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Boundary conditions and the Wigner equation solution

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Abstract We consider the existence and uniqueness of the solution of the Wigner equation in the presence of boundary conditions. The equation, describing electron transport in nanostructures, is analyzed in terms of the Neumann series expansion of the corresponding integral form, obtained with the help of classical particle trajectories. It is shown that the mathematical aspects of the solution can not be separated from the physical attributes of the problem. In the presented analysis these two sides of the problem mutually interplay, which is of importance for understanding of the peculiarities of Wigner-quantum transport. The problem is first formulated as the long time limit of a general evolution process posed by initial and boundary conditions. Then the Wigner equation is reformulated as a second kind of a Fredholm integral equation which is of Volterra type with respect to the time variable. The analysis of the convergence of the corresponding Neumann series, sometimes called Liouville–Neumann series, relies on the assumption for reasonable local conditions obeyed by the kernel.

Keywords Wigner equation · Monte Carlo method · Boundary conditions · Convergence

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1 Introduction

The Wigner equation describing electron transport in nanoelectronic structures is subject of an active research interest since more than 25 years. The Wigner picture offers many advantages related to the physical transparency of the phase space formulation of quantum mechanics and the analogy with the classical distribution function. However, the associated numerical aspects are rather difficult, comprised of many computational problems, which are gradually solved during these years. An important issue, subject to intensive speculations, is the existence and uniqueness of the solution of the Wigner equation. The stationary transport problem determined by boundary conditions is usually focused on, since it formulates the technologically important regime of operation of electronic nanostructures, corresponding to the question: What is the output from the structure under the condition of a given input. Thus, in general, the stationary equation is considered and the analysis relies on certain integral representations of the equation [1–3], with sometimes painful conclusions about the failure of the conventional boundary condition scheme to provide reasonable physical results [4]. The problem is actually related to the fact that the equation allows for unphysical solutions [5]. Conditions may be formulated, which identify the physically admissible phase space functions. For pure states such a condition reflects the fact that the density matrix, used to obtain the Wigner function, is a product of two functions, which are possible Schrödinger equation solutions, while for a mixed state the density matrix corresponds to a positive semi-definite operator [6]. This condition can be used to filter out the unphysical solutions: it can be shown that, if the initial condition is an admissible physical state, the Wigner equation maintains this property during the evolution. This shows the importance of a proper choice of the initial condition: The latter

must reflect the uncertainty relations, which means that the constant $\hbar$ must be involved in the problem since the very beginning [5]. Thus, unphysical solutions can be traced back to the time boundary as corresponding to unphysical initial conditions. Similarly, Wigner function values on spatial boundaries are entangled via the conditions for admissibility with certain function values defined on the rest of the domain of the function. Actually only the inflowing contribution from the boundaries [7] must be taken into account. As shown in the sequel, this is indeed the fact, however, nothing guarantees a physical solution, provided that the contributions from the boundaries are arbitrary changed. Thus the knowledge of the proper boundary conditions is a physical issue, needed to formulate the proper computational problem. As a rule, equilibrium conditions are assumed at the boundaries just because the equilibrium Wigner function is well-known. However, then the definition domain of the equation must be extended to infinity to avoid correlations with the non-equilibrium central region of the structure, where the electron flow occurs. In this respect, moving the boundaries arbitrarily close, or imposing arbitrary inflow boundary conditions on them, may lead to non-unique and unphysical solutions [4], which is a problem of a correct physical formulation of the computational task. Indeed, it may be shown that, for a class of periodic potentials with an interval of periodicity $\Omega = [-l/2, l/2]$ the computational problem is well-posed under arbitrary inflow boundary conditions specified at $-l/2$ ($v > 0$) and $l/2$ ($v < 0$) [3].

