Generalized Wigner Function Formulation
for Quantum Systems with Open Boundaries

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A rigorous microscopic theory for the description of quantum-transport phenomena in systems with open boundaries is proposed. We shall show that the application of the conventional Wigner-function formalism to this problem leads to unphysical results, like injection of coherent electronic states from the contacts. To overcome such basic limitation, we propose a generalization of the standard Wigner-function formulation, able to properly describe the incoherent nature of carrier injection at the device spatial boundaries as well as the interplay between phase coherence and energy relaxation/dephasing within the device active region. The proposed theoretical scheme constitutes the first rigorous derivation of the phenomenological injection model commonly employed in the simulation of open quantum devices.

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Present-day technology pushes device dimensions toward limits where the traditional semiclassical transport theory [1] can no longer be applied, and more rigorous quantum-transport approaches are required [2]. However, in spite of the quantum-mechanical nature of carrier dynamics in the core region of typical nanostructured devices—like semiconductor superlattices and double-barrier structures—the overall behaviour of such quantum systems is often the result of a complex interplay between phase coherence and energy relaxation/dephasing [3], the latter being primarily due to the presence of spatial boundaries [4]. It follows that a proper treatment of such novel nanoscale devices requires a theoretical modelling able to properly account for both coherent and incoherent—i.e., phase-breaking—processes on the same footing. To this end, a generalization to open systems—i.e., systems with open boundaries—of the well known Semiconductor Bloch Equations (SBE) [5] has been recently proposed [6]. However, the theoretical analysis presented in [6] is primarily related to the interplay between phase coherence and energy relaxation within the device active region, and—apart from its abstract formulation—no detailed investigation of the carrier-injection process (from the electrical contacts into the device active region) has been performed so far.

Aim of the present Letter is to provide a rigorous quantum-mechanical description of the coupling dynamics between the device active region and external charge reservoirs, able to account for the semi-phenomenological injection models commonly employed in state-of-the-art simulations of realistic one- and two-dimensional open quantum devices [7]. Among such simulation strategies it is worth mentioning the approach recently proposed by Fischetti and co-workers [8, 9]: By denoting with \( f_\alpha \) the carrier distribution over the electronic states \( \alpha \) of the device, the transport equation proposed in [9] is of the form:

\[
\frac{d}{dt} f_\alpha = \sum_{\alpha'} (W_{\alpha \alpha'} f_{\alpha'} - W_{\alpha' \alpha} f_\alpha) + \frac{f_{\alpha}^b - f_\alpha}{\tau_\alpha} . \tag{1}
\]

Here, \( f_\alpha^b \) denotes the equilibrium carrier distribution in the contacts while \( \tau_\alpha \) can be regarded as the device transit time for an electron in state \( \alpha \). As anticipated, in spite of a rigorous treatment of the scattering dynamics, the last (relaxation-time-like) term describes carrier injection/loss on a partially phenomenological level and does not depend on the real position of the device spatial boundaries.

In order to provide a fully microscopic real-space description of the carrier-injection process, we shall start revisiting the theoretical approach proposed in [9]. By applying to the conventional SBE for a closed system [10, 11]

\[
\frac{d}{dt} \rho_{\alpha_1 \alpha_2} = \sum_{\alpha'_1, \alpha'_2} L_{\alpha_1 \alpha_2, \alpha'_1 \alpha'_2} \rho_{\alpha'_1 \alpha'_2} \tag{2}
\]

the usual Weyl-Wigner transform

\[
u_{\alpha_1 \alpha_2}(r,k) = \int dr' \phi_{\alpha_1} \left( r + \frac{r'}{2} \right) \frac{e^{-ik \cdot r'}}{(2\pi)^2} \phi_{\alpha_2}^* \left( r - \frac{r'}{2} \right) \tag{3}
\]

one gets:

\[
\frac{d}{dt} f(r,k) = \int L(r,k; r',k') f(r',k') dr' dk' , \tag{4}
\]
FIG. 1: Schematic representation of the device active region sandwiched between its electrical contacts (a) and of the corresponding U boundary-condition scheme for a one-dimensional system. The latter implies, in particular, the knowledge of the incoming Wigner function $f(z_b, k)$, i.e., $f(z_{\text{left}}, k > 0)$ and $f(z_{\text{right}}, k < 0)$.

where

$$f(r, k) = \sum_{\alpha_1\alpha_2} u_{\alpha_1\alpha_2}(r, k) \rho_{\alpha_1\alpha_2}$$  \hspace{1cm} (5)$$

is the well-known Wigner function [4, 12] while the quantity $L(r, k; r', k')$ is the Liouville operator in the new phase-space representation $r, k$.

