Unphysical features in the application of the Boltzmann collision operator in the time-dependent modeling of quantum transport

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Abstract In this work, the use of the Boltzmann collision operator for dissipative quantum transport is analyzed. Its mathematical role on the description of the time-evolution of the density matrix during a collision can be understood as processes of adding and subtracting states. We show that unphysical results can be present in quantum simulations when the old states (that built the density matrix associated to an open system before the collision) are different from the additional states generated by the Boltzmann collision operator. As a consequence of the Fermi Golden rule, the new generated states are usually eigenstates of the momentum or kinetic energy. Then, negative values of the charge density may appear after the collision. This fact is originated by the different time-evolutions of the old and new states. This unphysical feature disappears when the Boltzmann collision operator generates states that were already present in the density matrix of the quantum system before the collision. Following these ideas, in this paper, we introduce an algorithm that models phonon–electron interactions through the Boltzmann collision operator without negative values of the charge density. The model only requires the exact knowledge, at all times, of the states that build the density matrix of the open system.

Keywords Quantum transport · Wigner function · Scattering · Negative probability · Wave packet
The consideration of the collision term in the modeling of quantum transport is of paramount importance because it converts a unitary and reversible equation of motion for the density matrix into a non-unitary and irreversible one, accounting for the phenomena of dissipation and decoherence. The proper treatment of such phenomena is mandatory for a realistic simulation of electron devices [10–13]. There are many proposals for the collision operator in the literature [14–20]. Some of such terms provide a quite accurate description of the phenomena at the price of a high requirement of computational resources. Because of that, such models are only applicable to very simple (idealized) systems. Other simpler versions of the collision term have a much wider practical applicability, but in some scenarios they can lead to unphysical results, in terms of negative values of the probability presence of electrons at some locations.

In this work, we discuss the possibilities that the Boltzmann collision operator, applied to quantum transport, can produce unphysical results. We will discuss negative charge densities with examples using the density matrix and the Wigner distribution function.

After this introduction, in Sect. 2, we explain briefly the mathematical definitions of the density matrix and the Wigner distribution function, and some unphysical problems found in the literature related with different types of collision operators. Then, in Sect. 3, we point out a problem inherent to the use of the Boltzmann collision operator in quantum systems and how to overcome it. In Sect. 4 we show numerical results for a very simple system (an electron in a double barrier interacting with a phonon) where the Boltzmann collision operator leads to unphysical negative charge (probability presence) density. In Sect. 5 we show numerically how this unphysical result can be removed by a careful treatment of the electron wave function before and after the scattering event. We conclude in Sect. 6.

2 The density matrix and Wigner distribution function formalisms for dissipative transport

Hereafter, we explain briefly the equation of motion of the density matrix and the Wigner distribution function to treat dissipation in nanodevices. For the sake of simplicity, we will assume a mean field approximation that allows us to discuss quantum transport in terms of a set of non-interacting individual electrons. In particular, we will consider one-dimensional (1D) physical space $x$ or a 1D phase space $x - k$. There would be no fundamental difference in our conclusions, if a many-particle or three-dimensional (3D) physical space were considered.

### 2.1 The density matrix formalism

The natural approach to model electrons in open systems is the density operator, which can be written as a weighted sum of states:

$$\hat{\rho}(t) = \sum_j p_j(t) |\psi_j(t)\rangle\langle\psi_j(t)|$$

where $p_j(t)$ specifies the probability that the open system is described by the pure state $|\psi_j(t)\rangle$. The density operator expressed in the position representation is the following,

$$\rho(x, x', t) = \langle x | \hat{\rho}(t) | x' \rangle = \sum_j p_j(t) \psi_j(x, t) \psi_j^*(x', t).$$

For a Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}'$, where $\hat{H}_0$ is the unperturbed Hamiltonian and $\hat{H}'$ accounts for the collision of the electron with other particles [7,21], the equation of motion of the density operator $\hat{\rho}$ is the so-called Liouville Von-Neumann equation:

$$\frac{\partial \hat{\rho}}{\partial t} = \frac{i\hbar}{\hbar} [\hat{H}, \hat{\rho}] = \frac{i\hbar}{\hbar} [\hat{H}_0, \hat{\rho}] + \hat{C}[\hat{\rho}]$$

where the first part of the right hand side of Eq. (3) is the unperturbed evolution of the quantum system and the second part, the collision term $\hat{C}[\hat{\rho}]$, describes the effect of the interaction with the environment. For the effective mass approximation $m^*$, Eq. (3) in the position representation becomes

$$i\hbar \frac{\partial \rho(x, x', t)}{\partial t} = -\frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2} \right) \rho(x, x', t) + \left((V(x) - V(x'))\rho(x, x', t) + C[\rho(x, x', t)] \right)$$

where $V(x)$ is the potential energy term and $C$ is the matrix representation of the $\hat{C}$ operator.

An important quantity in the modeling of electrical devices can be obtained by the trace of the density matrix:

$$Q(x, t) = tr(\hat{\rho}(t)) = \sum_j p_j(t) |\psi_j(x, t)|^2.$$
The function $Q(x, t)$ is often referred in the literature as the charge (or probability presence) density of the system. By definition, either interpreted as a probability presence or as the system charge, negative values\(^4\) cannot be accepted in Eq. (5).

