Quantum Non-Localilty in Systems with Open Boundaries: Failure of the Wigner-Function Formalism

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(Dated: March 23, 2022)

We shall revisit the conventional treatment of open quantum devices based on the Wigner-Function formalism. Our analysis will show that the artificial spatial separation between device active region and external reservoirs—properly defined within a semiclassical simulation scheme—is intrinsically incompatible with the non-local character of quantum mechanics. More specifically, by means of an exactly-solvable semiconductor model, we shall show that the application of the conventional boundary-condition scheme to the Wigner transport equation may produce highly non-physical results, like thermal injection of coherent state superpositions and boundary-driven negative probability distributions.

PACS numbers: 72.10.Bg, 85.30.-z, 73.40.-c

Current micro/nanoelectronics technology pushes device dimensions toward limits where the traditional semiclassical Boltzmann theory\textsuperscript{1} can no longer be applied, and more rigorous quantum-transport approaches are required\textsuperscript{2}. However, in spite of the genuine quantum-mechanical nature of carrier dynamics in the active region of typical nanostructured devices—like semiconductor superlattices and double-barrier structures—the overall behavior of such quantum systems is often the result of a non-trivial interplay between phase coherence and dissipation/dephasing\textsuperscript{3}, the latter being also due to the presence of spatial boundaries\textsuperscript{3}. 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 aim, a commonly used theoretical instrument is the so-called single-particle density matrix\textsuperscript{4,5}; however, while the latter is the ideal tool for the description of ultrafast phenomena in infinitely-extended/periodically-repeated nanostructures\textsuperscript{3}, it cannot be directly applied to quantum systems with open boundaries, for which a real-space treatment is imperative.

Such a real-space description is naturally provided by the Wigner-function formalism\textsuperscript{3}; within this approach the statistical quantum state of the electronic subsystem is fully described in terms of the so-called Wigner function, a function defined over the conventional phase-space as the Weyl-Wigner transform of the single-particle density matrix\textsuperscript{8,10}; for the case of a one-dimensional problem, the equation describing the time evolution of the Wigner function—often referred to as the Wigner transport equation— is of the form:

\[
d\frac{f(z,k)}{dt} = \int dz' dk' \mathcal{L}(z,k;z',k')f(z',k') , \tag{1}
\]

where \(\mathcal{L}(z,k;z',k')\) denotes the corresponding effective Liouville superoperator\textsuperscript{10} written in the Weyl-Wigner phase-space representation \(z,k\).

Different approaches for the study of quantum-transport phenomena in semiconductor nanostructures based on the Wigner-function formalism have been proposed. On the one hand, starting from the pioneering work by Frensley\textsuperscript{11}, a few groups\textsuperscript{12} have performed quantum-transport simulations based on a direct numerical solution of the Wigner equation in\textsuperscript{10} via finite-difference approaches by imposing to \(f(z,k)\) the standard boundary-condition scheme of the semiclassical device modelling, also called U-scheme\textsuperscript{10}. On the other hand, a generalization to systems with open boundaries of the well-known Semiconductor Bloch Equations (SBE)\textsuperscript{3,4}—the set of equations governing the time evolution of the single-particle density matrix— has been recently proposed\textsuperscript{10,13}; such generalized SBE—obtained again via the U-scheme previously mentioned—describe the open nature of the problem via a boundary source term and a corresponding renormalization of the Liouville superoperator. In addition to the two alternative simulation strategies previously recalled—both based on effective treatments of relevant interaction mechanisms—, Jacoboni and co-workers have proposed a fully quantum-mechanical simulation scheme for the study of electron-phonon interaction based on the so-called “Wigner paths”\textsuperscript{14,15}.

The generalized SBE approach previously recalled has been recently applied to prototypical semiconductor-based open systems. Preliminary results presented in\textsuperscript{15} seem to suggest an intrinsic limitation of the conventional Wigner function formalism in describing quantum-transport phenomena through systems with open boundaries. On the other hand, no clear evidence of such limitations has been reported so far via Wigner-function simulations based on finite-difference treatments\textsuperscript{3,12}.