For a closed system, the Wigner function $f$ is defined for any value of the real-space coordinate $r$ and its time evolution is fully dictated by its initial condition. In contrast, for a system with open boundaries $f$ is defined only within a given region $\Omega$ of interest and its time evolution is determined by the initial condition at $t_0$ inside such region as well as by the value of its incoming part on the boundary $r_b$ of the domain at any time $t' > t_0$. Such boundary-condition scheme [13]—also referred to as “U scheme”— is depicted in Fig. 1. More specifically, in order to properly impose the desired spatial boundary conditions, let us rewrite Eq. (4) as

$$\frac{d}{dt} f(r, k) = \int \tilde{L}(r, k; r', k') f(r', k') dr' dk' + S(r, k)$$  \hspace{1cm} (6)$$

by adding and subtracting a source term $S(r, k) = v(k) f^b(k) \delta(r - r_b)$ [14]. The latter is compensated by a renormal-
By applying the inverse of the Weyl-Wigner transform in (3) to Eq. (6) we get:

\[ \Delta L(r,k,r',k') = -v(k)\delta(r - r_0)\delta(r - r')\delta(k - k') , \]  

(7)

By applying the inverse of the Weyl-Wigner transform in (3) to Eq. (6) we get:

\[ \frac{d}{dt}\rho_{\alpha_1\alpha_2} = \sum_{\alpha'_1\alpha'_2} \hat{L}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2}\rho_{\alpha'_1\alpha'_2} + S_{\alpha_1\alpha_2} . \]  

(8)

Equation (8) is the desired generalization to open systems of the SBE in (2) \[16\].

In order to validate the theoretical approach presented so far, we shall focus on a very simple semiconductor nanostructure: a single-barrier equidistant from the device contacts (see Fig. 2). As basis states \( \alpha \) we adopt the scattering states of the device potential profile; moreover, to better identify the role played by carrier injection, we shall neglect all other sources of energy relaxation/dephasing in the device active region, like carrier-phonon and carrier-carrier scattering. Under these assumptions, Eq. (8) in steady-state conditions reduces to:

\[ \frac{i}{\hbar}(\epsilon_{\alpha_1} - \epsilon_{\alpha_2})\rho_{\alpha_1\alpha_2} - \sum_{\alpha'_1\alpha'_2} \Delta L_{\alpha_1\alpha_2,\alpha'_1\alpha'_2}\rho_{\alpha'_1\alpha'_2} = S_{\alpha_1\alpha_2} , \]  

(9)

where \( \epsilon_\alpha \) denotes the energy of the scattering state \( \alpha \) and \( \Delta L_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} \) is the renormalization term in (7) written in the density-matrix representation \( \alpha_1\alpha_2 \).

Figure 2 shows results for the single-barrier potential profile when carriers are primarily injected from left. Here, the simulated real-space charge distribution obtained from the phenomenological injection model in Eq. (1) (dashed curve) is compared to that of the microscopic model in (9) (solid curves). As we can see, the two models give completely different results. The phenomenological model gives almost exactly what we expect: since we have significant carrier injection from left only and since the potential barrier is relatively high, the carrier distribution is mainly located on the left side. In contrast, the microscopic model gives an almost symmetric charge distribution. In order to understand the origin of this unphysical result, let us focus on the nature of the source term in (8). Contrary to the phenomenological injection/loss term in (7), the latter is intrinsically non-diagonal, i.e., the injection of a carrier with well-defined wavevector \( k \) is described by a non-diagonal source contribution \( S_{\alpha_1\alpha_2} \). In other words, we inject into the device active region a coherent superposition of states \( \alpha_1 \) and \( \alpha_2 \), in clear contrast with the idea of injection from a thermal —i.e., diagonal— charge reservoir. More specifically, in this case the generic scattering state \( \alpha \) on the left comes out to be an almost equally weighted superposition of \( +k \) and \( -k \): \( \phi_k(z) = a_k e^{ikz} + b_k e^{-ikz} \). This, in turn, tells us that the generic plane-wave state \( k \) injected from the left contact is also an almost equally weighted superposition of the left and right scattering states. This is why the charge distribution (solid curve in Fig. 2) is almost symmetric: any electron injected from left couples to left as well as to right scattering states. The anomaly of the microscopic model is even more pronounced if we look at the carrier distribution in momentum space (see inset in Fig. 2). While for the phenomenological model (dashed curve) we get a positive-definite distribution showing, as expected, the two symmetric wavevector components of the scattering state, the microscopic result is not positive definite; this tells us that our boundary-condition scheme does not ensure that the solution of Eq. (1) is a “good” Wigner function.