2.2 The Wigner distribution function formalism

The Wigner distribution function is defined as the following Wigner–Weyl transform [22] of $\rho(x, x', t)$ in Eq. (2):

$$F_W(x, k, t) = \frac{1}{2\pi\hbar} \int \rho \left( x + \frac{x'}{2}, x - \frac{x'}{2}, t \right) e^{-ikx'} dx'.$$

(6)

The time evolution of the Wigner distribution function can be derived directly from Eq. (3). Therefore, the transport equation for the Wigner distribution function in Eq. (6) can be written as a sum of a term given by $\hat{L}_W [F_W(x, k, t)]$ plus a generic collision term $\hat{C}_W [F_W(x, k, t)]$ as

$$\frac{\partial F_W(x, k, t)}{\partial t} = \hat{L}_W [F_W(x, k, t)] + \hat{C}_W [F_W(x, k, t)].$$

(7)

The term $\hat{L}_W [F_W(x, k, t)]$ can be written as

$$\hat{L}_W [F_W(x, k, t)] = -\frac{\hbar k}{m^*} \frac{\partial F_W(x, k, t)}{\partial x}$$

$$- \frac{2}{\pi\hbar} \int_{-\infty}^{\infty} dk' \int_{0}^{\infty} dxx' e^{i(k-k')2x'}$$

$$\times \left[ V(x + x') - V(x - x') \right] F_W(x, k, t)$$

(8)

under the effective mass approximation. The collision term $\hat{C}_W [F_W(x, k, t)]$ has many different practical implementations (based on different approximation).

The charge density in Eq. (5) can also be obtained by integrating the Wigner distribution over all momenta:

$$Q(x, t) = \hbar \int F_W(x, k, t) dk.$$

(9)

2.3 Unphysical negative charge density found in the literature for quantum transport models

In the literature [23–28], there is a large list of different approaches that are used to define the collision operator, either in the density matrix formalism $\hat{C}[\hat{\rho}]$ or in the Wigner formalism $\hat{C}_W [F_W]$. As we said, the proper treatment of the interaction of electrons with the environment is mandatory for a realistic simulation of electron devices. However, since a direct simulation of all degrees of freedom is computationally inaccessible, the collision term cannot be treated exactly and some approximations are required. Such approximations do not only imply deviations from the exact result but, in some circumstances, they imply that the simulated results are unphysical (for example, the negative values of the charge density discussed in this paper).

In Table 1 we list some recent works of the literature explaining the negative values of the charge density, obtained from quantum transport formalisms dealing with the density matrix or the Wigner distribution function, with different implementations of the collision terms. Thus, there are many different reasons that explain why we can obtain negative charge densities. One can realize the important conceptual and practical difficulties of the proper modeling of the collision term with the recent work of Rossi and co-workers [29]. There, the authors show that a quite detailed treatment (including only a mean-field approximation) of electron-phonon scattering in the density matrix formalism leads to negative values of the charge. Surprisingly, such unphysical results disappear when a simpler treatment (including mean-field and Markovian approximations) is considered [29]. Similarly, a detailed treatment of scattering within the Barker-Ferry equation (or the Levinson equation) with a generalized Wigner distribution function formalism shows the relevance of the simulation times in the description of

\begin{table}[h]
\centering
\caption{Some unphysical behaviors found in the literature when modeling dissipative transport with the density matrix or Wigner distribution function formalisms using different implementations of the collision operator.}
\begin{tabular}{|c|c|c|}
\hline
Collision term & Unphysical problem & Reference \\
\hline
Non-Markovian treatment of collision & Without adding the Markovian approximation negative charge appears & [29] \\
Barker-Ferry equation and Levinson equation & The simulation time has to be small enough to avoid negative probability in the momentum space & [30] \\
Boltzmann collision operator, plus Fermi Golden rule & It can give negative charge in some scenarios due to the fact that the “rates derived based on the Fermi Golden rule rely on a well-defined kinetic energy pre- and post-scattering states” & [10] \\
Relaxation time approximation & The final (thermodynamical) equilibrium state used in the approximation can be unknown or unphysical & [12] \\
Any type of collision operator & A phenomenological injection model (without inclusion of a collision term) can provide negative charge & [13] \\
\hline
\end{tabular}
\end{table}
the collision interaction. For such approaches, unphysical results appear if the simulation time is not short enough (such limitation being related to the first order perturbation done in the development of the electron-phonon coupling) [30]. The implementation of the spatial boundaries conditions on the equation of motion of the density matrix at the borders of the simulation box can also be the origin of some unphysical results [13]. In this sense, it is very enlightening the discussion about mathematical and physical solutions of Eq. (7) done by Rossi and co-workers in [31]. We assume that \( f_a(x, k) \) is a physical (and mathematical) solution of Eq. (7), and that \( f_p(x, k) \) is another physical (and mathematical) solution. Then, because of the superposition principle, \( f(x, k) = c_a f_a(x, k) + c_p f_p(x, k) \) is by sure a mathematical solution of Eq. (7). However, we can select the coefficients \( c_a \) and \( c_p \) in such a way (for example, a negative value of \( c_p \)) so that \( f(x, k) \) may give rise to a negative charge distribution at some location, which means that \( f(x, k) \) will be an unphysical solution of Eq. (7), although it is a perfect mathematical solution.

