol{q}\cdot\boldsymbol{r}}-\mathbf{b}_{\boldsymbol{q}}^{\dagger}e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}), \tag{2.2}$$

where $F(\boldsymbol{q})$ is a function depending on the type of phonon scattering analyzed.

The generalized WF (Ref. 12) for an electron-phonon system is

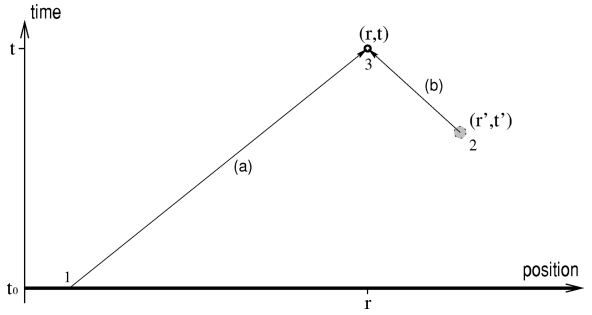

FIG. 1. Schematic representation of the integral equation for the Wigner function: the ballistic term [curve (a)] being the contribution to the Wigner function at $t=t_0$ from all phase-space points that do not suffer interactions from t_0 to t, while the second term [curve (b)] represents the contribution to the Wigner function from the last electron-phonon interaction in any $(\boldsymbol{r}',\boldsymbol{p}')$ and t' before t.

$$f_w(\boldsymbol{r},\boldsymbol{p},\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t) = \int d\boldsymbol{r}' e^{-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar}\langle \boldsymbol{r}+\boldsymbol{r}'/2,\{n_{\boldsymbol{q}}\}|\rho(t)|\boldsymbol{r}-\boldsymbol{r}'/2,\{n'_{\boldsymbol{q}}\}\rangle, \tag{2.3}$$

where ρ is the density operator of the electron-phonon system. For any given basis $\{|\varphi_n\rangle\}$ in the space of the electron states the coefficients[13]

$$f_{nn'}(\boldsymbol{r},\boldsymbol{p}) = \int d\boldsymbol{r}' e^{-i\boldsymbol{p}\cdot\boldsymbol{r}'/\hbar}\langle \boldsymbol{r}+\boldsymbol{r}'/2|\varphi_n\rangle\langle\varphi_{n'}|\boldsymbol{r}-\boldsymbol{r}'/2\rangle \tag{2.4}$$

connect the generalized WF to the density matrix $\rho(n,\{n_{\boldsymbol{q}}\};n',\{n'_{\boldsymbol{q}}\};t)$ and vice versa.[11]

Starting from the Liouville equation for the density matrix in the interaction picture, it is possible to derive the equation for the corresponding WF that is reported here in his compact form:[11]

$$\begin{aligned} f_w(t) &= \frac{1}{h^3}\mathcal{F}\mathcal{T}(t_0,t)\mathcal{F}^{\dagger}f_w^{(0)}(t_0) + \frac{1}{h^3}\mathcal{F}\int_{t_0}^{t} dt'\,\mathcal{T}(t',t) \\ &\quad\times\{\mathcal{H}'\mathcal{F}^{\dagger}f_w(t') - \mathcal{F}^{\dagger}f_w(t')\mathcal{H}'\} \\ &= f_w^{(0)} + \Delta f_w, \end{aligned} \tag{2.5}$$

where

$$\mathcal{T}(t_0,t) = \exp\{-i[\omega(n,\{n_{\boldsymbol{q}}\}) - \omega(n',\{n'_{\boldsymbol{q}}\})](t-t_0)\} \tag{2.6}$$

is the ''free-evolution'' operator, and $\mathcal{F}$ is the compact expression of the coefficients defined in Eq. (2.4). In Eq. (2.5) the first term $(f_w^{(0)})$ and the term containing $\mathcal{H}' = \mathbf{H}'/i\hbar(\Delta f_w)$ are, respectively, the ballistic contribution and the contribution to the WF due to the presence of scattering. The physical meaning of these two terms is illustrated in Fig. 1.

The above integral equation is linear in the unknown f_w. This property guarantees that if the WF at $t=t_0$ is the sum of several contributions, then each of them will evolve according to Eq. (2.5), and the solution of the equation at any given time $t>t_0$ will be given by the sum of the single contributions evaluated at the same time. This property will be used to our purposes in the next section.

III. WIGNER EQUATION FOR AN OPEN SYSTEM

For the sake of simplicity in the following we will consider a one-dimensional case in the space (z,p). There is no essential difference with the three-dimensional (3D) case, and the numerical examples presented in Sec. V have been actually realized in 3D with translational invariance along x and y.

As it can be seen by an iterative Neumann expansion, in order to solve Eq. (2.5) we need to know the WF at the initial time t_0 at each point (z,p) of the phase space. We will show that such initial condition can be substituted by the knowledge of the WF at the initial time t_0 inside the system and, at all times, on the boundary between the system and the environment. From the analytical point of view this transformation can be realized by splitting the integral over the z' coordinate in Eq. (2.5) (extended from $-\infty$ to $+\infty$) into three terms: $-\infty<z'<-A$, $-A\leqslant z'\leqslant +A$, and $A<z'<+\infty$, $\pm A$ being the boundary coordinates for the 1D system. The two space integrals over open domains not including the system must be transformed into time integrals at the two boundaries $\pm A$. In the following the proof will first be obtained assuming that the eigenstates of the unperturbed Hamiltonian are plane waves. Then the results will be extended to more general cases in Sec. III C.

