Neumann Series Analysis of the Wigner Equation Solution

I. Dimov, M. Nedjalkov, J.M. Sellier, and S. Selberherr

Abstract The existence and uniqueness of the electron transport Wigner equation solution, determined by boundary conditions, is analyzed in terms of the Neumann series expansion of the integral form of the equation, obtained with the help of Newton's trajectories. For understanding of the peculiarities of Wigner-quantum electron transport in semiconductor structures such mathematical issues can not be separated from the physical attributes of the solution. In the presented analysis these two sides of the problem mutually interplay.

The problem is first formulated from a physical point of view, where the stationary solution is considered as the long time limit of the general evolution problem posed by both initial and boundary conditions. The proof of convergence relies on the assumption for reasonable local conditions which may be specified for the kernel and on the fact that the Neumann series expansion corresponds to an integral equation of Volterra type with respect to the time variable.

Keywords Electron transport • Neumann series analysis • Semiconductor • Wigner equation

1 Introduction

The existence and uniqueness of the solution of the Wigner equation (WE) is subject of an active research interest [1–3] since the rising importance of a quantum description of the electron transport in the novel semiconductor nanoelectronics. An analysis of the regularity of the Wigner function and the existence and uniqueness of the solution of the by initial conditions posed evolution problem relevant for single-dimensional nanostructures is presented in [1] and used to proof the convergence of the suggested operator-splitting method. The analysis has been further augmented

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to account for the existence of boundary conditions characterizing the contacts of such structures. The well posedness of the transient problem, associated with time-dependent inflow boundary conditions has been shown in a mathematically rigorous way [2]. The integral form of the Wigner equation based on classical Newtonian trajectories for transient (posed by an initial condition, (IC)) and stationary (posed by boundary conditions, (BC)) problems has been used to investigate the corresponding Neumann expansion of the solution in connection with convergence proofs of the developed quantum Monte Carlo methods [4, 5]. In both cases the equation is of Volterra type with respect to the evolution time or the time to the boundary, so that the trajectory approach is straightforwardly generalized to the typical multidimensional structures of modern nanoelectronics. In a recent work [6] it has been shown that the stationary Wigner equation can be expressed as a Volterra type integral equation with respect to the spatial variable. It is argued that moving the boundaries arbitrary close, or imposing arbitrary inflow BCs on them, may lead to non-unique and unphysical solutions [6]. However, another recent work shows the well-posedness of the problem within the interval of periodicity $\Omega = [-l/2, l/2]$ of a certain class of periodic potentials, under arbitrary inflow BCs specified at $-l/2$ ($v > 0$) and $l/2$ ($v < 0$) [3]. Thus under certain physical settings the solution of the stationary Wigner equation is well defined by the boundary conditions, while in other circumstances the physical soundness of the problem becomes questionable. Alternatively stated, there circumstances where the stationary Wigner equation is of practical importance, while in other occasions the equation is of academic importance only.

Here we present an analysis, in which mathematical and physical aspects of the problem mutually interplay. This imposes a rather physical way of presentation with an accent on the application aspects of the results, on the expense of the mathematical rigor. The single-dimensional Wigner equation is considered, however the analysis holds for three-dimensional transport as in the case of classical transport [7, 8].

The problem is first formulated from a physical point of view, where the stationary solution is considered as the long time limit of the general evolution problem posed by both ICs and BCs. This implies the existence of a generic solution, determined partially by the ICs and partially by the BCs. The latter are interpreted in this scheme as a known part of the generic solution, which is complementary to the part corresponding to the IC's. If the contribution from the IC's does not vanish with time and only BCs are considered, the problem remains not well formulated already 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 WE can be relevant only after existence of physical arguments for that. As a matter of fact, physically relevant models in the Wigner formulation are the stargenvalue problem and the time-dependent Wigner equation, thoroughly discussed in [9–11].

These considerations are apart from the practical aspects of Wigner transport. Boundary conditions are known explicitly only in rare cases,. An exception is the equilibrium Wigner function, which is well known. Thus equilibrium conditions are routinely assumed at the boundaries. However, then the 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.

2 Integral Representation

The presented analysis is dimension-independent, so that for the sake of simplicity the single- dimensional formulation of the problem is considered. The equation for the Wigner function f reads:

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

where $v(k) = \hbar k/m$ 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 and parameterized backwards in time by $t' < t$. An important property of Newton trajectories is that they do not cross in the phase space, so that (3) is uniquely determined by the initialization point.

The Liouville operator becomes a full time differential over given characteristics, so that it is now possible to rewrite Eq. (1) as a set of equations parametrized by t', which can be furthermore integrated on t' in the limits $[0, t]$, giving rise to:

$$\begin{aligned} f(x,k,t) = &\int_0^t dt' \int dk' V_w(x(t'), k(t') - k') f(x(t'), k', t) \\ &+ f_i(x(0), k(0))\theta_\Omega(x(0)) + f_b(x(t_b), k(t_b))\theta(t_b). \end{aligned} \tag{4}$$

Here the domain indicator θ_Ω is unity, if the argument belongs to the closed interval Ω, and is zero otherwise, t_b is the time needed for $x(t')$ to reach the boundary.