In this work, we analyze, indeed, a much simpler and widely used treatment of the collision term. We discuss why in some circumstances the use of the Boltzmann collision operator can produce unphysical results. It is important to notice here that the Boltzmann collision operator is usually implemented through the use of the Fermi Golden rule that determines the scattering rates [3, 25, 32]. In our work, we do not discuss the range of validity of the approximation of the Fermi Golden rule, but only some inherent difficulties that can be found in the practical implementation of the Boltzmann collision operator in quantum simulators. To the best of our knowledge, although the idea was briefly mentioned in Ref. [10], the origin of the unphysical results presented in this paper has not been discussed in the literature explicitly.

3 The problem and the solution

The Boltzmann collision operator was initially proposed for classical systems [33]. For such systems, it has a very easy and understandable interpretation. The Boltzmann collision operator is just a rule for counting the number of electrons in and out of a volume of the phase space \( \Delta V \) due to a collision. The total number of electrons at time \( t + \Delta t \) in \( \Delta V \) is equal to the previous number of electrons that were there at \( t \), before the collision, plus the number of electrons that arrive at \( \Delta V \) from outside due to collision, minus the number of electrons that leave \( \Delta V \) during the collision.

Let us imagine a classical electron at \( x_0 \) with a velocity \( v_0 \) that interacts with another particle (for example, a phonon). Because of the interaction, the electron losses kinetic energy and its final velocity is \( v_f \). For simplicity, we assume that the initial position remains unchanged. Such collision process can be easily modeled in terms of the previous Boltzmann collision operator. The initial classical distribution function in phase space before the collision (apart from constant factors), at time \( t_0 \), is

\[
F_c(x, k, t_0) = \delta(x - x_0)\delta(k - k_0)
\]

being \( k_0 \) the wave vector associated to \( v_0 \). The Boltzmann collision operator generates the effect of the collision by subtracting an electron with momentum \( k_0 \) and adding a new electron with momentum \( k_f \). The final classical distribution function in phase space after the collision, at time \( t = t_0 + \Delta t \), is

\[
F_c(x, k, t_0 + \Delta t) = \delta(x - x_0)\delta(k - k_0) - \delta(x - x_0)\delta(k - k_f) + \delta(x - x_0)\delta(k - k_f) = \delta(x - x_0)\delta(k - k_f).
\]

The final results is obviously \( F_c(x, k, t_0 + \Delta t) = \delta(x - x_0)\delta(k - k_f) \). Up to here, the discussion seems very trivial. However, let us emphasize that it has been relevant that the negative part of the distribution function generated by the Boltzmann collision operator \( -\delta(x - x_0)\delta(k - k_0) \) is exactly compensated by the original positive one \( \delta(x - x_0)\delta(k - k_0) \). In this sense, the use of the Boltzmann collision operator in classical systems will always be unproblematic.

However, the application of the quantum version of the Boltzmann collision operator can be problematic because we have to add/subtract quantum states or wave functions, not point particles. As we will see next, the problem appears when we do not know the states that built the density matrix of the open system.

We consider an electron device as an open system with \( M \) electrons which are distributed in \( N \) different states. Say, there are \( M_1 \) electrons described by state \( |\psi_1\rangle \) where we define \( p_1 = M_1/M \). There are \( M_2 \) electrons with probability \( p_2 = M_2/M \) described by the state \( |\psi_2\rangle \) and so on. We construct a mixed state through the density matrix that describes our open system according to Eq. (1):

\[
\hat{\rho}_B(t_0) = \sum_{i=1}^{N} p_i(t_0) |\psi_i(t_0)\rangle \langle \psi_i(t_0)|
\]

with the conditions \( \sum_{i=1}^{N} p_i(t_0) = 1 \) and \( \sum_{i=1}^{N} M_i = M \). Because of the interaction of one electron with a phonon, the Boltzmann collision operator will add a new final state of
the electron $|\psi_F\rangle$ and will subtract another state associated to the electron $|\psi_O\rangle$. Then, the new density matrix after the scattering, at time $t_S = t_0 + \Delta t$, will be

$$
\dot{\rho}(t_S) = \dot{\rho}_B(t_0) - \frac{1}{M} |\psi_O\rangle\langle\psi_O| + \frac{1}{M} |\psi_F\rangle\langle\psi_F| \tag{13}
$$

In next Sect. 4.2, we will show explicitly with the Wigner formalism how the effect of collisions modeled by the Boltzmann collision operator can effectively be written as Eq. (13). The problem with the expression (13), due to Boltzmann collision operator, is that if we subtract a state $|\psi_O\rangle = |\psi_2\rangle$ that is not present in the density matrix before the collision, $\dot{\rho}_B(t_0)$, then we cannot simplify the density matrix to remove the negative sign that appears in the second term of the right hand side of Eq. (13). Then, by a simple computation, the new expression of the charge density with Eq. (5) using the density operator in Eq. (13) is

$$
Q(x, t) = \sum_{i=1}^{N} p_i |\psi_i(x, t)|^2 - \frac{1}{M} |\psi'_2(x, t)|^2 + \frac{1}{M} |\psi_F(x, t)|^2 \tag{14}
$$

