OPERATOR SPLITTING METHODS FOR THE WIGNER-POISSON EQUATION

Anton Arnold

Permanent address: Technische Universität Berlin, FB Mathematik, Straße des 17. Juni 136, W-1000 Berlin 12, Germany. Currently visiting at: Department of Mathematics, Purdue University, West Lafayette, IN 47907

and

Christian Ringhofer

Department of Mathematics, Arizona State University, Tempe, AZ 85287.

Abstract

The Wigner–Poisson equation is the most successful basis for transient simulations of quantum–effect semiconductor devices so far.

We present a (second order) operator splitting method for the time–discretization of this non–linear pseudo–differential equation. For the application to quantum devices some important model extensions are discussed (boundary conditions, many–body effects).

1. Introduction. In this paper we shall discuss operator splitting methods to discretize the linear Wigner equation and the coupled Wigner–Poisson system. The Wigner formalism, which represents a phase–space description of quantum mechanics, has in recent years attracted considerable attention of solid state physicists for including quantum effects in the simulation of ultra–integrated semiconductor devices, like resonant tunneling diodes, e.g. ([7], [8], [4]). Also, the Wigner (–Poisson) equation has recently been the objective of a detailed mathematical analysis ([11] and references therein).

The real–valued Wigner (quasi) distribution function $w = w(x, v, t)$ describes the motion of an electron ensemble in the $2d$–dimensional position–velocity (x, v)–phase space under the action of the electrostatic potential V. In the absence of collision and scattering, and in the effective–mass approximation, the time evolution is governed by the Wigner equation (q denotes the unit charge and m^* the effective mass of the electron):

$$w_t + v \cdot \nabla_x w + \tfrac{q}{m^*} \Theta[V] w = 0, \quad x, v \in \mathbb{R}^d, \quad d = 1, 2 \text{ or } 3, \tag{1.1}$$

with the pseudo–differential operator

$$\Theta[V] w = i\delta V\left(x, \tfrac{1}{i}\nabla_v, t\right) w = \tag{1.2}$$

$$= \tfrac{i}{(2\pi)^d} \int_{\mathbb{R}^d_\eta} \int_{\mathbb{R}^d_{v'}} \delta V(x, \eta, t) w(x, v', t) e^{i(v-v')\cdot\eta} dv' d\eta,$$

$$\delta V(x, \eta, t) = \tfrac{m^*}{\hbar} \left[V\left(x + \tfrac{\hbar}{2m^*}\eta, t\right) - V\left(x - \tfrac{\hbar}{2m^*}\eta, t\right) \right].$$

In this kinetic framework the particle density n and the current density J are defined by $n(x,t) = \int w(x,v,t)dv$ and $J(x,t) = -q \int v w(x,v,t)dv$. In order to account for electron–electron interactions in a simple mean–field approximation, (1.1) has to be coupled to the Poisson equation $\Delta V(x,t) = q/\varepsilon\,[n(x,t) - D(x)]$, where ε and $D(x)$ denote the permittivity and the doping profile of the semiconductor, respectively.

The Wigner function representation is equivalent to the conventional wave function formalism ([17], [10]), and any L^2–solution of the Wigner equation can be expanded into a series of pure states:

$$w = \sum_{j=1}^{\infty} \lambda_j w_j, \quad \lambda_j \geq 0, \quad \sum_{j=1}^{\infty} \lambda_j = 1, \tag{1.3}$$

where each w_j corresponds via

$$w_j(x,v,t) = (2\pi)^{-\frac{d}{2}} \int_{\mathbf{R}^d} \psi_j^* \left(x + \tfrac{\hbar}{2m}\eta, t\right) \psi_j \left(x - \tfrac{\hbar}{2m}\eta, t\right) e^{iv\cdot\eta} d\eta \tag{1.4}$$

to a pure state wave function ψ_j, whose time evolution is governed by the Schrödinger equation. Although theoretically equivalent, the Wigner formalism appears much more successful in the application of numerically simulating quantum–effect devices: In the kinetic framework boundary conditions can be formulated much more naturally, and this will be crucial for an effective coupling with (semi–) classical models (based on the Boltzmann equation, e.g.) away from the active region of the semiconductor. Moreover, a transient simulation based on the Schrödinger formalism would require to include a great number of pure states in (1.3) ([4]), which would compensate the higher dimensionality of the Wigner approach.