Here we present an analysis, where the the transport task is first formulated from a physical point of view. The stationary solution is considered as the long time limit of the general evolution problem posed by both initial and boundary conditions. This implies the existence of a generic solution comprised of two complementary parts determined by these conditions. To have a solution determined by boundary conditions only, the initial condition part must vanish with time. If the contribution from the initial condition does not vanish with time and only boundary conditions are considered, the problem remains ill-posed from a physical point of view. It follows that the time-dependent component of the field-less Liouville operator can not be neglected a priori, so that a restriction to the stationary Wigner equation can be relevant only under the existence of physical arguments for that. In the next section we formulate the computational problem in terms of the characteristics of the Liouville operator. As these are Newton trajectories, the presented analysis is dimension independent, that is why for simplicity the one-dimensional problem is considered. Section 3 is devoted to the computational aspects of the task, where we prove the existence and uniqueness of the solution posed by both boundary and initial conditions. A discussion of certain physical aspects along with the conclusions are presented in Sect. 4.

2 Wigner transport on trajectories

We consider a charged particle evolving into a single-dimensional structure under the action of an applied electric potential V. The phase space evolution is described by the Wigner equation:

$$\frac{\partial f(x,k,t)}{\partial t} + v(k)\frac{\partial f(x,k,t)}{\partial x} = \int dk' V_w(x, k-k') f(x,k',t), \tag{1}$$

where x and k are the position and wave vector variables, f is the Wigner function, often called also quasi-distribution function, since being the quantum counterpart of the classical distribution function, $v(k) = \hbar k/m$ and m are the electron velocity and effective mass, and V_w is the Wigner potential:

$$V_w(x,k) = \frac{1}{i\hbar 2\pi}\int ds e^{-iks}(V(x+s/2) - V(x-s/2)), \tag{2}$$

with $V(x)$ the electric potential of the structure determining the kernel of the equation. The differential component of (1) is given by the Liouville operator, whose characteristics are the field-less Newton trajectories.

$$x(t') = x - v(k)(t-t'); \qquad k(t') = k. \tag{3}$$

The trajectory (3) is initialized by x, m, t. Newton trajectories can not cross in the phase space, so that (3) is uniquely determined by the initialization point. The time $t' < t$ gives rise to a backward parametrization, which links the initial point $x(0)$ of the trajectory to the end point $x(t) = x$. An important property of this picture is that the wave vector remains unchanged during the evolution. This means that, if $k \neq 0$, a trajectory always leaves (after certain time) any bounded domain. We note that in more complicated physical pictures accounting for other types of interaction (e.g. phonon scattering) k can not remain constant. Furthermore, certain trajectories may remain trapped in some regions surrounded by hard walls, which is not a trivial situation especially in multi-dimensional considerations. The consequences of this fact will be discussed in the sequel. The Liouville operator becomes a full time differential over given characteristics, that is, with the help of (3), it is possible to rewrite (1) as a set of equations parametrized by t'.

$$\frac{df(x(t'),k(t'),t')}{dt'} = \int dk' V_w(x(t'), k(t')-k') f(x(t'),k',t'). \tag{4}$$

We pursue the idea to integrate both sides in certain time limits. Apparently for $t' = t$ we obtain $f(x,k,t)$, which is the supremum of t'. The time t' may be reduced to the infinimum $t' = 0$, which, as already discussed follows the trajectory backwards in time. This links $f(x,k,t)$ with the initial condition, unless at a certain time t_b a boundary point is encountered. Thus we can formulate a task, where we look for the solution in an interval Ω, where the initial condition $f_i(x,k)$ is known at time $t = 0$, with boundaries at points $\pm l/2$, where the values of

$$f_b(-l/2,k,t), \text{ for } k > 0; \qquad f_b(l/2,k,t) \text{ for } k < 0 \tag{5}$$

are known at any time $t > 0$ (and are equal zero at $t = 0$). We note that, if going backwards over a trajectory from an internal point we encounter a boundary point, in the forward picture this trajectory is injected into Ω, thus only positive (negative) k values on the left (right) boundary are involved. To summarize: an integration of (1) on t' in the limits $[0,t]$ gives

$$\begin{aligned} &f(x,k,t) \\ &= \int_0^t dt' \int dk' V_w(x(t'),k(t')-k') f(x(t'),k',t') \\ &\quad + f_i(x(0),k(0))\theta_\Omega(x(0)) + f_b(x(t_b),k(t_b))\theta(t_b). \end{aligned} \tag{6}$$