This charge density is a sum of positive and negative terms. The dramatic problem with Eq. (14) is that, when the time-evolution of the negative term $\psi'_2(x, t)$ is not perfectly balanced by the positive term $\psi_2(x, t)$ (or by other states that build $\dot{\rho}_B$) at every time and position, the possibility of getting negative values $Q(x, t)$ is opened. The solution of the unphysical result originated by a negative charge density is, in principle, quite simple. If we subtract a state $|\psi_O\rangle$ which is present in the density matrix $\dot{\rho}_B(t_0)$, for example, $|\psi_O\rangle = |\psi_2\rangle$, then, we can write the density matrix in Eq. (13) at any time $t$ after the scattering time $t_S$ as

$$
\dot{\rho}(t) = \sum_{i=1}^{N} p_i |\psi_i(t)|^2
+ \frac{M_2 - 1}{M} |\psi_2(t)|^2 + \frac{1}{M} |\psi_F(t)|^2 \tag{15}
$$

The relevant point now is that, by construction, the term $(M_2 - 1)/M$ will be positive at any time $t$. Obviously, in the selection of the scattering process we have to ensure that $M_2 \geq 1$, because if not, we would be subtracting a non-existent state. If the condition $|\psi_O\rangle = |\psi_2\rangle$ is satisfied during the collision, then, independently of the time-evolution of all the states, the charge density computed from Eq. (5) using the density operator in Eq. (15) is just a sum of positive terms:

$$
Q(x, t) = \sum_{i=1; i \neq 2}^{N} p_i |\psi_i(x, t)|^2 + \frac{M_2 - 1}{M} |\psi_2(x, t)|^2 + \frac{1}{M} |\psi_F(x, t)|^2 \tag{16}
$$

Let us mention, however, that this procedure requires a knowledge of the pure states that build the density matrix (or the Wigner distribution function) of our open system. This information is usually not available in most quantum transport simulations. An exception being the BITLLES simulator, where each electron inside the device has its own (conditional) wave function [34].

### 4 Numerical example of the problem

In this section, we will show with numerical results the potential drawbacks of the combination of the Wigner distribution function and the Boltzmann collision operator discussed in the previous section. In some scenarios, such combination can lead to negative values of the charge density. Later, in Sect. 5, we will develop a novel scattering model (taking care of adding and subtracting states present in the density matrix of the open system) where the previous unphysical feature disappears by construction.

#### 4.1 Boltzmann collision operator for Hamiltonian eigenstates

The Boltzmann collision operator in the Wigner formalism is given in the literature [3] by

$$
\dot{C}_W[F_W(x, k, t)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left\{ W_{kk'} F_W(x, k', t) - W_{k'k} F_W(x, k, t) \right\} dk'
$$

(17)

where $W_{kk'}$ is the rate of scattering from the (unperturbed Hamiltonian) eigenstate with eigenvector $k'$ to the (unperturbed Hamiltonian) eigenstate with eigenvector $k$. The transition probabilities $W_{kk'}$ are obtained from the Fermi Golden rule according to [35]:

$$
W_{kk'} = \frac{2\pi}{\hbar} |M_{kk'}|^2 \delta(E_k - E_{k'} + \hbar \omega)
$$

(18)

where $M_{kk'}$ are the matrix elements for the transitions from state $k'$ to $k$, and $\omega$ is the frequency of the phonon for inelastic scattering. The bold symbols represent vectors in the 3D space. For technical reasons, since only one dimension is considered in our work, the 3D scattering rates must be “projected” onto the one-dimensional model to find $W_{kk}$ defined in Eq. (17):

$$
W_{kk'} = \frac{\lambda^2}{(2\pi)^2} \int_{-\infty}^{\infty} d^2k' \int_{-\infty}^{\infty} d^2k', W_{kk'} \exp \left( -\frac{\lambda^2 k^2}{2} \right)
$$

(19)
where \( k \) and \( k' \) are now the 1D initial and final states respectively.\(^6\) A very relevant point in our discussion is that the Fermi Golden rule Eq. (18) forces us to use Hamiltonian eigenstates (of the Hilbert space without the interacting potential) to compute the matrix elements \( M_{kk'} \).

In following Sect. 4.2, we will show a simple example of the application of Eq. (7) for a simple initial state and scattering rates \( W_{kk'} \), that, surprisingly, gives unphysical results in the form of negative charge density evaluated according to Eq. (9).

### 4.2 Electron in a double barrier with a collision event

We note here that we are not interested in the simulation of realistic nanodevices, but only in showing with a very simple example an unexpected result when combining the Boltzmann collision operator and the Fermi Golden rule. The violation of the requirement \( Q(x, t) \geq 0 \) in only one simple system is enough to warn that such implementation of the collision operator can lead to unphysical results in more complex or realistic simulations.

As seen in the inset of Fig. 1, we consider an electron that suffers a collision with a phonon while traveling through a typical double barrier potential. We consider a 1D Hilbert space with the following uniform grid 

\[
x_j = j \Delta x, \quad j = 1, 2, \ldots, M
\]

with \( \Delta x = 0.2 \) nm the spatial step and \( M = 3000 \) the number of grid points. The simulation box is large enough (it extends from 0 till 600 nm) to avoid any spurious interaction of the wave packet with the spatial boundaries. In the simulation, the temporal step is \( \Delta t = 3 \) fs.