Finally (3) has been used to set $x(t) = x$, $k(t) = k$. The solution is sought in the interval Ω, where the initial condition (IC) $f_i(x,k)$ is known at time $t = 0$ and the BCs $f_b(-l/2,k,t)$, $k > 0$, $f_b(l/2,k,t)$, $k < 0$ are known at any time $t > 0$ (and zero at $t = 0$). Here we assume stationary physical conditions, in particular the BCs and the potential profile V are time independent. Furthermore boundaries, usually associated with certain physical interfaces, have now the meaning of points, where the function f, the unique solution of a generic evolution problem, is known.

3 Convergence

The second kind Fredholm integral equation (1) has a free term given by the IC and BCs. 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

$$f(x,k,t) = \int_{t_0}^{t} dt' \int dk' V_w(x(t'),k(t') - k') f(x(t'),k',t) + f_1(x,k,t_0), \tag{5}$$

where itself the free term

$$f_1(x,k,t_0) = f(x(t_0),k(t_0),t_0) \tag{6}$$

of (5) satisfies Eq. (4) 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, reasonable local conditions may be specified for the kernel, in order to guarantee the convergence of the series. In [7] the necessary conditions for the convergence of such a kind of iterative expansion are given. These conditions concern the kernel of the equation V_w. We consider a typical condition for V_w after the following remark. Frequently authors use the term *mild conditions*. However, since one is interested in computational convergence, we also need to have a mild condition number. If the solution convergence is mild, then the solution can be confidently declared as non-singular. Since the convergence behavior and the condition number can be affected by poor scaling, the definition of *mild* is problem dependent. Simply speaking, mildness means confidence in the convergence to the true non-singular solution [12]. Now, one sufficient condition for convergence is the boundedness of the Wigner potential, $|V_w| < C$, where C is a constant. Indeed, if Δt_1 is small enough, the iterative terms have an upper limit given by the corresponding terms of a geometric

progression defined by

$$C\Delta t_1 < 1. \tag{7}$$

In this way the solution f of (5) 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. It is important to show that these intervals can cover the whole evolution interval, which ensures that the initial time is reached. The next estimation addresses this problem. By assuming that the Fourier transform $\tilde{V}$ of the electric potential V is bounded by a constant $\hbar C/4$ and using the definition (2) it may be shown that:

$$|V_w(x,k)| < C, \tag{8}$$

Thus, it is sufficient to request that the potential V is an absolutely integrable function, as the Fourier transform of such a function is bounded and continuous. The result (8) used in (7), shows the existence of an infimum of the set Δt_i, which can be used as a global decomposition time Δt.

Finally, this procedure links f to the free term in (4): the initial and the boundary conditions, which uniquely determine the solution of the equation.

4 Physical Analysis

The physical aspects of this proof may be associated to the Markovian character of the Wigner evolution. Furthermore we note that the solution has two complementary contributions from the IC and the BCs. In general, for small evolution times t the main contribution to the solution in an internal point of Ω is given by the IC. For large 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.

An important conclusion follows from this analysis: In the case when the initial condition 'leaks' through the boundaries: $f_i = 0$ after given time t_s, the electron system enters into a stationary regime and it is legitimate to consider the stationary equation as physically relevant. However, from a physical point of view it is clear that if there are electronic states which remain insulated away from the boundaries, they can not be controlled by the boundaries and the time dependent factor in the Wigner equation can not be neglected. Such are the bound eigenstates of the Hamiltonian related e.g. to periodic in time solutions or electrons with zero momenta. From a mathematical point of view, states which commute with the system Hamiltonian give rise to the 'bound state problem' for the von Neumann or Wigner equations [13]. The particular manifestation of this problem within the developed approach, is the fact that such states can not be

associated with trajectories which reach the boundaries: the wave vector of bounded states is undefined. In particular, zero momentum electrons are routinely neglected in the mathematical approaches. Indeed they have zero contribution to certain physical mean values like velocity, energy, and current, however, they affect the electrostatics.

The requirement for V to be an absolute integrable function is satisfied by a large class of potentials. Indeed the physical quantities are usually assumed to be smooth functions of their variables. In particular the existence of the first derivative, the electric force, guarantees the continuity of V almost everywhere, besides the fact that discontinuities are considered as convenient for the mathematical treatment of limiting cases. Furthermore one must assume that V approaches zero far away from the structure, which correctly accounts for the recovery of the equilibrium [14].

Finally 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.

We conclude with a remark concerning the fact that boundaries are considered as a part of a global Wigner function. There are conditions for both pure and mixed states, which, if satisfied, allow to interpret a phase space function as a physically acceptable quasi-distribution, or Wigner function [13]. In this respect, an inconsistent change of the values at the boundaries will lead to unphysical results.

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