ADAPTIVE METHODS FOR THE SOLUTION OF THE WIGNER-POISSON SYSTEM*

CHRISTIAN RINGHOFER**

Abstract. A numerical method, based on spectral collocation, for the solution of the Wigner-Poisson system is presented. A numerical example is briefly discussed.

1. Introduction. Quantum mechanical transport phenomena in small semiconductor devices, such as c. f. resonant tunneling diodes, can be described either by the Schrödinger equation or equivalently by the Wigner-Poisson system [3], [6]

\[
\begin{align*}
\text{a)} & \quad \partial_t w + \frac{1}{m} p \cdot \nabla_x w - \theta[V_E + V_B]w = 0 \\
\text{b)} & \quad -\epsilon \Delta_x V_E + q(n - D(x)) = 0, \\
\text{c)} & \quad n(x, t) = \int_{\mathbb{R}^d_p} w(x, p, t) dp.
\end{align*}
\]

Here \( x \) denotes position, \( p \) momentum, and \( t \) denotes time. \( d \) is the dimensionality of the problem (i.e. \( d = 1, 2 \) or \( 3 \) holds). \( w(x, p, t) \) is the Wigner distribution function (WDF), \( V_E(x, t) \) is the electric potential and \( n(x, t) \) denotes the charge density. \( V_B \) is a time independent step function modelling the quantum barriers. \( D(x) \) models the doping profile of the device. The pseudo differential operator \( \theta[V] \) in (1)a), given by

\[
\theta[V] = \frac{1}{i\hbar} \left[ V \left( x + \frac{i\hbar}{2} \nabla_p, t \right) - V \left( x - \frac{i\hbar}{2} \nabla_p, t \right) \right],
\]

models the impact of the electric field \( -\nabla_x V \) on the WDF. Here \( \hbar \) denotes Planck's constant. (See [3] for alternative definitions of \( \theta \).) The system (1) reduces to the classical Boltzmann transport equation in the classical limit for \( \hbar \to 0 \). However, for very small devices with an active region of the order of \( 10^{-8} m \), the system (1) is quite far from the classical regime [2].

In this paper we discuss the numerical solution of the Wigner - Poisson problem. In Section 2 we review a pseudospectral discretization of the Wigner - Poisson problem which was previously presented and analyzed in [4], [5]. In Section 3 we discuss the use of adaptive meshes in the context of this method to reduce the over all computational cost. In Section 4 we present some numerical results.

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

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2. Numerical method. Because of the definition of the pseudo differential operator $\theta$ in (1) via Fourier transforms, spectral methods using trigonometric basis functions are a natural choice for its discretization. Thus the WDF is approximated by

$$u(x, p, t) = \sum_{|\mu| \leq N} \tilde{u}(x, \mu, t) \exp(i\alpha \mu \cdot p),$$

where $\alpha$ denotes a small parameter. Choosing the values of $u$ at the collocation points $p_j = \frac{\pi}{\alpha N} j, j = (j_1, \ldots, j_d)$ as variables, we obtain the following discretization of $\theta$:

a) $\theta[V]u(x, p_j, t) = \sum_{|k| \leq N} A_{jk}(x, t)u(x, p_k, t)$

b) $A_{jk}(x, t) = (2N)^{-d} \sum_{|\mu| \leq N} \frac{i}{\hbar} \delta V\left( x, \frac{i\hbar}{2} \mu, t \right) \exp[i\alpha \mu \cdot (p_j - p_k)]$

c) $\delta V(x, z, t) := V(x + z, t) - V(x - z, t)$.

After truncation of the integral in (1)c) outside the cube $[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}]^d$ the charge density $n$ is given by

$$n(x, t) = \left( \frac{2\pi}{\alpha} \right)^d \tilde{u}(x, 0, t) = \left( \frac{\pi}{\alpha N} \right)^d \sum_{|k| \leq N} u(x, p_k, t).$$

This yields the mixed hyperbolic-elliptic systems

a) $\partial_t u_j + \frac{1}{m} p_j \cdot \nabla_x u_j - \sum_{|k| \leq N} A_{jk} u_k = 0, \quad u_j(x, t) := u(x, p_j, t)$

b) $-\epsilon \Delta_x V_E + q \left[ \left( \frac{\pi}{\alpha N} \right)^d \sum_{|k| \leq N} u(x, p_k, t) - D(x) \right] = 0$.

This system can be discretized by any standard discretization method for hyperbolic systems. Multiplication with the matrix $A$ in (6)a) can be performed in $O(N \log N)$ operations using FFT algorithms. It is important to notice that the matrix $A(x, t)$ is skew, i.e. that $x^* A x = 0$ holds for all vectors $x$. This implies that the Poisson equation can be solved on the previous time step without any additional step restriction [4].

To obtain convergence of the solution of (6) to the solution $w$ of the Wigner–Poisson problem (1) it is necessary to let the diameter of the simulation domain $[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}]^d$ tend to infinity together with the number of modes. From [5] we have the following theorem establishing a spectral order of convergence for finite but arbitrary time intervals.