Mainly due to the non–local pseudo–differential operator, the numerical solution of the Wigner equation represents a major computational task, especially for multi–dimensional structures and with the model extensions discussed later in §3. It is, therefore, of paramount importance to develop efficient and accurate numerical schemes, which should also reflect the conservation of some important physical quantities.

During the last few years various numerical methods have been used for the Wigner equation: finite difference schemes ([7], [12]), spectral collocation methods ([13]) and a deterministic particle method ([1]). In this paper we shall discuss operator splitting methods, which have been first used by plasma physicists ([16]). In §2 we present the numerical scheme for the Wigner (–Poisson) equation and its stability and convergence properties from the mathematical point of view. In §3 the quantum transport model will be extended to be suitable for simulations of quantum devices and the corresponding modifications of the splitting scheme will be outlined.

2. Operator Splitting Scheme.

In this section, we present the basic ideas of the operator splitting method for the Wigner–Poisson equation, which reads in scaled form

$$w_t + v \cdot \nabla_x w + \Theta[V]w = 0, \tag{2.1a}$$

$$\Delta V(t) = n(t) - D. \tag{2.1b}$$

For the mathematical details and proofs we refer the reader to [2], [3].

First we will illustrate the scheme for the linear, whole space case with a prescribed, constant–in–time potential $V = V(x) \in L^\infty(\mathbf{R}^d)$. The splitting method for (2.1a) consists in splitting the transport operator $A = -v \cdot \nabla_x$ and the pseudo–differential operator $B = -\Theta[V]$ for each time step of length Δt. Then the resulting evolution equations are solved successively:

$$\begin{cases} u_t = Au, & t_n \leq t \leq t_{n+1} \\ u(t_n) = w_n, & \\ w_{n+\frac{1}{2}} := u(t_{n+1}), & \end{cases} \tag{2.2}$$

$$\begin{cases} u_t = Bu, & t_n \le t \le t_{n+1} \\ u(t_n) = w_{n+\frac{1}{2}}, & \\ w_{n+1} := u(t_{n+1}) & \end{cases} \tag{2.3}$$

where w_n and w_{n+1} denote approximations of $w(t)$ at t_n and $t_{n+1} = t_n + \Delta t$. This splitting method is particularly suitable for the Wigner equation since the operators A and B act in orthogonal directions of phase–space, and since the two split evolution equations can be solved explicitly:

$$w_{n+\frac{1}{2}}(x,v) = w_n(x - v\Delta t, v), \tag{2.4}$$

$$(\mathcal{F}_v w_{n+1})(x,\eta) = (\mathcal{F}_v w_{n+\frac{1}{2}})(x,\eta) e^{-i\Delta t\ \delta V(x,\eta)}, \tag{2.5}$$

where $\mathcal{F}_v$ denotes the Fourier transform with respect to v. Because of this explicit solvability, we shall first consider the convergence properties of the semi–discretization (2.2), (2.3). The conservation of total charge $\iint w\,dx\,dv$ and the L^2–norm is readily obtained from the above solution formulas: $\|w_{n+1}\|_2 = \|w_{n+\frac{1}{2}}\|_2 = \|w_n\|_2$, which yields stability of the splitting scheme. Since A and B generate C_0–groups of isometries on $L^2(\mathbf{R}^{2d})$ $(e^{tA}, e^{tB}; t \in \mathbf{R})$, the L^2–convergence is an immediate consequence of Trotter's product formula for linear semigroups (see [5] e.g.):

$$w(t) = e^{t(A+B)} w^I = \lim_{N\to\infty} \left[e^{\frac{t}{N}B} e^{\frac{t}{N}A} \right]^N w^I. \tag{2.6}$$

THEOREM 2.1. *Let $V \in L^\infty(\mathbf{R}^d)$ and the initial Wigner function $w^I \in L^2(\mathbf{R}^{2d})$. Then, the operator splitting method* (2.2), (2.3) *converges in $L^2(\mathbf{R}^{2d})$ as $\Delta t \to 0$.*