The scenario previously discussed is highly non-physical; it can be mainly ascribed to the boundary-condition scheme employed so far, which implies injection of plane-wave electrons [see source term in Eq. (1)], regardless of the shape of the device potential profile. This is an intrinsic limitation of the conventional Wigner-function representation \( r, k \). It is then clear that, in order to overcome this limitation, what we need is a boundary-condition scheme realizing diagonal injection over the scattering states \( \alpha \) of the device potential profile.

To this end, in this Letter we propose a generalization of the Wigner-function formulation considered so far. The key idea is to extend the Weyl-Wigner transform in (3) from the \( k \) to a generic basis set \( \{|\beta\rangle\} \) according to (17):

\[ u^{01\alpha_2}_{\beta_1\beta_2}(r) = \Omega \int dr' \phi_{\alpha_1}(r + r') \chi^*_{\beta_1}(r + r') \chi_{\beta_2}(r - r') \phi^*_{\alpha_2}(r - r') . \]  

(10)

In analogy to (3), our generalized Wigner function is given by (18):

\[ f^{\beta_1\beta_2}_{\alpha_1\alpha_2}(r) = \sum_{\alpha_1\alpha_2} u^{01\alpha_2}_{\beta_1\beta_2}(r)\rho_{\alpha_1\alpha_2} . \]  

(11)
FIG. 2: Comparison between the real-space charge distribution obtained from the phenomenological injection model in (1) $n(r) = \sum \alpha \phi \alpha(r)^2$ — dashed curve and the microscopic model in (9) $n(r) = \sum \alpha_1 \alpha_2 \rho \alpha_1(r) \phi \alpha_2(r)$ — solid curve for a GaAs-based single-barrier structure (height $V_o = 0.5$ eV and width $a = 4$ nm) equidistant from the electrical contacts. In this room-temperature simulation, due to a misalignment $\Delta \mu = 0.2$ eV of the left and right chemical potential, carriers are primarily injected from left. The corresponding charge distribution in momentum space is also reported in the inset (see text).

By adopting as basis states $|\beta\rangle$ the scattering states of the device potential profile and assuming a diagonal source term of the form

$$S_{\beta_1,\beta_2}(r) = v_{\beta_1} f_{\beta_1}^{\beta_2} \delta_{\beta_1,\beta_2} \delta(r - r_b),$$

its equation of motion will be

$$\frac{d}{dt} f_{\beta_1,\beta_2}(r) = \sum_{\beta_1',\beta_2'} \int d r' L_{\beta_1,\beta_2,\beta_1',\beta_2'}(r, r') f_{\beta_1',\beta_2'}(r') + S_{\beta_1,\beta_2}(r)$$

with a renormalization $\Delta L_{\beta_1,\beta_2,\beta_1',\beta_2'}(r, r')$ given by

$$- v_{\beta_1} \delta_{\beta_1,\beta_2} \delta_{\beta_1,\beta_2'} \delta(r - r_b) \delta(r - r').$$

We stress that now the source term in (12) describes diagonal injection over the scattering states (with velocity $v_\beta$), as requested. Indeed, if we now integrate Eq. (13) over the real-space coordinate $r$, we get again the density-matrix...
equation in (8), but with a diagonal source term $S_{\alpha_1\alpha_2} = v_{\alpha_1} f^b_{\alpha_1} \delta_{\alpha_1\alpha_2}$ and a much simpler —i.e., partially diagonal— renormalization term $\Delta L_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} = -v_{\alpha_1} \delta_{\alpha_1\alpha_2} u^\alpha_{\alpha_1\alpha_2} (r_b)$. In the scattering-free case, the stationary solution is again described by Eq. (9). However, due to the diagonal nature of the new source term as well as of the partially diagonal structure of $\Delta L$, Eq. (9) has now a diagonal solution: $\rho_{\alpha_1\alpha_2} = f_{\alpha_1} \delta_{\alpha_1\alpha_2}$. More specifically, the diagonal density-matrix elements $f_{\alpha}$ obey the following steady-state equation:

$$T_{\alpha\alpha'} f_{\alpha'} = f^b_{\alpha}$$

with $T_{\alpha\alpha'} = u^\alpha_{\alpha'\alpha'} (r_b)$. Equation (15) is semiclassical in nature, i.e., it involves diagonal density-matrix terms only [19].