At the initial time \( t_0 \) we consider an arbitrary initial pure state \( \langle x | \psi_B \rangle \) whose support fits perfectly inside the simulation box. Since we are interested in describing such system with the Wigner distribution function, the density matrix of this initial pure state is given by \( \hat{\rho}_B = |\psi_B\rangle \langle \psi_B| \), and the Wigner distribution function just needs the Wigner-Weyl transform given by Eq. (6). The time-evolution of the Wigner distribution function can be computed directly by solving the Schrödinger equation (plus a Wigner-Weyl transform) or by solving the Eq. (7) without the collision operator. Then, at time \( t_S \), a scattering process takes place according to the Boltzmann collision operator.

\[\text{Hamiltonian eigenstates scattering approach:}\]

- 1st term: \( F_W(x, k, t) \)
- 2nd term: \( W_{kk'} F_W(x, k', t) \)
- 3rd term: \( W_{kk'} F_W(x, k', t) \)

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\[\text{Fig. 1} \quad \text{Schematic representation of the Hamiltonian eigenstates scattering process. a Simulation of a wave packet impinging on double barriers, the collision is performed at time } t_S \text{ before the wave packet touches the barriers. b A simple physical picture of the Hamiltonian eigenstates scattering process in the } x-k \text{ space discussed in Sect. 4. During the collision, one term (3rd term) is eliminated and a new term (2nd term) is added. The eliminated state does not coincide with any of the old (before the collision) states of the system.}\]

It is usually assumed in the literature that the scattering process is sufficiently instantaneous\(^7\) that we can assume that the evolution of the Wigner distribution function from the \( t_S \) till \( t_S + \Delta t \) is

\[
\frac{\partial F_W(x, k, t)}{\partial t} \bigg|_{t=t_S} \approx \frac{F_W(x, k, t_S + \Delta t) - F_W(x, k, t_S)}{\Delta t}
\]

\[
= \frac{1}{2\pi} \int \left\{ W_{kk'} F_W(x, k', t_S) - W_{k'k} F_W(x, k, t_S) \right\} dk'
\]

\[\text{Eq. (21)}\]

\[\hbar^2\]

\[
\lambda_T = \frac{\hbar^2}{KTm^*}
\]

\[\text{where } K \text{ is the Boltzmann constant and } T \text{ is the absolute temperature.}\]
A further elaboration of Eq. (21) requires the specification of the scattering rates \( W_{kk'} \) and \( W'_{kk} \). In this case, for simplicity, we will account just for one collision process of one electron with one phonon. In particular, we will consider that, because of the collision, the initial wave vector of the electron \( k_0 \) changes to a final value \( k_F \). By using the Fermi Golden rule in Eq. (19), such electron–phonon interaction can be associated to the terms:

\[
W_{kk'} = \alpha \delta(k' - k_0) \lim_{\sigma \to 0} e^{-\frac{(i-k_F)^2}{\sigma^2}} \tag{22a}
\]

\[
W'_{kk} = \alpha \delta(k' - k_F) \lim_{\sigma \to 0} e^{-\frac{(i-k_0)^2}{\sigma^2}} \tag{22b}
\]

where the parameter \( \alpha \) takes into account all (irrelevant for our simple example) details of the specific computation of the Fermi Golden rule. The parameter \( \sigma \rightarrow 0 \) means that rates \( W_{kk'} \) and \( W'_{kk} \) are localized closely to momentum \( k = k_F \) and \( k = k_0 \), respectively. For numerical reasons, we avoid writing explicitly delta functions in the right hand side of Eq. (22a) and Eq. (22b). In simple words, \( W_{kk'} \) is the transition rate associated to an electron initially in \( k = k_0 \) that appears finally at \( k = k_F \) (see 2nd term in Fig. 1), and \( W'_{kk} \) is associated to an electron initially in \( k = k_0 \) that finally disappears from \( k_0 \) (see 3rd term in Fig. 1). The summary of this scattering process described in Eq. (21) (or in the sum in Fig. 1) is just that an electron with initial momentum \( \hbar k_0 \) gets a final momentum to \( \hbar k_F \) because of the interaction with a phonon. This is the quantum version of the classical collision explained in Sect. 3.

Substituting the scattering rates written in Eq. (22a) and Eq. (22b) into Eq.(21) and rearranging it, we obtain

\[
\hat{F}_W(x, k, t_S + \Delta t) = \hat{F}_W(x, k, t_S) + \frac{\alpha \Delta t}{2\pi} \hat{F}_W(x, k_0, t_S) e^{\frac{(i-k_F)^2}{\sigma^2}}
\]

\[
- \frac{\alpha \Delta t}{2\pi} \hat{F}_W(x, k_0, t_S) e^{\frac{(i-k_0)^2}{\sigma^2}} \tag{23}
\]

Since there is a one-to-one correspondence between the Wigner distribution function and the density matrix [22,37], one can obtain the density matrix by the inverse Wigner–Weyl transform of the Wigner distribution function as

\[
\rho(x, x', t) = \int_{-\infty}^{\infty} \hat{F}_W \left( \frac{x + x'}{2}, k, t \right) e^{ik(x-x')} dk \tag{24}
\]