A. Ballistic free electrons

We will analyze first the transformation of the ballistic term:

$$\begin{aligned} f_w^{(0)}(z,p,\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t) &= \frac{1}{(2\pi)^2 h}\int dk \int dk' f_{kk'}(z,p) \\ &\quad\times\exp\{-i[\omega(k,\{n_{\boldsymbol{q}}\}) - \omega(k',\{n'_{\boldsymbol{q}}\})](t-t_0)\} \\ &\quad\times\int dz' \int dp' f^{*}_{kk'}(z',p') f_w(z',p',\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t_0), \end{aligned} \tag{3.1}$$

where $f_{kk'}$ are the coefficients in Eq. (2.4) that, for the case of a basis set of plane waves, are given by

$$\begin{aligned} f_{kk'}(z,p) &= \int dz' e^{-ipz'/\hbar} e^{ik(z+z'/2)} e^{-ik'(z-z'/2)} \\ &= \hbar e^{i(k-k')z}\delta\left(p - \hbar\frac{k+k'}{2}\right). \end{aligned} \tag{3.2}$$

In Eq. (3.1) for clarity we have explicitly inserted the integral symbols. By substituting the coefficients in Eq. (3.2) into Eq. (3.1), the ballistic evolution of the WF after some straightforward calculations, results to be

$$f_w^{(0)}(z,p,\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t) = f_w\left(z-\frac{p}{m}(t-t_0),p,\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t_0\right) \times\exp\{-i[\omega(\{n_{\boldsymbol{q}}\})-\omega(\{n'_{\boldsymbol{q}}\})](t-t_0)\}, \tag{3.3}$$

where $\hbar\omega(\{n_{\boldsymbol{q}}\})$ is the total energy of the phonon bath in the state $\{n_{\boldsymbol{q}}\}$. The two factors on the right-hand-side of Eq. (3.3) describe the free trajectory of the electron and the time evolution of the free-phonon bath, respectively. Equation (3.3) shows that if the initial WF is considered as the integral of δ-like contributions, each of them, in absence of external forces, carries its value following a classical trajectory. Thus, the ballistic contribution to the WF shown symbolically in Fig. 1 has to be considered as ''carried'' along a classical trajectory in absence of external forces. This concept of Wigner paths[11] has guided us in developing the following derivation.

Let us consider the range $-\infty<z'<-A$ in the integral in Eq. (3.1) and call $f_L^{(0)}$ the corresponding part of $f_w^{(0)}$. Making use of the properties of the coefficients $f_{kk'}$ (Ref. 11) we insert into the considered term the factor (equal to unity):

$$\frac{1}{(2\pi)^2 h}\int dk''\int dk'''\int dz\int dp f_{kk'}(z,p)f^*_{k''k'''}(z,p)\,. \tag{3.4}$$

Then, substituting the explicit expression of the coefficients f given by Eq. (3.2) we obtain

$$f_L^{(0)}(z,p,\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t)=\frac{\hbar^2}{(2\pi)^6}\int dk\int dk' e^{i(k-k')z}\delta\left(p-\hbar\frac{k+k'}{2}\right)\exp\left(-i(k-k')\frac{\hbar}{m}\frac{k+k'}{2}(t-t_0)\right) \times\exp\left(-i\sum_{\boldsymbol{q}}(n_{\boldsymbol{q}}-n'_{\boldsymbol{q}})\omega_{\boldsymbol{q}}(t-t_0)\right)\int dk''\int dk'''\int_{-\infty}^{-A}dz'\int dp' e^{-i(k-k')z'} \times\delta\left(p'-\hbar\frac{k+k'}{2}\right)e^{i(k''-k''')z'}\delta\left(p'-\hbar\frac{k''+k'''}{2}\right)\int dz''\int dp'' e^{-i(k''-k''')z''}\delta\left(p''-\hbar\frac{k''+k'''}{2}\right) \times f_w(z'',p'',\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t_0). \tag{3.5}$$

In order to proceed we introduce the variable transformations

$$\overline{K}=\frac{k+k'}{2}\quad\text{and}\quad\overline{k}=k-k' \tag{3.6}$$

and transform the integrals over k and k' into integrals over the new variables. By use of the delta function we obtain

$$f_L^{(0)}(z,p,\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t)=\frac{1}{(2\pi)^5}\int_{-\infty}^{-A}dz'\int dp'\,\delta\left(z-z'-\frac{p'}{m}(t-t_0)\right)\delta(p-p') \times\exp\left(-i\sum_{\boldsymbol{q}}(n_{\boldsymbol{q}}-n'_{\boldsymbol{q}})\omega_{\boldsymbol{q}}(t-t_0)\right)\int dk''\int dk''' e^{i(k''-k''')z'}\delta\left(p'-\hbar\frac{k''+k'''}{2}\right) \times\int dz''\int dp'' f^*_{k''k'''}(z'',p'')f_w(z'',p'',\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t_0). \tag{3.7}$$

Using again the properties of the δ function we get the following constraints on the space variables z and z':

$$z'<-A\Rightarrow z-\frac{p'}{m}(t-t_0)<-A, \tag{3.8}$$

which, in turn, imply constraints on the time variable:

$$t>t_0+\frac{z-(-A)}{\frac{p'}{m}}\quad\text{if } p'>0,$$

$$t<t_0+\frac{z-(-A)}{\frac{p'}{m}}\quad\text{if } p'<0. \tag{3.9}$$

Since we are interested in the WF inside the device then $z>-A$ and $z-(-A)>0$. As a consequence, being $t>t_0$, the second condition of Eq. (3.9) is never verified. As it regards the first-time constraint in Eq. (3.9) we may notice that

$$t'=t-\frac{z-(-A)}{\frac{p'}{m}}=t_0-\frac{z'-(-A)}{\frac{p'}{m}}, \tag{3.10}$$

is the time at which the path crosses the boundary at $z=-A$. Thus, the constraints mean that contributions from the left must have positive momentum. By using the crossing time t' as a new integration variable in place of z' in Eq. (3.7) it is obtained:

$$f_L^{(0)}(z,p,\{n_q\},\{n'_q\},t)=\frac{1}{(2\pi)^4h^2}\int_{t_0}^{t}dt'\int_0^{+\infty}dp'\frac{p'}{m}h\int dk\int dk' f_{kk'}(z,p)$$

$$\times e^{-i[\omega(k,\{n_q\})-\omega(k',\{n'_q\})](t-t')}f^*_{kk'}(-A,p')h\int dk''\int dk''' f_{k''k'''}(-A,p')$$

$$\times e^{-i[\omega(k'',\{n_q\})-\omega(k''',\{n'_q\})](t'-t_0)}\int dz''\int dp'' f^*_{k''k'''}(z'',p'')f_w(z'',p'',\{n_q\},\{n'_q\},t_0). \tag{3.11}$$