Here the domain indicator θ_Ω is unity, if the argument belongs to the closed interval Ω. Note that due to the two θ functions f_i and f_b provide two complementary contributions to f. Besides, in the first iteration of the kernel with the boundary term, the lower limit of the time integration is cast to t_b due to the function $\theta(t_b)$. Furthermore, all higher order iterations are characterized by a descend ordering of the consecutive times of integration, having a bottom limit t_b. We conclude the section by further assuming stationary physical conditions, in particular we assume that the boundary conditions and the potential profile V are time independent.

3 Analysis of the convergence

The second kind Fredholm integral Eq. (1) has a free term f_1 given by the sum of f_i and f_b. The solution can be presented as a Neumann series of the consecutive iteration of the kernel on the free term and is uniquely determined by the latter provided the series converges. The proof of the convergence relies on the fact that (1) is of Volterra type with respect to the variable t. This allows to rewrite the equation as

$$\begin{aligned} f(x,k,t) = &\int_{t_0}^t dt' \int dk' V_w(x(t'),k(t')-k') f(x(t'),k',t) \\ &+ f_1(x,k,t_0), \end{aligned} \tag{7}$$

where itself the free term

$$f_1(x,k,t_0) = f(x(t_0),k(t_0),t_0) \tag{8}$$

of (7) satisfies Eq. (6) at $t_0 = t - \Delta t_1$, which is a time of the past with respect to the initialization time, $t > t_0$. Under the assumption that f_1 is known, local conditions may be specified for the kernel, in order to guarantee the convergence of the series [1,8]. A sufficient condition for convergence is the boundedness of the Wigner potential, $|V_w| < C$, by a given constant C. Under this assumption and if Δt_1 is small enough, the iterative terms have an upper-bound limit given by the corresponding terms of a geometric progression defined by

$$A\Delta t_1 < 1. \tag{9}$$

In this way the solution f of (7) is uniquely determined by the free term f_1.

The procedure can be repeated for f_1, which introduces the free term f_2 and so on, giving a decomposition of the backward evolution into the time intervals Δt_i. Next we show that these time intervals do not converge to certain point of compression, but actually cover the whole evolution interval, thus reaching the initial time after finite steps in the procedure. The next estimation addresses this problem. From (2) it follows that:

$$\begin{aligned} |V_w(x,k)| &= \left| \frac{1}{i\hbar 2\pi} \int dx' e^{-ix'k} \right. \\ &\quad \left. \times \int ds \left(e^{-i(x+x'/2)s} - e^{-i(x-x'/2)s} \right) \tilde{V}(s) \right| \\ &= \left| \frac{2}{i\hbar} \left(e^{i2xk} \tilde{V}(-2k) - e^{-i2xk} \tilde{V}(2k) \right) \right| < A. \end{aligned} \tag{10}$$

The last estimate comes from the assumption that the Fourier transform $\tilde{V}$ of the potential V is bounded by a constant $\hbar A/4$. By recalling that the Fourier transform of an absolutely integrable function is is a bounded and continuous function, we request that the potential V is an absolutely integrable function. In this case (9), and (10) guarantee the existence of an infinimum of the set Δt_i. This minimum can be used as a global decomposition time Δt.

This procedure, based on the Markovian character of the Wigner equation and a reasonable assumptions for the potential V, uniquely determines the solution of the equation by linking the solution f at given time in a given phase space point (with a spatial coordinate belonging to Ω) to the free term f_1 in (6). This means that, if the initial and the boundary conditions are known, they uniquely determine the solution of the equation. With this result we address the computational aspects of the problem. Questions, whether it is possible to formulate the boundary conditions and if they can alone

determine the solution, must be addressed from a physical point of view.