Figure 3 shows again results for the single-barrier potential profile previously considered. Here, the simulation based on the phenomenological injection model in Eq (1) (dashed curves) is compared to that of the new microscopic model in (15) (solid curves). As we can see, the highly non physical behaviours of Fig. 2 (solid curves) have been completely removed. Indeed, the momentum distribution in the inset is always positive-definite and the two models exhibit a very similar behaviour. We find relatively small deviations close to the device spatial boundaries, which can be ascribed to the interlevel injection coupling $T_{\alpha\alpha'}$ [see Eq. (15)], not present in the phenomenological injection model.

In conclusion, we have proposed a rigorous description of quantum-transport phenomena in systems with open boundaries. Our analysis has shown that the conventional Wigner-function formalism leads to unphysical results,
like injection of coherent superpositions of states from the device spatial boundaries. This basic limitation has been removed by introducing a generalization of the standard Wigner-function formulation, able to properly describe the incoherent nature of carrier injection. The proposed theoretical scheme constitutes a rigorous derivation of the phenomenological injection models commonly employed in the simulation of open quantum devices.

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[1] See, e.g., C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulations* (Springer, Wien 1989).

[2] See, e.g., *Theory of Transport Properties of Semiconductor Nanostructures*, edited by E. Schöll (Chapman & Hall, London 1998).

[3] See, e.g., R.C. Iotti and F. Rossi, Phys. Rev. Lett. 87, 146603 (2001).

[4] See, e.g., W. Frensley, Rev. Mod. Phys. 62, 3 (1990) and references therein.

[5] See, e.g., F. Rossi and T. Kuhn, Rev. Mod. Phys. 74 (2002) and references therein.

[6] F. Rossi, A. Di Carlo, and P. Lugli, Phys. Rev. Lett. 80, 3348 (1998).

[7] See, e.g., *Special Issue on Computational Electronics*, VLSI design 13 (2001).

[8] M.V. Fischetti, Phys. Rev.B 59, 4901 (1999) and references therein.

[9] This is grounded on a Master Equation description derived from a rigorous density-matrix formulation of the problem, and can be regarded as the diagonal (i.e., semiclassical) limit of the theoretical scheme proposed in [6].

[10] Here, \( \rho_{\alpha\beta} \) is the single-particle density matrix written in our single-particle basis \( \{ \phi_{\alpha} \} \). Its diagonal elements correspond to the usual distribution function \( f_{\alpha} \) of the semiclassical theory [1] while the off-diagonal terms \( \alpha \neq \beta \) describe the degree of quantum-mechanical phase coherence between states \( \alpha \) and \( \beta \).

[11] Within such formalism, the Liouville superoperator \( L \) describes—in addition to the single-particle quantum-mechanical evolution—various energy-relaxation and dephasing processes in terms of generalized in- and out-scattering operators [2].

[12] See, e.g., F.A. Buot, Phys. Rev.B 10, 3700 (1974).

[13] P. Bordone et al., Phys. Rev.B 59, 3060 (1999).

[14] Here, \( v(k) \) denotes the negative or incoming part of the carrier group velocity normal to the boundary surface and \( f^b(k) \) is the Wigner function describing the distribution of the injected carriers.

[15] Indeed, it is easy to show that Eqs. (4) and (6) coincide, provided that \( f(r, k) = f^b(k) \), i.e., the desired boundary conditions.

[16] The open character of the system results in a non-Hermitian correction \( \Delta L \) to the Liouville operator \( L \), whose effect is equivalent to a purely dissipative process within the simulated region, as originally pointed out in [4].

[17] Here, the set of basis functions \( \chi_\beta(r) \equiv \langle r | \beta \rangle \) is, in general, different from the basis set \( \phi_\alpha \). It is easy to show that if we consider as basis states \( | \beta \rangle \) conventional plane waves, the standard Weyl-Wigner transform in [4] is recovered.

[18] In analogy to the conventional Wigner-function theory [4, 12], the real-space charge distribution (see solid line in Fig. 3) is now given by \( n(r) = \sum_{\alpha\beta} f_{\beta\beta}(r) \).

[19] We stress that, by replacing the \( T \) with the identity operator \( (T_{\alpha\beta} = \delta_{\alpha\beta}) \), the usual phenomenological model in [1] is recovered; indeed for the scattering-free case \( (W_{\alpha\beta} = 0) \) in steady-state conditions we get \( f_{\alpha} = f_{\alpha}^b \).