A mixed spectral-collocation and operator splitting method for the Wigner-Poisson equation

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ABSTRACT. The Wigner-Poisson equation is a kinetic pseudo-differential equation to model quantum transport. A combined spectral-collocation and operator splitting method is presented and analyzed.

1. Introduction

In this paper we present and analyze an operator splitting method for the Wigner-Poisson (WP) equation. The Wigner formalism ([10,6]), which represents a phase-space description of quantum mechanics, has in recent years received a lot of attention as a tool to simulate transport phenomena in ultra-integrated quantum effect semiconductor devices.

The real-valued Wigner distribution function $w(x,v,t)$ describes the motion of an electron ensemble in position-velocity (x,v)-phase space under the action of the electrostatic potential $V(x,t)$. The time evolution of w is governed by the Wigner equation, which reads in scaled form

$$\partial_t w + v\partial_x w + \Theta[V]w = 0 \quad , \quad x \in (-\pi,\pi),\, v \in I\!R, \tag{1.1}$$

with the pseudo-differential operator (PDO)

$$\Theta[V]w = \frac{i}{2\pi}\int\int \delta V(x,\eta,t)w(x,v',t)e^{i(v-v')\eta}\,dv'd\eta, \tag{1.2}$$

$$\delta V(x,\eta,t) = V(x+\frac{\eta}{2},t) - V(x-\frac{\eta}{2},t).$$

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To incorporate many-body effects in a simple mean-field approximation, the potential V is selfconsistently coupled to the Poisson equation

$$\partial_x^2 V(x,t) = \rho(x,t) - D(x), \tag{1.3}$$

with the particle density $\rho = \int w dv$ and some fixed ion density D.

Mainly for simplicity of the presentation we will here only consider the $1D$-problem, which we supplement with periodic boundary conditions (BC) in x. For realistic simulations of resonant tunneling diodes ([4]) absorbing BCs ([8]) have given very satisfactory results, but the analysis of the resulting initial-boundary value problem is still under investigation ([1]). In order for the Poisson equation to be solvable with periodic BCs, charge neutrality of the initial state, i.e.,

$$\int_{I\!R} \int_{-\pi}^{\pi} w^I(x,v)\, dx\, dv = \int_{-\pi}^{\pi} D(x)\, dx, \tag{1.4}$$

has to hold, which will then persist under temporal evolution. Also we will require the potential V to satisfy the normalization $\int_{-\pi}^{\pi} V\, dx = 0$ for all time t.

In §2 we will present the numerical scheme for the solution of the coupled system (1.1) - (1.3), and outline its stability and convergence proof in §3 (for mathematical details we refer to [2,3]).

2. Numerical scheme

From the numerical point of view, the major problem in the discretization of the WP system stems from the PDO which is nonlocal in v. In [2] an operator splitting method has been analyzed (first used in [9]), which consists in separating the transport operator $A = -v\partial_x$ and the nonlinear PDO $Bw = -\Theta[V[w]]$ ($V[w]$ is the solution of (1.3) with periodic BCs) for each time step:

$$\partial_t f = Af \quad , \quad t_s \le t \le t_{s+1} = t_s + h; \quad f(t_s) = w_s \quad , \quad w_{s+\frac{1}{2}} = f(t_{s+1}), \tag{2.1}$$

$$\partial_t f = Bf \quad , \quad t_s \le t \le t_{s+1}; \quad f(t_s) = w_{s+\frac{1}{2}} \quad , \quad w_{s+1} = f(t_{s+1}). \tag{2.2}$$

The advantage of this operator splitting method lies in the fact that, at least theoretically, both steps can be carried out explicitly, since the density $\rho[f]$, and thus also $V[f]$, stay constant during the second evolution step (2.2) :

$$w_{s+\frac{1}{2}}(x,v) = w_s(x-hv,v), \quad \hat{w}_{s+1}(x,\eta) = \hat{w}_{s+\frac{1}{2}}(x,\eta)e^{-ih\delta V_s(x,\eta)}, \tag{2.3}$$

where $\hat{w}$ denotes the Fourier transform with respect to v.