4 Physical aspects

The initial and boundary conditions give two complementary contributions to the solution. To reach a stationary regime, with boundary contributions only, the initial counterpart must vanish in the domain Ω with the increase of the evolution time. In the ideal case the initial condition 'leaks' through the boundaries and the electron system enters a stationary regime. It is worth to mention the following peculiarities: In general, for small evolution times t the main contribution to the solution in an internal point of Ω is given by the initial conditions, since the 'backward' end of the trajectory (3) also belongs to Ω. For larger times (3) encounters the boundary, so that the BCs determine the solution. Moreover, since the trajectory evolves backward in time, the function f outside Ω contributes to the solution inside Ω by these values of k only, which guarantee the injecting character of f_b. In this case it is legitimate to consider the stationary equation as physically relevant. However, there could be trajectories which never reach a physical boundary, that is a place where injecting boundary conditions have to be specified. We consider a potential which becomes zero at the boundaries (and remains such at infinity), but is characterized by a potential well around the origin. From a physical point of view the solutions inside the well may demonstrate periodic or stationary behavior and form the subspace of bound states. Actually these states are asymptotically bounded in a region around the well, which may be adjusted according to a desired precision due to the exponential damping of the wave functions away from the well. Thus a physical density can not leak trough the boundaries. A good example are the eigenstates of an harmonic oscillator with a frequency ω, which in Wigner representation are products of Laguerre polynomials with an exponentially decaying function of the argument

$$\xi = x^2 + k^2, \tag{11}$$

where, for convenience we assume $m\omega = 1$. From a mathematical point of view, bound states determine the zero space for evolution operators based on the commutator with the Hamiltonian like the Wigner and density matrix representations [9]. These states remain invariant under the action of these operators. The time evolution of the the harmonic oscillator states is given by a simple rotation of any initial condition f_i.

$$f(x,k,t) = f_i\left(xcos(\omega t) - ksin(\omega t), xsin(\omega t) + kcos(\omega t)\right) \tag{12}$$

This can be seen by applying the operations of (1) on (12) and taking into account that the operator with the Wigner potential of a harmonic oscillator can be equivalently formulated as a force term, which completes the left hand side of (1) to a general Liouville operator. In this case there is no difference between classical and quantum evolution, and quantum mechanics enters via the initial condition which must obey the uncertainty relations. The argument ξ, (11), of an eigenstate considered as an initial condition then does not change with time as can be seen from (12). Such Wigner states can be introduced as initial conditions only, and since they cannot be modified by the kernel of the equation, they remain as a part of the computational task forever. If we cast the physical task to the stationary, boundary condition problem, such states remain empty by default, unless the boundary is intentionally moved in the well and begins to fill them. Thus by moving the boundary we may obtain completely different solutions, which, however is not due to the unphysical nature of the Wigner equation, but rather to our approach to it. This conclusion is consistent with the results reported in [10] and [11], where the problem is investigated from an alternative point of view and peculiar effects are displayed. A manifestation of the bound state problem in our approach is that there is no way to specify boundary conditions for states in the potential well. These states are associated with zero or negative kinetic energies and according to (5) and (3) we can not inject trajectories with zero or imaginary wave vectors.

Here we consider as important the following remark. It looks like the picture of a conservation of the physical density into a given domain heavily contradicts to our previous considerations. Indeed, provided that k is not zero after some time, any trajectory (3) can reach any distance from the origin point, and according to the classical case a trajectory means a physical density moving away from Ω. However, this is the essential difference with quantum mechanics in the phase space. In the latter case trajectories are associated with numerical particles, which may abandon Ω in such a way that no physical density leaks outside Ω. Considering the picture of signed particles, (a recent overview is given in [12]) associated to the Wigner formulation of quantum mechanics, one can easily imagine a couple of a positive and a negative particles which in total gives zero physical density leaving the domain.

Finally the requirement for V to be an absolute integrable function is satisfied by a large class of potentials. The existence of the first derivative, the electric force, guarantees the continuity of V almost everywhere, Furthermore one must assume that V approaches zero far away from the structure, which correctly accounts for the recovery of the equilibrium [13]. Almost everywhere continuous functions which become zero at infinity are absolutely integrable, showing that this condition does not restrict, but rather characterize the physically relevant potentials.

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