Since the operators A and B do not commute, the algorithm is accurate only to first order. For a given time dependent potential, $V(t)$ has to be evaluated at $\bar{t}_n = (t_n + t_{n+1})/2$ for the split evolution equation (2.3). We then obtain the following convergence result:

THEOREM 2.2. *Let $V \in C^1([0,T], L^\infty(\mathbf{R}^d)) \cap C([0,T], W^{1,\infty}(\mathbf{R}^d))$, $\Delta V \in C([0,T], L^\infty(\mathbf{R}^d))$, and w^I, vw^I, $\nabla_x w^I$, $Aw^I \in L^2(\mathbf{R}^{2d})$. Then*

$$\left\| w(t) - \left[e^{\frac{t}{N}B} e^{\frac{t}{N}A} \right]^N w^I \right\|_2 \le \frac{C}{N} \tag{2.7}$$

holds, with C independent of $t \in [0,T]$.

An algorithm based on the step–forward operator $e^{\frac{\Delta t}{2}A} e^{\Delta t B} e^{\frac{\Delta t}{2}A}$ ("Strang splitting") is second order accurate. But since the adjacent applications of the operator $e^{\frac{\Delta t}{2}A}$ can be combined into one operation (except for the first and last half–step in a calculation), this algorithm is almost only as expensive as the above first order scheme.

A simple calculation, based on the expansion (1.3), (1.4), shows that the presented operator splitting method for the Wigner equation is equivalent to splitting the operators $i\hbar/2m^*\Delta_x$ and $iq/\hbar V(x,t)$ in the Schrödinger equation for every pure state ψ_j. (In [6], a Strang splitting method for the Schrödinger equation was used in the simulation of lateral surface superlattices.) Therefore, the expansion coefficients λ_j of the numerical iterates w_n will stay constant in time, which shows that all w_n are physical Wigner functions

($\lambda_j \geq 0, \sum_j \lambda_j = 1$). Since the particle density is expressed as $n(x,t) = \sum_j \lambda_j |\psi_j(x,t)|^2$ in the Schrödinger formalism, this also implies the positivity conservation of $n = \int w\, dv$ in the numerical scheme (although the Wigner function w takes negative values).

Although, theoretically, both steps of the splitting method can be carried out exactly, approximations will have to be made if a concrete finite dimensional representation of the solution is chosen. Because of the definition of the pseudo–differential operator via Fourier transforms it is natural to expand the Wigner function in trigonometric functions in the velocity direction (which are eigenfunctions of $\Theta[V]$). The resulting spectral collocation method is then of spectral accuracy ([**13**], [**14**]). For notational simplicity we just illustrate the one–dimensional situation:

$$w(x, v_m, t) \sim \sum_{\mu=-M}^{M} \hat{w}(x,\mu,t) e^{i\alpha\mu v_m}, \quad v_m = \frac{m\pi}{\alpha M} \quad m = -M+1, \ldots, M, \tag{2.8}$$

with the inverse Fourier transform

$$\hat{w}(x,\mu,t) = (2M\beta(\mu))^{-1} \sum_{m=-M+1}^{M} w(x, v_m, t) e^{-i\alpha\mu v_m}, \quad \beta(\mu) = 1 + \delta(|\mu| - M). \tag{2.9}$$

In this framework (2.5) is discretized as

$$\hat{w}_{n+1}(x,\mu) = \begin{cases} \hat{w}_{n+\frac{1}{2}}(x,\mu) e^{-i\Delta t\ \delta V(x,\alpha\mu)}, & |\mu| < M \\ \hat{w}_{n+\frac{1}{2}}(x,\mu), & |\mu| = M, \end{cases} \tag{2.10}$$

and $n(x,t) \sim \frac{2\pi}{\alpha} \hat{w}(x,0,t)$ holds.

When the Wigner function is discretized in x–direction with a grid spacing Δx, such that Δt is an integer multiple of $\frac{\alpha M}{\pi} \Delta x$, then the discretization of (2.4) can be carried out exactly. In this case, no artificial diffusion (normally inherent to difference methods) is introduced by the numerical scheme. For smaller time steps, however, interpolation between neighboring x–gridpoints has to be used.