For the linear Wigner equation with a given potential $V \in L^\infty(I\!R)$ the L^2-convergence (this is the natural framework for the Wigner function [5]) of this splitting scheme as $h \to 0$ is an immediate consequence of Trotter's product formula for linear semigroups, yielding a first-order method (second-order for 'Strang splitting', [2]).

We will now specify the finite-dimensional representation of w_s. Because of the definition of the PDO via Fourier transforms it is natural to expand the Wigner function in the trigonometric functions $\Phi(n,v) = \sqrt{\frac{\alpha}{2\pi}}\exp(i\alpha n v)$ which are eigenfunctions of $\Theta[V]$. Since we discuss here the case of periodic BCs, we will expand the Wigner function in trigonometric functions in the spatial direction as well:

$$(2.4) \quad w_s(x,v) \sim u_s(x,v) = \sum_{n=-N+1}^{N} \hat{u}_s(x,n)\Phi(n,v) = \sum_{m=-M+1}^{M} \overline{u}_s(m,v)e^{imx}$$

$$= \sum_{m=-M+1}^{M} \sum_{n=-N+1}^{N} \tilde{u}(m,n)e^{imx}\Phi(n,v),$$

where $\hat{u}_s(x,-n) = \hat{u}_s(x,n)^*$ for $|n| < N$ and $\hat{u}_s(x,N) \in \mathbb{R}$, and similarly for $\overline{u}_s$. As the shift step in (2.3) will in general not preserve the structure of $\overline{u}_s$, it will have to be carried out by collocation. We define the collocation points x_k and v_j by

$$(2.5) \quad x_k = \frac{k\pi}{M} \quad , \quad k = -M+1, ..., M, \quad v_j = \frac{j\pi}{\alpha N} \quad , \quad j = -N+1, ..., N.$$

For the approximation of (1.3) the integral over w has to be truncated at $v = \pm\frac{\pi}{\alpha}$:

$$(2.6) \qquad \rho_s(x) \sim \int_{-\frac{\pi}{\alpha}}^{\frac{\pi}{\alpha}} u_s(x,v)dv = \sqrt{\frac{2\pi}{\alpha}}\hat{u}_s(x,0).$$

After also expanding ρ_s, V_s, and D into trigonometric polynomials in x, the fully discretized fractional step (2.3) takes the form $u_{s+\frac{1}{2}} = G(h)u_s$, $u_{s+1} = F_M(h, u_{s+\frac{1}{2}})$, with

$$(2.7) \qquad [G(h)u](x, v_j) = \sum_{m=-M+1}^{M} \overline{u}(m, v_j)e^{-imhv_j}e^{imx},$$

$$(2.8) \qquad V(x) = \sum_{m\neq 0} \frac{[\overline{D}(m) - \sqrt{\frac{2\pi}{\alpha}}\tilde{u}(m,0)]}{m^2}e^{imx},$$

$$[F_M(h,u)](x_k, v_j) = \sum_{n=-N+1}^{N} \hat{u}(x_k, n)e^{-ih\delta V(x_k, \alpha n)}\Phi(n, v_j).$$

Here, $\overline{V}(0) = 0$ reflects the chosen normalization of the potential.

When taking $\frac{\alpha N}{2\pi} \in \mathbb{N}, \delta V(x, \alpha N) = 0$ follows, and the scheme (2.7), (2.8) can easily be seen to preserve the total charge $\sqrt{\frac{2\pi}{\alpha}}\frac{\pi}{M}\tilde{u}(0,0)$ and the discrete L^2-norm of u_s. This will be the basis for the stability obtained in §3.