As a consequence, we can rewrite Eq. (23) as,

\[
\rho(x, x', t_S + \Delta t) = \rho_B(x, x', t_S)
\]

\[
+ \frac{\alpha \Delta t}{2\pi} \hat{F}_W \left( \frac{x + x'}{2}, k_0, t_S \right) e^{i k_F (x-x')}
\]

\[
- \frac{\alpha \Delta t}{2\pi} \hat{F}_W \left( \frac{x + x'}{2}, k_0, t_S \right) e^{i k_0 (x-x')} \tag{25}
\]

which can be rewritten in the form of positive and negative summands discussed in Eq. (13) as

\[
\hat{\rho}(t) = \hat{\rho}_B(t) + \hat{\rho}_P(t) - \hat{\rho}_N(t)
\]

\[
= |\psi_B\rangle\langle\psi_B| + |\psi_P\rangle\langle\psi_P| - |\psi_N\rangle\langle\psi_N| \tag{26}
\]

where the first term in the right-hand side, \( \hat{\rho}_B \), describes the density matrix before the collision, the second and third terms are the terms generated (by the Boltzmann Collision operator) due to the collisions. It is important to underline that we are selecting \( \alpha \) small enough to ensure that the charge density of the density matrix \( \rho(x, x', t_S + \Delta t) \) in Eq. (25) is strictly non-negative everywhere just after the scattering. As commented previously, it would be a nonsense to subtract more probability presence than what we have in one specific location at \( t_S \). Even with this important requirement, the problem may appear later when the time evolution of \( \rho_P(x, x', t_S) \) and \( -\frac{\alpha D}{2\pi} \hat{F}_W \left( \frac{x + x'}{2}, k_0, t_S \right) e^{i k_0 (x-x')} \) in Eq. (25) (or \(-|\psi_N\rangle\langle\psi_N|\) in Eq. (26)) becomes different.

We compute the charge probability distribution from Eq.(9) at four different times corresponding to the initial time \( t_0 = 0 \) ps, just after the scattering time \( t_S = 0.006 \) ps, at \( t_2 = 0.315 \) ps when the wave packets \( \psi_B \) and \( \psi_N \) are interacting with the barriers, and at time \( t_3 = 0.66 \) ps when the interaction is nearly finished and the initial wave packets \( \psi_B \) and \( \psi_N \) are clearly split into transmitted and reflected components. The information corresponding to these four times is plotted in Fig. 2.

In order to enlarge the typical interference effects, at the initial time \( t_0 = 0 \) we consider the following initial state \( \langle x | \psi_B \rangle = C \langle x | \psi_1 + \psi_2 + \psi_3 \rangle \) with \( C \) a normalization constant. Each wave function \( \psi_j(x, t_0) \) at the initial time \( t_0 \) is a Gaussian wave packet \( \psi_j(x, t_0) = \left( \frac{2}{\pi a_0^2} \right)^{1/4} e^{ik_0(x-x_0)} \exp \left( \frac{-(x-x_0)^2}{a_0^2} \right) \) but with different initial central positions \( x_0 \). In particular, the left wave packet \( \psi_1 \) has \( x_0_1 = 250 \) nm, the middle wave packet \( \psi_2 \) has \( x_0_2 = 280 \) nm and the right wave packet is \( \psi_3 \) has \( x_0_3 = 310 \) nm. The initial spatial variance of the three wave packets is \( a_0 = 15 \) nm, its central wave vector \( k_0 = 0.69 \) nm\(^{-1} \) and the effective mass \( m^* = 0.2 \) m with \( m \) being the free electron mass. The center of the barriers is at \( x = 350 \) nm. Both barriers have a 0.8 nm width, the energy height is 0.2 eV, and they are separated by 4 nm.

After the scattering process, the evolution of the whole density matrix in Eq. (26) implies the new term \( \psi_P \) with new momentum \( \hbar k_F \) (associated to the density matrix is \( \hat{\rho}_P \) in Eq. (26)) and the new terms \( \psi_N \) with the old momentum \( \hbar k_0 \) (associated to the density matrix \( \hat{\rho}_N \) in Eq. (26)). The two additional wave packets \( \psi_N \) and \( \psi_B \) are Gaussian wave packets with the same very large dispersion \( a_{0s} = 2a_0 \left( \sqrt{1 + \frac{4\hbar^2 k_F^2}{m^* a_0^4}} \right) \) (to mimic a plane wave) and the same
Fig. 2 Evolution of Gaussian wave packets coupled with the Hamiltonian eigenstates scattering approach moving towards barriers. a, c, e, g are the Wigner distribution function and b, d, f, h are the corresponding probability (charge) density at four different times: initial time \( t_1 = 0 \) ps, scattering time \( t_S = 0.006 \) ps before touching the barriers, time \( t_2 = 0.315 \) ps when wave packets are interacting with the barriers and time \( t_3 = 0.66 \) ps when the interaction is completely done. The simulation parameters are \( E = 0.09 \) eV, \( m^* = 0.2 \) \( m_0 \), where \( m_0 \) is the free electron mass, the barrier height is 0.2 eV, the barrier width is 0.8 nm and the well depth is 4 nm. The collision is implemented with the Hamiltonian eigenstates scattering model discussed in Sect. 4. Because of such model, negative charge density appears (Color online).