We will now proceed to the coupled Wigner–Poisson problem (2.1a,b). Again, transport operator and pseudo–differential operator are split like in (2.2), (2.3). But the nonlinear operator B is now defined by $Bu = -\Theta[V[u]]u$, where the potential $V[u]$ solves the Poisson equation (2.1b), supplemented with appropriate decay or boundary conditions on infinite or bounded (spatial) domains, respectively. Since $\int_{\mathbf{R}^d} (Bu)(x,v) dv = 0$ holds, the nonlinear evolution equation

$$u_t = Bu, \quad t_n \leq t \leq t_{n+1} \tag{2.11}$$

shows that the density and hence the potential $V[u]$, associated to its solution $u(t)$, are constant in time. Therefore (2.11) can be solved explicitly like in the linear case by using the potential $V[w_{n+\frac{1}{2}}]$ in (2.5).

First order convergence of the scheme (2.2), (2.11) and second order convergence of the corresponding "Strang splitting" have been established in [**2**]. For the nonlinear analysis in $1D$, the weighted L^2–space $L^2(\mathbf{R}^2; 1+|v|)$ has to be chosen in the underlying framework to allow for a proper definition of $n = \int w\, dv$.

3. Model Extensions for Quantum Device Simulations.

In this section we discuss some approaches to incorporate important physical mechanisms into the Wigner–Poisson model to enable a more realistic description of quantum transport

in semiconductor devices. We will present three different aspects, for simplicity separately, and their possible realizations in the framework of operator splitting methods.

a) *boundary conditions:* For the simulation of resonant tunneling diodes most authors ([4], [7]) supplemented the Wigner equation (2.1a), posed on a finite x–domain $\Omega \subseteq \mathbf{R}^d$, with inflow boundary conditions (BC):

$$w(x,v,t) = w_D(x,v,t) \text{ for } x \in \partial\Omega, \quad v \in \mathbf{R}^d, \quad r \cdot v < 0, \tag{3.1}$$

where r is the outward normal vector on $\partial\Omega$. If these simulation (or device–) boundaries are posed too close to the source of quantum effects (heterojunctions), they represent artificial constraints for the dynamic of the system: outgoing waves may be artificially reflected by the boundary, instead of being 'absorbed' by the contact. This introduced constraint also affects the analytical behavior of the exact Wigner function (less regularity) and its discretization. In the splitting scheme (2.2), (2.3) the (spatial) BC (3.1) only supplements $u_t = Au$, but no BC is needed for (2.3), since B acts in v–direction only. However, the numerical iterates w_n will not satisfy the BC (3.1), and each step of form (2.2) will transport this boundary–discontinuity into the domain Ω. Hence, the order of convergence of this t–discretization is reduced to $\frac{1}{2}$.

The following scheme modification raises the order of convergence to 1, but still retains a decoupled evolution for different velocities:

$$\begin{aligned} &u_t = Au + Bw_n, \quad u(t_n) = w_n, \quad w_{n+1} := u(t_{n+1}), \\ &u(x,v,t) = w_D(x,v,t), \quad x \in \partial\Omega, \quad v \in \mathbf{R}^d, r \cdot v < 0. \end{aligned} \tag{3.2}$$

In one dimension with $\Omega = (-1,1)$, the solution is given by

$$w_{n+1}(x,v) = \tilde{w}_n(x - v\Delta t, v) + \tfrac{1}{v} \int_{[x-v\Delta t, x] \cap \Omega} (Bw_n)(\xi, v) d\xi, \tag{3.3}$$

where $\tilde{w}_n$ denotes the extension of w_n by the inflow boundary data for $x < -1$, $v > 0$, and $x > 1$, $v < 0$.