The last part of the above expression describes the free evolution of the WF outside the domain of interest corresponding to the Wigner paths (a) 1-2 in Fig. 2, so that $f_L^{(0)}$ can be finally written as

$$f_L^{(0)}(z,p,\{n_q\},\{n'_q\},t)=\frac{1}{(2\pi)^2h}\int dk\int dk' f_{kk'}(z,p)\int_{t_0}^{t}dt' e^{-i[\omega(k,\{n_q\})-\omega(k',\{n'_q\})](t-t')}$$

$$\times\int_0^{+\infty}dp'\frac{p'}{m}f^*_{kk'}(-A,p')f_w^{(0)}(-A,p',\{n_q\},\{n'_q\},t'). \tag{3.12}$$

The space integral over the variable z' has been substituted by a time integral over the crossing time t' from the initial time t_0 to the observation time t, with the WF evaluated at the left boundary of the system ($z=-A$), as desired.

Similar calculations can be performed for the case $+A<z'<+\infty$, so that Eq. (3.1) becomes

$$f_w^{(0)}(z,p,\{n_q\},\{n'_q\},t)=\frac{1}{(2\pi)^2h}\int dk\int dk' f_{kk'}(z,p)$$

$$\times\Bigg\{e^{-i[\omega(k,\{n_q\})-\omega(k',\{n'_q\})](t-t_0)}\int_{-A}^{+A}dz'\int dp' f^*_{kk'}(z',p')f_w(z',p',\{n_q\},\{n'_q\},t_0)$$

$$+\int_{t_0}^{t}dt' e^{-i[\omega(k,\{n_q\})-\omega(k',\{n'_q\})](t-t')}\Bigg[\int_0^{+\infty}dp'\frac{p'}{m}f^*_{kk'}(-A,p')f_w(-A,p',\{n_q\},\{n'_q\},t')$$

$$+\int_{-\infty}^{0}dp'\frac{p'}{m}f^*_{kk'}(-A,p')f_w(A,p',\{n_q\},\{n'_q\},t')\Bigg]\Bigg\}, \tag{3.13}$$

which is the expected result. Contributions coming from paths that at $t=t_0$ start from inside the region of interest are given by the first term in the above equation left unchanged with respect to the original description. In Eq. (3.13) the boundary of the evolution equation of the ballistic term $f_w^{(0)}$ is the bold line in Fig. 2(a).

B. Phonon scattering

We consider now the collision term:

$$\Delta f_w(z,p,\{n_q\},\{n'_q\},t>0)=\frac{1}{(2\pi)^3h}\int dk\int dk' f_{kk'}(z,p)\int_{t_0}^{t}dt' e^{-i[\omega(k,\{n_q\})-\omega(k',\{n'_q\})](t-t')}$$

$$\times\sum_{m_q}\int dk''\int dz'\int dp'[\mathcal{H}'(k,\{n_q\},k'',\{m_q\})f^*_{k''k'}(z',p')f_w(z',p',\{m_q\},\{n'_q\},t')$$

$$-f^*_{kk''}(z',p')f_w(z',p',\{n_q\},\{m_q\},t')\mathcal{H}'(k''\{m_q\},k'\{n'_q\})]. \tag{3.14}$$

We shall again be guided by the concept of Wigner path, since it has been shown[11] that each electron-phonon interaction vertex maintains the propagation along a Wigner path with a momentum transfer equal to half of the phonon momentum ($q/2$). As it was done in the previous case, Eqs. (3.2) and (3.4) are substituted into Eq. (3.14), and the integral over z' is split into three parts. Let us consider first the range $z'<-A$ corresponding to an electron-phonon interaction occurring outside the left boundary of the region of interest. Introducing the transformation in Eq. (3.6) the integrals $\int dk \int dk'$ can be transformed into $\int d\bar{k} \int d\bar{K}$ and the second one can be performed using delta functions contained in the coefficients in Eq. (3.2). Then we introduce the time variable t'' (corresponding to the time at which the path crosses the left boundary) defined through the space coordinate z':

$$z' = -A - (t''-t')\frac{p'}{m}. \tag{3.15}$$

When $z'<-A$ and $p'>0$ we are led to the following constraints on the variable t'': $t' \leqslant t'' \leqslant t_0$ (corresponding to particles entering the system from the left boundary). The integral over z' can be easily transformed into an integral over t'' and the following change in the integral limits is used:

$$\int_{t_0}^{t} dt' \int_{t'}^{t} dt'' = \int_{t_0}^{t} dt'' \int_{t_0}^{t''} dt'. \tag{3.16}$$

By inserting the identity $\hbar \int dK \delta(p-\hbar K)=1$ and considering the inverse variable transformation of Eq. (3.6) we are left with