Aim of this Letter is to solve this apparent contradiction,
thus shedding light on the real limitations of the conventional Wigner-function picture applied to open-device modelling. Our analysis will show that the artificial spatial separation between device active region and external reservoirs is intrinsically incompatible with the non-local character of quantum mechanics.

In order to gain more insight into this highly non-trivial problem, let us start considering the explicit form of the Wigner equation in stationary conditions and in the absence of any scattering mechanism:

$$v(k) \frac{\partial}{\partial z} f(z, k) + \int dk' \mathcal{V}(z, k - k') f(z, k') = 0 \quad (2)$$

where

$$\mathcal{V}(z, k) = \int_{-\infty}^{\infty} dz' e^{-\frac{2ikz'}{\hbar}} [V(z + z') - V(z - z')] \quad (3)$$

is the Weyl-Wigner superoperator corresponding to the device potential profile $V(z)$, while $v(k)$ denotes the electron group velocity. Following the standard U-scheme, we shall now impose the desired spatial boundary conditions for $f$ at the left ($z = -\frac{z_0}{2}$) and right ($z = +\frac{z_0}{2}$) contacts, specifying the “incoming” electron distribution $f_b(k) = f(z_0, k)$, where $z_0(k) = \frac{\hbar}{\pi V_0} (\theta(-k) - \theta(+k))$. The corresponding propagator $W$ (which is the Weyl-Wigner superoperator corresponding to the current point $z$) to the current point $z$ we get:

$$f(z, k) = f_b(k) - \int_{z_0(k)}^z dz' \int dk' \frac{\mathcal{V}(z', k - k')}{v(k)} f(z', k') = f_b(k) + \int dz' dk' \mathcal{W}(z, k; z', k') f(z', k') \quad (4)$$

with $\mathcal{W}(z, k; z', k') = -\theta(z' - z_0(k)) \theta(z - z') \frac{\mathcal{V}(z', k - k')}{v(k)}$. In a compact notation we have:

$$f = f_b + \mathcal{W} f \quad \text{or} \quad f = \frac{1}{1 - \mathcal{W}} f_b \quad (5)$$

By expanding the above formal solution in powers of the interaction superoperator/propagator $\mathcal{W}$ —and therefore of the potential $\mathcal{V}$— we get the well-known Neumann series:

$$f = \sum_{n=0}^{\infty} \mathcal{W}^n f_b \quad (6)$$

Let us now focus on the case of a symmetric potential profile ($V(z) = V(-z)$), which in turn corresponds to an antisymmetric potential superoperator, i.e., $\mathcal{V}(z, k) = -\mathcal{V}(-z, k)$. Using this property together with the symmetric nature of our spatial boundaries, i.e., $z_0(k) = -z_0(-k)$, it is possible to show that the interaction propagator $\mathcal{W}$ is also preserving the potential symmetry. This result is extremely important: it implies that for any symmetric potential profile and spatial boundaries the Neumann expansion in gives always a Wigner function symmetric in the spatial coordinate: $f(z, k) = f(-z, k)$. Therefore, in total agreement with the numerical results of the generalized SBE presented in [12], the spatial charge density $n(z) = \int f(z, k) dk$ is always symmetric, no matter which is the shape of the injected carrier distribution $f_0(k)$. As anticipated, such symmetric behavior—which is an exact result of the treatment presented so far—has never been observed via finite-difference calculations.

In order to solve this apparent contradiction, let us now focus on a particular choice of the device potential profile: $V(z) = V_0 [1 + \cos(2\kappa z)]$. The corresponding superoperator in is simply given by:

$$\mathcal{V}(z, k) = \pi V_0 \sin(2\kappa z) [\delta(k - \kappa) - \delta(k + \kappa)] \quad (7)$$

For this particular potential superoperator—characterized by a factorization/decoupling of position ($z$) and momentum ($k$) coordinates—it is possible to obtain the spatial charge distribution analytically:

$$n(z) = \int dk f_b(k) I_{F_2} \left[ \frac{1}{2}; 1 + \alpha(k), 1 - \alpha(k); q(z) \right]$$

$$q(z) = \frac{2m^* V_0^2}{\kappa^2} \sin[\kappa (z - \frac{l}{2})] \sin[\kappa (z + \frac{l}{2})] \quad (8)$$

Here, $m^*$ is the electron effective mass, $\alpha(k) = k/\kappa$, and $I_{F_2}$ denotes the generalized hypergeometric function of type $(1, 2)$.