When the WP system is discretized in the v-direction only, we obtain the hyperbolic system

$$\partial_t u(x,v_j,t) + v_j \partial_x u(x,v_j,t) + (\Theta[V]u)(x,v_j,t) = 0, \tag{2.9}$$

$$\partial_x^2 V(x,t) = \frac{\pi}{\alpha N} \sum_{j=-N+1}^{N} u(x,v_j,t) - D(x). \tag{2.10}$$

In [7] it has been shown that the solution u of (2.9), (2.10) converges to the solution of the WP system with spectral accuracy for $\alpha \to 0$ and $\alpha N \to \infty$. Therefore, we will here only focus on the convergence of the splitting method (2.7), (2.8) to the solution of the hyperbolic system (2.9), (2.10) .

3. Stability and convergence

In the mathematical analysis of the WP system one has to require w and $vw \in L^2$, in order to allow for a proper definition of ρ. In the stability analysis of (2.7), (2.8) we have to establish a discrete analogue of this framework. The potential in (2.8) satisfies the estimate

$$||V||_{1,\infty}^2 \le \text{const}\,[\frac{2\pi}{\alpha} \sum_{m=-M+1}^{M} |\tilde{u}(m,0)|^2 + 1], \tag{3.1}$$

with a constant independent of α, M and N. The approximation for the density $\rho[u]$ can be estimated by

$$\frac{2\pi}{\alpha} \sum_{m=-M+1}^{M} |\tilde{u}(m,0)|^2 \le \text{const}||u||_{X_0}^2, \quad ||u||_{X_0}^2 = ||u||_2^2 + ||Hu||_2^2, \tag{3.2}$$

for all $u \in B_{MN}$, which is the space of functions represented by (2.4). Here the operator $H : B_{MN} \to B_{MN}$, defined by $Hu = \frac{\exp(i\alpha v_j)-1}{\alpha} u$, is the discrete approximation for ivu.

The scheme (2.7), (2.8) conserves $||u_s||_2$, and the shift step also conserves $||Hu_s||_2$. A straightforward estimate of (2.8) gives

$$||HF_M(h,u)||_2^2 \le \text{const}(1+h)(1+||V||_{1,\infty}^2)||u||_{X_0}^2, \tag{3.3}$$

which then yields a uniform bound for $||u_s||_{X_0} + ||V_s||_{1,\infty}$, $sh \le T$. In order to obtain nonlinear stability of the numerical scheme, one can show that (2.8) is locally Lipschitz in the X_0-norm.

To discuss the consistency of the method, we introduce the projection (by collocation at x_k) $P_M : B_N \to B_{MN}$, with $B_N = \{\sum_n \hat{u}(x,n)\Phi(n,v), \hat{u}(\cdot,n) \in L^2(-\pi,\pi)\}$. Now we extend the fractional step (2.7), (2.8) to B_N : G is defined like in (2.7), but the nonlinear operator F now involves the exact solution of the Poisson equation with periodic BCs. For the formulation of the main result of this section we need the periodic (in x) Sobolev space $X_r = \{u \in B_N | u(\cdot,v),\, Hu(\cdot,v) \in H_p^r(-\pi,\pi)\}$.

Theorem 3.1 *Let* $u \in C^1([0,T],X_r)$, $\partial_x u$, $v_j u \in C([0,T],X_r)$, $\int_{-\pi}^{\pi} \int_{-\frac{\pi}{\alpha}}^{\frac{\pi}{\alpha}} u^I \,dxdv = \int_{-\pi}^{\pi} D\,dx$, *and* $D \in B_{MN} \cap H_p^{r+1}(-\pi,\pi)$. *Then*

$$\|P_M u(t+h) - F_M(h, G(h) P_M u(t))\|_{X_0} \leq \text{ const } h(h + M^{-r}). \tag{3.4}$$

The left-hand side of (3.4) can be split as $P_M[u(t+h) - F(h, G(h)u(t))] + P_M[\{F(h, G(h)\cdot) - I\} \circ (I - P_M)u(t)]$, where the first term represents the error of the operator splitting in B_N, and the second term is due to the collocation projection of $u(t)$.

Combining this theorem with the above nonlinear stability result shows the first-order convergence of the scheme with respect to h, and the spectral accuracy of the spacial discretization.

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