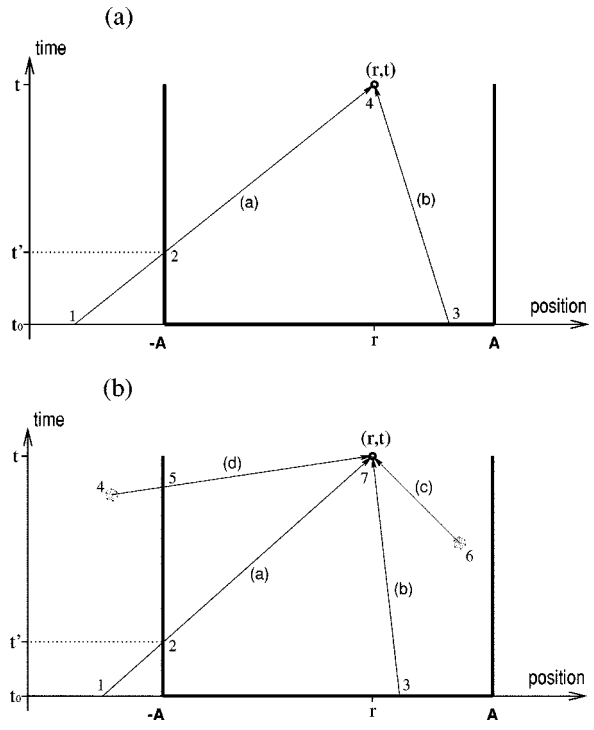

FIG. 2. Schematic representation of the integral equation for the Wigner function with the boundary conditions. The integration contour of the evolution equation of the Wigner function is the bold line. (a) Ballistic evolution: Wigner paths coming from outside [curve (a)] and from inside [curve (b)] the domain of interest. (b) Ballistic contributions [curve (a) and curve (b)] and contributions of the perturbation term having the last electron-phonon interaction inside [curve (c)] and outside [curve (d)] the domain of interest. The terms of type (a) and (d) can be summed to give the total Wigner function on the boundary. Therefore, to consider the contribution to the Wigner function coming from the boundary corresponds to take into account all the terms of type (a) and (b).

$$\begin{aligned}
\Delta f_{w,L}(z,p,\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t) = {} & \frac{1}{(2\pi)^5 h} \int dk \int dk' f_{kk'}(z,p) \int_0^{+\infty} dp' \int_{t_0}^{t} dt'' \int_{t_0}^{t''} dt' \frac{p'}{m} \\
& \times \exp\{-i[\omega(k,\{n_{\boldsymbol{q}}\}) - \omega(k',\{n'_{\boldsymbol{q}}\})](t-t'')\} f^*_{kk'}(-A,p') \\
& \times \exp\{-i[\omega(\{n_{\boldsymbol{q}}\}) - \omega(\{n'_{\boldsymbol{q}}\})](t''-t')\} \int dk'' \int dk''' \\
& \times \exp\{-i(k''-k''')p'/m(t''-t')\} f_{k''k'''}(-A,p') \sum_{m_{\boldsymbol{q}}} \int dk^{iv} \int dz'' \int dp'' \\
& \times [\mathcal{H}'(k''\{n_{\boldsymbol{q}}\},k^{iv}\{m_{\boldsymbol{q}}\}) f^*_{k^{iv}k'''}(z'',p'') f_w(z'',p'',\{m_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t') \\
& - f^*_{k''k^{iv}}(z'',p'') f_w(z'',p'',\{n_{\boldsymbol{q}}\},\{m_{\boldsymbol{q}}\},t') \mathcal{H}'(k^{iv}\{m_{\boldsymbol{q}}\},k'''\{n'_{\boldsymbol{q}}\})],
\end{aligned} \tag{3.17}$$

where we have used once more the expression in Eq. (3.2) for the f coefficients. After some straightforward manipulations using the delta functions and remembering Eq. (3.14) we are left with the following result:

$$\Delta f_{w,L}(z,p,\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t)=\frac{1}{(2\pi)^2\hbar}\int dk\int dk' f_{kk'}(z,p)\int_{t_0}^{t}dt''$$
$$\times e^{-i[\omega(k,\{n_{\boldsymbol{q}}\})-\omega(k',\{n'_{\boldsymbol{q}}\})](t-t'')}$$
$$\times\int_0^{+\infty}dp'\frac{p'}{m}f^*_{kk'}(-A,p')\Delta f_w(-A,p',\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t''). \tag{3.18}$$

Similar calculations can be performed for the case $z'>A$ (and $p'<0$). The final result is

$$\Delta f_{w,R}(z,p,\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t)=\frac{1}{(2\pi)^2\hbar}\int dk\int dk' f_{kk'}(z,p)\int_{t_0}^{t}dt''$$
$$\times e^{-i[\omega(k,\{n_{\boldsymbol{q}}\})-\omega(k',\{n'_{\boldsymbol{q}}\})](t-t'')}$$
$$\times\int_{-\infty}^{0}dp'\frac{-p'}{m}f^*_{kk'}(A,p')\Delta f_w(A,p',\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t''). \tag{3.19}$$

Equations (3.18) and (3.19) show that the interaction term in the integral equation (2.5) corresponding to the last e-ph interaction occurring outside the region of interest can be substituted by a free coherent propagation of the interaction term Δf_w of the ω frequence from the boundary to the observation point. This term will be summed to the term (3.13) previously analyzed, corresponding to the free propagation of the WF without e-ph interactions.

Finally the term in Eq. (3.14) associated to the range $-A\leqslant z'\leqslant A$ corresponds to interactions occurring inside the region of interest and needs not to be changed to our purposes.

By collecting the above results we can rewrite Eq. (2.5) as follows:

$$f_w(z,p,n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t)=\frac{1}{(2\pi)^2\hbar}\int dk\int dk' f_{kk'}(z,p)\int_{t_0}^{t}dt'\exp\{-i[\omega(k,\{n_{\boldsymbol{q}}\})-\omega(k',\{n'_{\boldsymbol{q}}\})](t-t')\}$$
$$\times\left\{\int_0^{+\infty}dp'\frac{p'}{m}f^*_{kk'}(-A,p')f_w(-A,p',\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t')\right.$$
$$\left.-\int_{-\infty}^{0}dp'_z\frac{p'}{m}f^*_{kk'}(A,p')f_w(A,p',\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t')\right\}$$
$$+\frac{1}{(2\pi)^2\hbar}\sum_{kk'}f_{kk'}(z,p)\exp\{-i[\omega(k,\{n_{\boldsymbol{q}}\})-\omega(k',\{n'_{\boldsymbol{q}}\})](t-t_0)\}$$
$$\times\int_{-A}^{A}dz'\int dp' f^*_{kk'}(z',p')f_w(z',p',\{n_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t_0)$$
$$+\frac{1}{(2\pi)^3\hbar}\int dk\int dk' f_{kk'}(z,p)\int_{t_0}^{t}dt'\exp\{-i[\omega(k,\{n_{\boldsymbol{q}}\})-\omega(k',\{n'_{\boldsymbol{q}}\})](t-t')\}$$
$$\times\int d\tilde{k}\left\{\mathcal{H}'(k,\{n_{\boldsymbol{q}}\},\tilde{k},\{m_{\boldsymbol{q}}\})\int_{-A}^{A}dz'\int dp' f^*_{\tilde{k}n'}(z',p')f_w(z',p',\{m_{\boldsymbol{q}}\},\{n'_{\boldsymbol{q}}\},t')\right.$$
$$\left.-\int_{-A}^{A}dz'\int dp' f^*_{\tilde{k}\tilde{k}}(z',p')f_w(z',p',\{n_{\boldsymbol{q}}\},\{m_{\boldsymbol{q}}\},t')\mathcal{H}'(\tilde{k},\{m_{\boldsymbol{q}}\};k',\{n'_{\boldsymbol{q}}\})\right\}, \tag{3.20}$$

where the initial condition at t_0 over the space domains $z<-A$ and $z>A$ has been substituted with the boundary condition at the system boundaries $\pm A$ both in the ballistic and in the scattering terms. The change from initial (for closed systems) to boundary conditions (for open systems) is symbolically illustrated in Fig. 2(a).

C. Phonons and potential profile

In this section we analyze the case in which the perturbation term is again given by the electron-phonon interaction, while the unperturbed Hamiltonian $\mathbf{H}_0$ contains, besides the free-electron and free-phonon Hamiltonians also a potential profile and an applied bias defined in the region of interest. The eigenstates of $\mathbf{H}_0$ are no longer plane waves but if, as we assume in our case, the potential is flat outside the region of interest, they can be taken as scattering states, and the coefficients $f_{kk'}(z,p)$ do not have the simple form presented in

Eq. (3.2). For this general case the validity of Eq. (3.20) will be extended on the basis of physical and analytical considerations. This will allow us to solve the problem for the case of an arbitrary potential profile taking advantage of the result obtained in the previous section. To this purpose we can use the linearity of the equation of motion for the WF [Eq. (2.5)] and decompose the WF into a sum of a number of initial contributions well localized in phase space. Furthermore, we set the boundaries of our system where the potential is constant, far from the region where the potential is rapidly varying. Under these hypotheses a single contribution to the WF evolves in a constant potential profile while it is entering the device from the boundary.

Let us now consider the time evolution of the WF:

$$i\hbar\frac{\partial}{\partial t}f_w(z,p,t)=\int dz' e^{ipz'/\hbar}\times\left\{\overline{i\hbar\frac{\partial\Psi(z-z'/2,t)}{\partial t}\Psi^*(z+z'/2,t)}+\overline{i\hbar\Psi(z-z'/2,t)\frac{\partial\Psi^*(z+z'/2,t)}{\partial t}}\right\},\tag{3.21}$$

where the overbar means ensemble average, and substitute the time derivative of the wave function by means of the time-dependent Schödinger equation:

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}f_w(z,p,t)=&-\frac{\hbar^2}{2m}\int dz' e^{ipz'/\hbar}\times\left\{\overline{\frac{d^2\Psi(z-z'/2,t)}{dz^2}\Psi^*(z+z'/2,t)}-\overline{\Psi(z-z'/2,t)\frac{d^2\Psi^*(z+z'/2,t)}{dz^2}}\right\}\\&+\int dz' e^{ipz'/\hbar}\{V(z-z'/2)-V(z+z'/2)\}\times\overline{\Psi^*(z+z'/2,t)\Psi(z-z'/2,t)}.\end{aligned}\tag{3.22}$$

The time evolution of the WF in this case is written as the sum of two terms: the first one corresponds to the ballistic evolution, the second one represents the scattering with the potential profile. For a WF localized in a region of the real space where the potential is constant, the term including the scattering potential gives no contribution. In fact, from the properties of the WF deriving from its definition, it follows that, in the real-space region where the WF is zero for any value of the momentum, $\overline{|\Psi|^2}=0$ and therefore all the corresponding wave functions of the ensemble are zero. Therefore, since either $V(z-z'/2)-V(z+z'/2)=0$ or $\overline{\Psi^*(z+z'/2,t)\Psi(z-z'/2,t)}=0$ for each z and z', the scattering term is zero. As a consequence, the contributions to the WF entering the device across the boundaries move, in the region of constant potential, according to a free evolution. Moreover, assuming perfectly thermalizing contacts, these contributions can be supposed to be distributed according to the equilibrium distribution when they enter the boundaries. Then we may assume such a distribution to correspond to the initial condition at t_0. This means that the contribution provided by the initial condition at t_0 for an interval dz around z, is transferred to the one provided by the boundary condition for an interval dt around t through the path transformation $dz=(p/m)dt$, where p/m is the velocity corresponding to the Wigner variable p.

Since the explanation given above may result somehow involved, it can be useful to summarize it. The time evolution of the WF can be written as the sum of the time evolutions of its single contributions, and they move ''free'' in the real-space region where the potential is constant. Perfectly thermalizing contacts allow to consider them distributed according to an equilibrium distribution that can be supposed to derive directly from the initial condition $f_w(z',p',t_0)$. Then the same considerations developed in the previous sections apply, and the initial condition can be substituted by the boundary conditions.

Concerning the evolution of the contributions to the WF starting inside the device at t_0, they are accounted for, as for the case discussed in the previous section, by integrating the position variable between $-A$ and A.