In order to investigate the main features of the analytical results obtained so far, let us start by considering extremely simple spatial boundary conditions: a monoenergetic carrier injection from left only, i.e., $f_b(k) \propto \delta(k - k_0)$. Moreover, we choose a potential periodicity $\kappa = \frac{\pi}{2}$ corresponding to just one maximum within the device active region, so as to mimic the single-barrier device considered in [13]. Figure B shows a comparison between the analytical spatial charge distribution in and the phenomenological result obtained via conventional scattering-state calculations. As we can see, the two curves differ significantly: while the phenomenological charge distribution (dashed curve) —describing an extremely small tunnelling dynamics through the potential maximum—exhibits a clear and non-ambiguous asymmetric behavior, the analytical result of the Wigner-function approach (solid curve) is always symmetric, in total agreement with the analysis proposed in [13]. This implies that, also for an infinitely high potential barrier and for a monoenergetic injection from left only, carriers are “instantaneously” present also on the right part of the device, a typical non-local feature of our quantum-mechanical calculation. More important, within the Wigner-function treatment (solid curve) we deal with a
spatial charge/probability distribution with negative values, which tells us that the analytical solution $f(z, k)$ of the differential equation in (1) is not necessarily a Wigner function [18].

Let us finally come to potential discrepancies between exact and finite-difference results. Figure 2 shows a comparison between the conventional finite-difference solution of Eq. (2) proposed in [8] (dashed curve) and a numerical iterative solution of Eq. (4) (solid curve); for both cases the same $80 \times 80$ phase-space discretization has been employed. As we can see, while the iterative solution coincides with the analytical result (see solid curve in Fig. 1), the finite-difference result comes out to be strongly asymmetric. A closer inspection (not reported here) reveals that such anomalous behavior is mainly ascribed to the usual non-symmetric discretization (left or right derivative) of the kinetic/diffusion term in Eq. (2), which may result in a fictitious decoherence/damping dynamics [19]. This seems to indicate that the more regular—and physically-sound—results obtained so far via finite-difference calculations may be ascribed to such non-symmetric discretization procedure, which in turn tends to limit the highly non-physical features of the Wigner-function formalism applied to systems with open boundaries.

The analysis presented so far allows us to draw a few important conclusions. First of all, the results of the analytically solvable device model previously considered clearly show that the usual boundary-condition scheme—successfully applied to semiclassical device modelling—is intrinsically incompatible with the non-local nature of quantum mechanics. More specifically, from a strictly mathematical point of view it is true that the Wigner equation (2) is a first-order equation in $z$ parameterized by the wavevector $k$ and, as such, it is sufficient to specify the value of the Wigner function at the device boundaries; on the other hand, from a physical point of view the separation between active region and external reservoirs/contacts is only apparent, since the action of the potential superoperator $V$ [see Eq. (2)] is local in space, but its value inside the device depends on the properties of the potential $v(z)$ both inside and outside the device active region [see Eq. (3)]. We are forced to conclude that the application of the standard boundary-condition scheme to the Wigner equation in (2) is not physically justified, since it may provide solutions which are not Wigner functions, i.e., which do not correspond to the state of a quantum system. A clear and unambiguous proof of such non-physical outcomes are the negative values of the electron probability distribution reported in Figs. 1 and 2. Generally speaking, what is intrinsically wrong in the usual Wigner-function treatment of open devices is the spatial separation between active region and reservoirs. This is similar to isolate a portion of a given energy spectrum, and try to treat such subset of energy levels as an independent subsystem. In contrast, in order to provide a rigorous description of open quantum devices it is imperative to introduce a clear separation between the degrees of freedom of the subsystem of interest (i.e., electrons primarily localized within the device active region) and those of the external reservoirs (i.e., carriers primarily localized within the electrical contacts). Given such separation, it is possible to obtain an effective transport equation for the subsystem of interest via a suitable statistical average over the coordinates of the “environment”. Following such reduction procedure, one gets again the Wigner equation (11), where now the Liouville superoperator is the sum of a contribution describing the subsystem/device of interest plus an effective superoperator describing the interaction of the device with external reservoirs: $\mathcal{L} = \mathcal{L}^{\text{dev}} + \mathcal{L}^{\text{dev-res}}$. 