The central position \( x_0S = x_0 + \frac{\hbar k_0}{m^*} t_S \). The wave vectors for \( \psi_N \) and \( \psi_P \) are \( k_0 \) and \( -k_0 \) (here we assume \( k_F = k_0 \)), respectively.

The results of the charge (or probability presence) densities in the right hand side of the Fig. 2 are just Eq. (9), that is the integral of the Wigner distribution function in the left-hand side of the figure over all momenta (for a fixed position). The negative values of the Wigner distribution function in the figures is not at all problematic as far as the marginal integral in Eq. (9) satisfies \( Q(x, t) \geq 0 \) [38]. Before and just after
the collision, there is not unphysical evolution of the charge. Just after the collision, the new state $|\psi_P\rangle$ gives only positive charge density and the negative contribution of the new state $|\psi_N\rangle$ is, obviously, smaller than the positive one provides by $|\psi_B\rangle$ at each location. Figs. 2(e) and (f) show the same information at the new time $t_2 = 0.315$ ps when the wave packets $\langle x|\psi_B\rangle$ and $\langle x|\psi_N\rangle$ have evolved with time and interacting with the barriers. At position $x = 300$ nm, negative charge (presence probability) appears. This result is unphysical in the same sense that a wave function with a negative modulus will be unphysical, i.e. inconsistent with the probabilistic (Born law) interpretation of quantum mechanics. After the interaction is completed, at time $t_2 = 0.66$ ps, the spurious phenomenon becomes even worse. In this particular simple example, there are more positions (for example, $x = 492$ nm) with negative value probabilities.

We have also performed simulations (not shown in the present paper) where the scattering process is strictly performed according to Eq. (25) using $-\frac{a\Delta t}{2\pi} F_W \left( \frac{x+x'}{2}, k_0, t_S \right) e^{ik_0(x-x')}$ instead of $|\psi_N\rangle\langle \psi_N|$. The results are quite similar to the ones show in Fig. 2, but because of the own positive/negative oscillation of the $F_W \left( \frac{x+x'}{2}, k_0, t \right)$, the charge probability results are even worse than the ones plotted here. The amplitude where the negative probability occurs is larger and such negative values appear in more positions, which is affected by the factor $\frac{a\Delta t}{2\pi} F_W(x, k_0, t_S)$ describing the scattering strength. It is important to point out that the unphysical spurious behaviors become even worse with longer time evolutions (related to the device active region). In conclusion, the presence of negative charge is not because of the exact shape of the $\rho_N$ and $\rho_P$, either pure states or mixed states, but because the time-evolution of the states $\rho_N$ is different from $\rho_B$ because, at some times $t$, their positive and negative contribution cannot be compensated (even if they were compensated at $t_0$).

5 Numerical example of the solution

As indicated in Sect. 3, the solution to avoid these unphysical results of Fig. 2, while still using the Boltzmann collision operator, is having an exact knowledge of the states involved in the description of the density matrix. By construction, this way of working will not provide any negative charge density.

5.1 Boltzmann collision operator for general states

Let us assume that we have a perfect knowledge of all states, $|\psi_i\rangle$ with $i = 1, \ldots, N$, that are needed to build our density matrix of the open system in Eq. (12). We define first $F_W(x, k, t)$ as the Wigner-Weyl transform with respect to the element of the density matrices $p_i |\psi_i\rangle\langle \psi_i|$ in Eq. (12). Then, because of the linearity of the Wigner distribution function with respect to the density matrix, before the collision, we can write the whole Wigner distribution function as follows:

$$ F_W(x, k, t) = \sum_{i=1}^{N} F_W^i(x, k, t) $$

Inspired in the classical application of the Boltzmann collision operator, we define a collision operator in Eq. (17) that provides transitions between different states as

$$ \hat{C}_W \left[ F_W(x, k, t) \right] = \frac{1}{2\pi} \sum_{i=1}^{N^*} \sum_{j=1}^{N^*} \left( Z_{ij} F_W^i(x, k, t) - Z_{ji} F_W^j(x, k, t) \right) $$

where the terms $Z_{ij}$ provides the scattering rate (for the general states used in each case) from the $j$—state $|\psi_j\rangle$ to the $i$—
Fig. 4 Evolution of Gaussian wave packets coupled with general states scattering approach moving toward barriers. \(a, c, e, g\) are Wigner distributions and \(b, d, f, h\) are the corresponding probability density values of states at different times, which are identical to the times in Fig. 2: \(t_1 = 0\) ps, \(t_5 = 0.006\) ps, \(t_2 = 0.315\) ps, and \(t_3 = 0.66\) ps. The simulation parameters are \(E = 0.09\) eV; \(m^* = 0.2 m_0\), where \(m_0\) is the free electron mass; the barrier height is 0.2 eV; the barrier width is 0.8 nm; and the well depth is 4 nm. The collision is implemented with the general states scattering model discussed in Sect. 5. Because of such model, charge density is always non-negative (Color online)
state $|\psi_i\rangle$. The sums in Eq. (28) are carried out over the $N^a$ possible existent terms (which are in principle infinite, but we can limit to a reasonable number of possible states in a practical application). We do not use $W_{kk'}$ in Eq. (28) because, in principle, they are computed only for Hamiltonian eigenstates, while we define $Z_{ij}$ using our general states $|\psi_j\rangle$.