We can conclude that Eq. (3.20) describes the time evolution of the WF also in presence of an arbitrary potential profile far from the boundaries, and in this case a proper basis set of scattering states is used in place of plane waves. The change from initial (for closed systems) to boundary conditions (for open systems) is symbolically illustrated for this general case in Fig. 2(b).

IV. THE ITERATIVE EXPANSION

In order to solve the integral equation for the WF [Eq. (3.20)], a Neumann expansion has been obtained by iterative substitution of Eq. (3.20) into itself. In the compact formalism introduced in Eq. (2.5) this expansion results to be

$$\begin{aligned}f_w(t)=&f_w^{(0)}(t_0,t)+\frac{1}{h^3}\mathcal{F}\int_{t_0}^{t}dt'\mathcal{T}(t',t)\times\left\{\mathcal{H}'\mathcal{F}^\dagger\left[f_w^{(0)}(t_0,t')+\frac{1}{h^3}\mathcal{F}_2\int_{t_0}^{t'}dt''\mathcal{T}_2(t'',t')\times\{\mathcal{H}_2'\mathcal{F}_2^\dagger f_w^{(0)}(t_0,t'')-\mathcal{F}_2^\dagger f_w^{(0)}(t_0,t'')\mathcal{H}'\}\right]\right.\\&\left.-\mathcal{F}^\dagger\left[f_w^{(0)}(t_0,t')+\frac{1}{h^3}\mathcal{F}_2\int_{t_0}^{t'}dt''\mathcal{T}_2(t'',t')\times\{\mathcal{H}_2'\mathcal{F}_2^\dagger f_w^{(0)}(t_0,t'')-\mathcal{F}_2^\dagger f_w^{(0)}(t_0,t'')\mathcal{H}'\}\right]\mathcal{H}'+\cdots\right\},\end{aligned}\tag{4.1}$$

where

$$f_w^{(0)}(t_0,t)=\frac{1}{h^3}\mathcal{F}\mathcal{T}(t_0,t)\mathcal{F}^\dagger f_w^{(0)}(t_0),\tag{4.2}$$

and pairs of adjacent $\mathcal{F}\mathcal{F}^\dagger$ can be simplified using the unitarity relations defined in Ref. 11. At the initial time t_0 electrons and phonons are assumed to be at equilibrium and noninteracting, so that the total WF is diagonal in the phonon

variables. This assumption is equivalent to assume that the electron-phonon interaction is switched on at t_0. In practice, the effect of such an assumption becomes negligible if the dynamical evolution of the system is studied for sufficiently long times and the boundaries of the system are sufficiently far from the region of interest.

Since, at the observation time t, the trace over phonons must be performed when electron variables are investigated, only diagonal terms in the phonon variables of the generalized WF in Eq. (3.20) are to be evaluated. This implies that only even-order terms of the Neumann expansion contribute to our solution, and only terms corresponding to real and virtual phonon interactions,[14] where twice the same mode q is considered in the factors $\mathcal{H}'$ in Eq. (4.1).

For each phonon mode q the matrix elements of the interaction Hamiltonian between the states $|k,\{n_q\}\rangle$ and $|k',\{n_q'\}\rangle$ (where k is the incoming wave vector of the electron scattering state, and n_q the phonon occupation number) are given by

$$\begin{aligned}\mathcal{H}'(k',\{n_{\mathbf{q}}'\};k,\{n_{\mathbf{q}}\})&=\langle\phi_{k'},\{n_{\mathbf{q}}'\}|F(q)(\mathbf{b}_{\mathbf{q}}e^{iqz}-b_{\mathbf{q}}^{\dagger}e^{-iqz})|\phi_k,\{n_{\mathbf{q}}\}\rangle\\&=\sqrt{n_{\mathbf{q}}}\mathcal{C}(k',q,k)-\sqrt{n_{\mathbf{q}}+1}\mathcal{C}^*(k,q,k')\end{aligned}\tag{4.3}$$

where $\mathcal{C}(k',q,k)$ is the matrix element of e^{iqz} between the electron states $|k\rangle$ and $|k'\rangle$. As it regards the square roots of the phonon occupation numbers appearing in the above equation, they become n_q or n_q+1 when the second-order contributions of interest are considered. They correspond to the phonon occupation numbers which specify the actual phonon state at the considered time. However, when the trace operation over the phonon variables is performed and the thermal bath is assumed at equilibrium they must be substituted by their average values, given by the Bose-Einstein distribution.[14]

The perturbative contributions to the integral equation for the WF still maintain very complex expressions involving several integrations, so that, before their numerical evaluation, analytical manipulations are necessary. In particular, the time integrals have been performed analytically and the following identities have been used:

$$\int dk''\mathcal{C}(k,\pm q,k'')f^*_{k'',k'}(z,p)=e^{\pm iqz}f^*_{k,k'}\left(z,p\pm\hbar\frac{q}{2}\right)\tag{4.4}$$

that can be easily obtained using the analytical properties of the quantities involved.