\begin{figure}[h]
\centering
\includegraphics[width=\columnwidth]{fig1}
\caption{Quantum-transport through a GaAs-based device active region ($l = 40$ nm) with a cosine-like potential profile ($V_0 = 150$ meV) sandwiched between its electrical contacts: comparison between the analytical charge distribution (solid curve) and the corresponding phenomenological result (dashed curve) for the case of a monoenergetic carrier injection from left ($E_0 = 70$ meV).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\columnwidth]{fig2}
\caption{Finite-difference result (dashed curve) and a corresponding iterative numerical solution of Eq. (4) (see text).}
\end{figure}
We stress that within the proposed alternative approach there is no need to impose any spatial boundary condition: as for the case of a closed system the spatial domain is again \(-\infty < z < +\infty\). The only boundary condition is the Wigner function \(f(z, k)\) at the initial time \(t\); it follows that—contrary to the case of spatial boundary conditions—the homogeneous Liouville dynamics in (1) provides/maintains a “good” Wigner function at any later time \(t\), thus preventing from non-physical behaviors, like those reported in Fig. I.

We finally stress that the alternative simulation scheme described so far may be concretely realized following the prescription recently proposed in [20]: the basic idea is to replace the usual open description of quantum devices based on spatial boundaries (i.e., source/loss terms) with a closed-system treatment, where the interaction of the device electrons with the external reservoirs is simply described in terms of effective scattering rates acting on the device electrons only.

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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] It is worth mentioning that an equivalent and alternative approach to the density-matrix formalism is provided by the nonequilibrium Green’s function technique [1]. Following this approach, Lake, Datta, and co-workers have proposed an efficient quantum-transport simulation scheme for the study of open semiconductor devices [7].

[5] See, e.g., H. Haug and S.W. Koch, *Quantum Theory of the Optical and Electronic Properties of Semiconductors*, 3rd Edn., World Scientific, Singapore (1994).

[6] See, e.g., H. Haug and A.-P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, Berlin, 1996).

[7] See, e.g., R. Lake and S. Datta, Phys. Rev. B 45, 6670 (1992).

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

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

[10] F. Rossi et al., Phys. Rev. Lett. 80, 3348 (1998).

[11] W.R. Frensley, Phys. Rev. Lett. 57, 2853 (1986).

[12] See, e.g., N. C. Klusdahl et al., Phys. Rev. B 39, 7720 (1989);

[13] R. Proietti Zaccaria and F. Rossi, Phys. Rev. B 67, 113311 (2003).

[14] See, e.g., M. Pascoli et al., Phys. Rev. B 58, 3503 (1998).

[15] This approach is intrinsically able to overcome the standard approximations of the semiclassical scattering theory; however, due to the huge amount of computation required, its applicability is often limited to short time-scales and extremely simplified situations.

[16] The above formal solution can be also regarded as a sort of Schwinger-Dyson equation linking the desired Wigner function \(f\) to the free-particle one \((f_b(z, k) = f_b(k))\) through the potential superoperator \(V\).

[17] More specifically, by applying the interaction superoperator \(W\) to any symmetric function \((a(z, k) = a(-z, k))\), we get as a result again a symmetric function of \(z\), i.e.,

\[
\begin{align*}
   b(z, k) &= -\int_{z(k)}^z dz' \int dk' V(z', k' - k') a(z', k') \\
   &= b(-z, k). 
\end{align*}
\]

(10)

[18] Indeed, it is well known that a “good” Wigner function, i.e., obtained as the Weyl-Wigner transform of a density matrix, will never give rise to negative charge distributions.

[19] We stress that this problem does not affect the iterative solution of Eq. (4), since in this case the kinetic part of the dynamics is treated exactly.

[20] R. Proietti Zaccaria et al., Appl. Phys. Lett. 84, 139 (2004); R. Proietti Zaccaria et al., Phys. Rev. B 70, 195311 (2004).