In order to obtain a more accurate t–discretization, a higher order approximation for the BC has to be employed (like 'absorbing BC' in [15]).

b) *electron-electron interaction:* Most transient simulations of quantum devices use a mean–field approximation (via self–consistent coupling to the Poisson equation) to incorporate many–body effects into the system, at least in a rudimentary fashion. In the framework of the non–linear operator splitting (2.2), (2.11) a refined coupling can readily be included, as long as it gives rise to an effective potential $V_{\text{eff}}[n]$ to be inserted in the pseudo–differential operator $\Theta[V]$. So it is easy to incorporate local exchange–correlation potentials ([9]), which, in basic models, are of the form $V_{\text{ex}}(x,t) = -\alpha n(x,t)^{\frac{1}{3}}$.

c) *relaxation-time models:* The relaxation–time (RT) approximation is the simplest model to account for electron–phonon scattering, but it still yields remarkable results in device simulations. In [8] the phenomenological relaxation term $1/\tau\ [w_0(x,v) - w(x,v,t)]$ serves as the right hand side of (2.1a), coupled to (2.1b). w_0 is a steady state of the system, satisfying

$$v \cdot \nabla_x w_0 + \Theta[V_0] w_0 = 0, \quad \Delta V_0 = n_0 - D. \tag{3.4}$$

In this situation $w(t)$ converges to w_0 for 'small' τ. To reflect this convergence behavior in the numerical scheme we symmetrize the RT–Wigner–Poisson equation by subtracting (3.4) and split:

$$(w - w_0)_t = -v \cdot \nabla_x (w - w_0) - \frac{1}{\tau(v)}(w - w_0), \tag{3.5}$$

$$(w - w_0)_t = -\Theta[V]w + \Theta[V_0]w_0, \quad \Delta(V - V_0) = n - n_0. \tag{3.6}$$

Even by allowing for a (more realistic) v–dependence of the RT $\tau(v)$, (3.5) can be solved explicitly.

In [4] the more theoretically justified relaxation term

$$\frac{1}{\tau}\left[\frac{n(x,t)}{n_0(x)} w_0(x,v) - w(x,v,t)\right] \tag{3.7}$$

was employed. The resulting RT–Wigner–Poisson equation shows no obvious asymptotic behavior for large time and can be split as:

$$w_t = -v \cdot \nabla_x w, \tag{3.8}$$

$$w_t = -\Theta[V]w + \frac{1}{\tau}\left[\frac{n}{n_0} w_0 - w\right], \quad \Delta V = n - D. \tag{3.9}$$

Integrating over v again shows that V stays constant during the step (3.9), which can thus be solved explicitly.

References

1. A. Arnold and F. Nier, Math. of Comp. **58** (1992), 645–669.
2. A. Arnold and C. Ringhofer, *An operator splitting method for the Wigner–Poisson problem*, submitted (1992).
3. A. Arnold and C. Ringhofer, *On the convergence of a combined operator splitting and fractional step method for the Wigner–Poisson equation*, manuscript.
4. F. A. Buot and K. L. Jensen, Phys. Rev. B **42** (1990), 9429–9457.
5. A. J. Chorin, T. J. Hughes, M. F. McCracken, and J. E. Marsden, Comm. Pure Appl. Math. **31** (1978), 205–256.
6. M. H. Degani and J. P. Leburton, Superlattices and Microstructures **11** (1992), 79–82.
7. W. R. Frensley, Phys. Rev. **B36** (1987), 1570–1580.
8. N. Kluksdahl, A. M. Kriman, D. K. Ferry, and C. Ringhofer, Phys. Rev. B **39** (1989), 7720–7735.
9. W. Kohn and L. J. Sham, Phys. Rev. **140** (1965), 1133–1138.
10. P. A. Markowich, Math. Meth. in the Appl. Sci. **11** (1989), 459–469.
11. P. A. Markowich, C. Ringhofer and C. Schmeiser, "Semiconductor Equations," Springer Verlag, Wien–New York, 1990.
12. V. Ravaioli, M. A. Kriman, W. Plötz, N. Kluksdahl, and D. K. Ferry, Physica **134B** (1985), 36–40.
13. C. Ringhofer, SIAM J. Numer. Anal. **27** (1991), 32–50.
14. C. Ringhofer, M^3AS **2** (1991), 91–112.
15. C. Ringhofer, D. Ferry, and N. Kluksdahl, Transport Theory and Statistical Physics **18 (3,4)** (1989), 331–346.
16. N. D. Suh, M. R. Feix, and P. Bertrand, J. Comput. Phys. **94** (1991), 403–418.
17. V. I. Tatarskii, Sov. Phys. Usp. **26** (1983), 311–327.