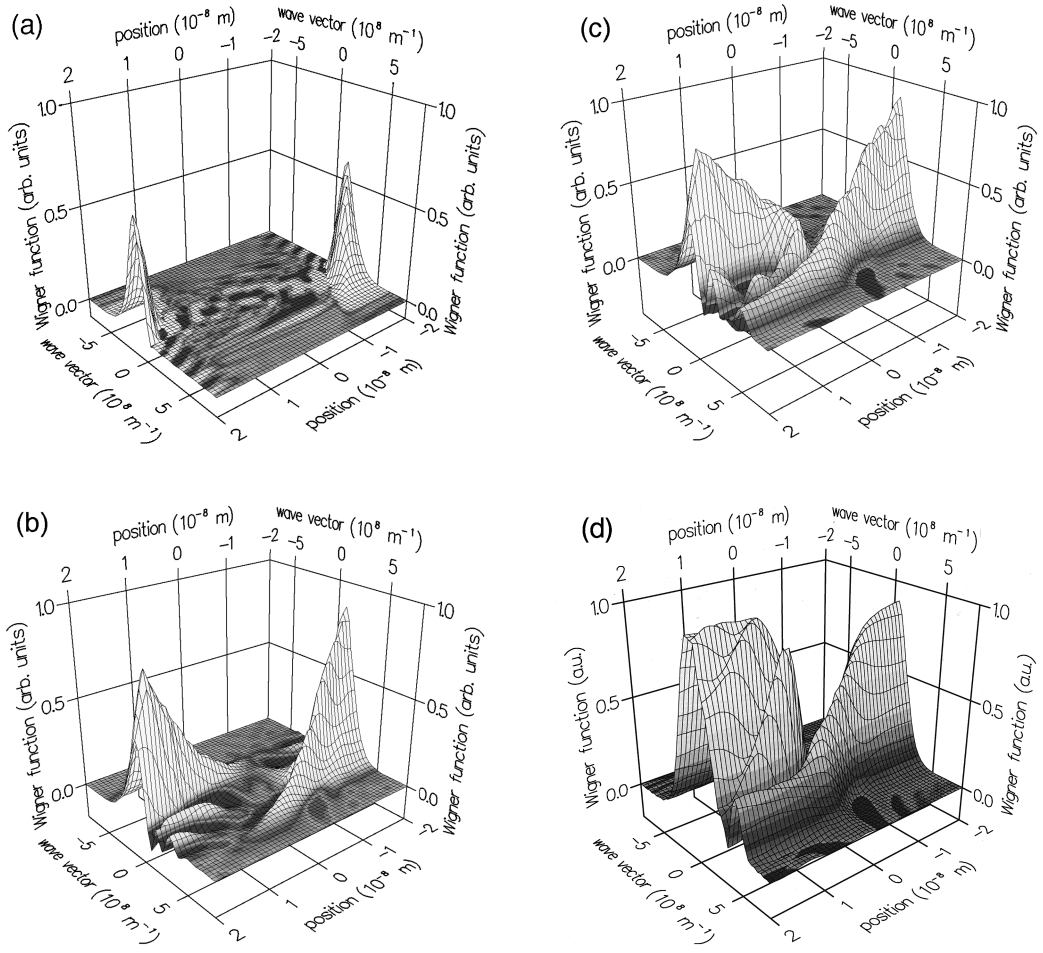

FIG. 3. ''Ballistic invasion''of the Wigner function into an empty device with local equilibrium boundary conditions at $t=10$ fs (a), $t=40$ fs (b), $t=80$ fs (c) for electrons entering from the boundaries into a region with a potential step and stationary Wigner function (d), as obtained by means of an equilibrium density matrix diagonal over the scattering states for a 0.1-eV step potential.

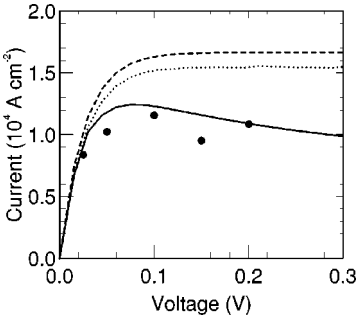

FIG. 4. Electron current across step potential as a function of the step height. In the figure a comparison between quantum and semiclassical calculations with and without e-ph interaction is shown. The following cases are reported: Wigner-ballistic curve (solid line), Wigner curve with e-ph scattering (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 $n = 10^{16}\,\mathrm{cm}^{-3}$ has been assumed.

V. NUMERICAL RESULTS

The theory described in the previous sections has been applied to investigate electron transport in GaAs-based mesoscopic heterostructures. Numerical calculations have been performed for a three-dimensional system. The electronic unperturbed states have been chosen as the scattering states of the considered potentials as it regards the direction orthogonal to the interfaces, obtained as numerical solutions of the corresponding Schrödinger equation. Along the plane of the interface plane waves have been assumed. For simplicity the effective mass has been assumed to be the same all over the structure ($m^* = 0.067 m_0$).

Electron interaction with polar-optical phonons has been considered in this paper, characterized by a coupling function $F(\mathbf{q})$ in Eq. (2.2) given by

$$F(q) = \left[\frac{e^2 K_B \theta_{pop}}{2\hbar^2 \varepsilon_0} \left\{ \frac{1}{\varepsilon(\infty)} - \frac{1}{\varepsilon(0)} \right\} \right]^{1/2} \frac{1}{q}, \qquad (5.1)$$

where $K_B \theta_{pop}$ is the energy of the polar optical phonons in GaAs ($\theta_{pop} = 410\,\mathrm{K}$), and $\varepsilon(\infty) = 10.92$ and $\varepsilon(0) = 12.9$ are the high- and low-frequency dielectric constant, respectively.

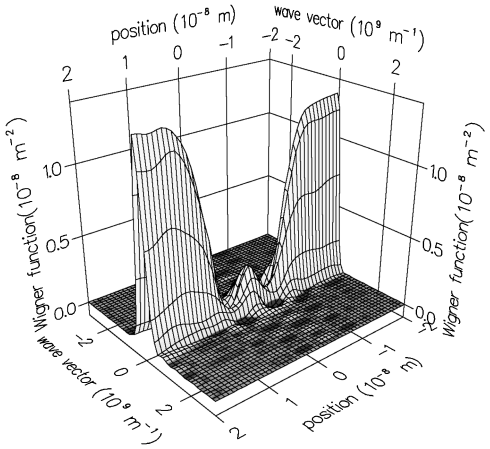

FIG. 5. Wigner function for a double-barrier potential profile, at a 160-mV applied bias, including the effect of an e-ph scattering switched on 50 fs before the ''observation'' time.