5.2 Electron in a double barrier with a collision event

We discuss here the same numerical example presented in Sect. 4, but here with our new collision operator in Eq. (28). We use the same initial density matrix $\rho_B(t_0) = |\psi_B\rangle\langle\psi_B|$ in Eq. (12). We consider that there are two electrons with such state, $M_1 = M = 2$. Then, when the scattering takes place, one of the two electrons with initial state $|\psi_B\rangle$ changes its state, while the other remains unaffected. The new density matrix in Eq. (13) is $\hat{\rho}(t_S) = \hat{\rho}_B - (1/2)|\psi_B\rangle\langle\psi_B| + (1/2)|\psi_F\rangle\langle\psi_F|$. The new density matrix after scattering can be greatly simplified to $\hat{\rho}(t_S) = (1/2)|\psi_B\rangle\langle\psi_B| + (1/2)|\psi_F\rangle\langle\psi_F|$ because $|\psi_N\rangle \equiv \sqrt{1/2}(|\psi_B\rangle + |\psi_F\rangle)$. This collision process is explained in Fig. 3.

Before the collision, both electrons are described by identical states that share the same $-k$ support because the two electrons have the same (mean) momentum. After the collision, one electron has higher (mean) momentum than that of the other. Thus, electrons are described by different states with different $-k$ supports.

In our numerical example, we use the same initial wave packet $|\psi_B\rangle$ discussed in Fig. 2. At the initial time $t_1 = 0$ ps, the information of the Wigner function and the charge probability distribution obtained in Fig. 4 are different to that in Fig. 2. Then, at time $t_S = 0.006$ ps, the new collision operator in Eq. (28) acts on the Wigner distribution function. After the scattering, the system state is $\hat{\rho} = |\psi_B\rangle\langle\psi_B| + |\psi_F\rangle\langle\psi_F| - |\psi_N\rangle\langle\psi_N| = \frac{1}{2}|\psi_B\rangle\langle\psi_B| + \frac{1}{2}|\psi_F\rangle\langle\psi_F|$. As a consequence, the negative values disappear. Therefore, the unphysical results are removed. These conclusions are perfectly corroborated by Fig. 4.

We remark also that this new algorithm for collision explained here is relevant for time-dependent modeling of quantum transport. In addition, since it requires a perfect knowledge of the states that build the density matrix, its practical implementation fits perfectly well with the BITLLES simulator developed with conditional wave functions [2,39–41]. Then, the mentioned algorithm for dissipative quantum transport can be straightforwardly implemented for quantum transport by directly including the interaction between electrons and phonons in the kinetic part of the Hamiltonian that describes the wave function of each electron. For a preliminary description of this method, see Refs. [42,43].

### 6 Conclusions

In this work, we have discussed the combination of the Boltzmann collision operator and the Fermi Golden rule to simulate dissipative processes in quantum electron devices. In general, the Fermi golden rule provides the transition rates $W_{kk'}$ and $W_{kk''}$ for (unperturbed) Hamiltonian eigenstates. We have shown that this combination can provide negative unphysical values for the charge (probability) in some simple scenarios, as we proved in Sect. 4 (Fig. 2).

We have also discussed the ultimate reasons of such unphysical results: the different time-evolutions of the states that build the density matrix in the Wigner distribution function and the Hamiltonian eigenstates generated by the Boltzmann collision operator after a collision. This problem will never occur if the transition between states during the collision process is done according to the set of states that built the density matrix. In Table 2, the numerical results show negative values of the charge density when the Boltzmann collision operator is applied with Hamiltonian eigenstates.

In principle, the unphysical results can be avoided by means of more elaborated forms of the collision operator [10]. However, then, the intuitiveness and the computational simplicity offered by the Boltzmann collision operator would be missed. We mentioned in Sect. 5 that by construction, an approach based on the generalization of the Boltzmann collision operator as written in Eq. (28) will always avoid such unphysical feature. An algorithm based on these ideas will still retain the intuitiveness and the computational simplicity of the Boltzmann collision operator. However, it will require the knowledge of the states that conform the density matrix or Wigner distribution function. This detailed knowledge of the states that build the density matrix is trivially accessible in a formulation of quantum transport in terms of conditional wave functions. See, for instance, the BITLLES simulator [34]. Then, the collision process can be applied directly into the Hamiltonian of the equation of motion that determines the evolution of the conditional wave function (just by adding

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8 As a reasonable approximation, if the general wave packet has (a more or less) well defined momentum (for example, the mean momentum of the wave packet) the terms $W_{kk'}$ can be numerically used instead of $Z_{ij}$ in Eq. (28) by using some relations between $i$ and $j$ and $k$ and $k'$. 

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Table 2 Norm of the system state (positive, negative, and total probability density) at $t_3 = 0.66$ ps when using the Hamiltonian eigenstates (H.E.) discussed in Sect. 4 or the general states (G.S.) scattering discussed in Sect. 5

| Type          | Positive Probability | Negative Probability | Total Probability |
|---------------|----------------------|-----------------------|------------------|
| H.E. scattering | 1.025                | -0.025                | 1                |
| G.S. scattering | 1                    | 0                     | 1                |
an additional term in the kinetic part of the Hamiltonian). For more details, see [42] and [43].

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