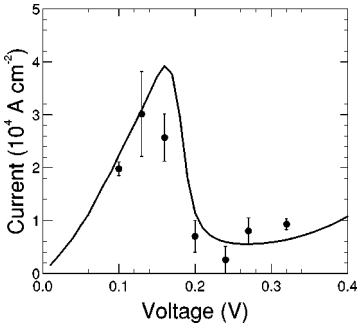

FIG. 6. Electron current as a function of the applied bias for the case of a double-barrier potential profile. A comparison is shown between the results obtained using the ballistic Wigner function (solid line) and the Wigner function corrected by the effect of an electron-phonon scattering process (full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

As first application we have evaluated the ballistic evolution of an electron flux across a step potential profile. The following initial and boundary conditions have been assumed: $f_w = 0$ at $t = t_0$ inside the device and a Maxwellian local equilibrium incoming distribution at the left and right boundaries. Results are shown in Figs. 3(a)–3(d) at different times after the initial condition. At the longest times we recover for f_w the same result, which is obtained without using boundary conditions for a stationary infinite system, where f_w is evaluated by means of an equilibrium density matrix diagonal over the scattering states.

In order to evaluate the effect of a single electron-phonon scattering event on the otherwise coherent electron propagation across the step we have evaluated the second-order contribution in the e-p perturbation Hamiltonian to the iterative expansion of Eq. (3.20).

The integral over the phonon modes has been performed by means of a Monte-Carlo sampling. All the other integrals appearing in the perturbative terms have been performed numerically by means of finite-difference and fast-Fourier algorithms. Space correlations for the evaluation of the coefficients in Eq. (3.2) have been considered up to 40 nm, and in some cases the results have been verified assuming twice this value.

Owing to the formidable computational burden associated to the numerical integrations, we have developed and implemented a parallel algorithm suitable to exploit the features of modern supercomputers. Typical computer CPU times required for the evaluation of a point in the $I(V)$ characteristics of the considered structures are of the order of 30 h on a 100 CPU-Cray T3E machine.

Figure 4 shows the electron current as a function of the step-potential height as obtained with the ballistic WF (solid curve) and with the WF corrected by the effect of an e-ph scattering process (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 than the corresponding semiclassical one, and instead of reaching a saturation value, 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 coefficient, that is, to a decrease of the current intensity. Finally, in both quantum and semiclassical calculations the effect of the e-ph interaction is, as expected, a reduction of the current with respect to the ballistic case.

As a second case we considered a double-barrier structure. The two AlGaAs barriers are 0.28-eV high and 2.8-nm wide, and they are separated by a GaAs layer of 5 nm. A constant external electric field has been applied to the considered structure.

The steady-state WF for a double barrier potential profile, at a 160-meV applied bias, including the effect of an e-ph scattering is presented in Fig. 5. In Fig. 6, the current is displayed as a function of the applied bias for such a potential profile. The solid curve is obtained with the ballistic WF, whilst the full circles (with the error bars) are the results of the calculations performed using the WF corrected for effects of an e-ph scattering mechanism. Even considering the uncertainty introduced by problems of numerical accuracy, the effect of the e-ph scattering process on the characteristics 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 increased. These results can be interpreted in terms of the loss of coherence and of the broadening of the resonance states, and are in agreement with those obtained by Frensley[15] and by Ragazzi *et al.* using a semiclassical Boltzmann collision operator.[16]

VI. CONCLUSIONS

We have developed a general method for the solution of quantum electron transport problems for an open system containing an arbitrary potential profile and electron-phonon interaction with thermalizing contacts located in regions with constant potential profile. In particular, we have proved that in order to evaluate the Wigner equation including electron-phonon interaction the initial condition of the WF over the whole space can be substituted by a suitable boundary condition. The analytical proof has been initially given for the case in which the eigenstates of the unperturbed Hamiltonian are plane waves and then extended to the more general case of scattering states. From the physical point of view this new result provides a natural description of an open system by imposing at the boundaries the correct conditions determined by the environment. The theory has been applied to calculate the current associated with electron quantum transport across a potential step and a double barrier in presence of single phonon-scattering process.

ACKNOWLEDGMENTS

This work has been partially funded by A.R.O. and O.N.R. through E.R.O.

[1] *Nanostructures and Mesoscopic Systems*, edited by W. P. Kirk and M. A. Reed (Academic Press, San Diego, 1992).

[2] *Quantum Transport in Ultrasmall Devices*, edited by D. K. Ferry, H. L. Grubin, C. Jacoboni, and A. P. Jauho (Plenum Press, New York, 1994).

[3] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge Press, Cambridge, 1995).

[4] H. Haug and A. P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, Berlin, 1996).

[5] E. Wigner, Phys. Rev. **40**, 749 (1932).

[6] N. C. Kluksdahl, A. M. Kriman, D. K. Ferry, and C. Ringhofer, Phys. Rev. B **39**, 7720 (1989).

[7] W. R. Frensley, Rev. Mod. Phys. **62**, 745 (1990).

[8] R. Brunetti, C. Jacoboni, and M. Nedjalkov, in *Hot Carriers in Semiconductors*, edited by K. Hess (Plenum Press, New York, 1996), p. 417.

[9] C. Jacoboni, A. Abramo, P. Bordone, R. Brunetti, and M. Pascoli, VLSI Design **8**, 185 (1998).

[10] P. Bordone, A. Abramo, R. Brunetti, M. Pascoli, and C. Jacoboni, Phys. Status Solidi B **204**, 303 (1997).

[11] M. Pascoli, P. Bordone, R. Brunetti, and C. Jacoboni, Phys. Rev. B **58**, 3503 (1998).

[12] F. Rossi, C. Jacoboni, and M. Nedjalkov, Semicond. Sci. Technol. **9**, 934 (1994).

[13] P. Carruthers and F. Zachariasen, Rev. Mod. Phys. **55**, 245 (1983).

[14] R. Brunetti, C. Jacoboni, and F. Rossi, Phys. Rev. B **39**, 10 781 (1989).

[15] W. R. Frensley, Solid-State Electron. **31**, 739 (1988).

[16] S. Ragazzi, A. Di Carlo, P. Lugli, and F. Rossi, Phys. Status Solidi B **204**, 339 (1997).