Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 2198-5855

A class of stochastic algorithms for the Wigner equation

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submitted: March 15, 2016

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No. 2239
Berlin 2016

2010 *Mathematics Subject Classification.* 65C05, 60J25, 81Q05.

Key words and phrases. Wigner equation, stochastic algorithms, numerical experiments .

Edited by
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Abstract

A class of stochastic algorithms for the numerical treatment of the Wigner equation is introduced. The algorithms are derived using the theory of pure jump processes with a general state space. The class contains several new algorithms as well as some of the algorithms previously considered in the literature. The approximation error and the efficiency of the algorithms are analyzed. Numerical experiments are performed in a benchmark test case, where certain advantages of the new class of algorithms are demonstrated.

Contents

1 Introduction

The Wigner equation [24] has the form

$$\frac{\partial}{\partial t} f(t,x,k) + \frac{\hbar}{m} (k \cdot \nabla_x) f(t,x,k) = \int_{\mathbb{R}^d} V_W(x, k-k') f(t,x,k') \, dk' , \tag{1.1}$$

where $t > 0$ is time, $\mathbb{R}^d$ is the d-dimensional Euclidean space, $x \in \mathbb{R}^d$ is a position, $k \in \mathbb{R}^d$ is a wave-vector, $\hbar$ is Planck's constant (divided by 2π) and m is mass. The central dot denotes the scalar product and ∇ is the gradient. The initial condition is

$$f(0,x,k) \quad = \quad f_0(x,k) , \tag{1.2}$$

where f_0 is an integrable function. The solution f is real-valued, but not necessarily non-negative. It is related to the solution ψ of the Schrödinger equation

$$i\,\hbar \frac{\partial}{\partial t} \psi(t,x) = -\frac{\hbar^2}{2m} \Delta_x \psi(t,x) + V(x) \psi(t,x) ,$$

where i is the imaginary unit, V is potential energy and Δ denotes the Laplace operator. In particular, under some restrictions on ψ , the function f satisfies

$$\int_{\mathbb{R}^d} f(t,x,k) \, dk = |\psi(t,x)|^2 \qquad \forall\, t \geq 0 , \quad x \in \mathbb{R}^d . \tag{1.3}$$

The Wigner kernel V_W is determined via the relation

$$V_W(x,k) = \frac{1}{i\,\hbar\,(2\pi)^d} \int_{\mathbb{R}^d} \exp(-i\,k \cdot y) \, \left[V\left(x + \frac{y}{2}\right) - V\left(x - \frac{y}{2}\right) \right] dy . \tag{1.4}$$

It is real-valued and anti-symmetric with respect to k .

Over the last decade there has been a growing interest in modelling quantum effects in nanoelectronic devices. In this context, the Wigner equation (1.1) turned out to be convenient, since it can be coupled easily to the scattering part of the semiconductor Boltzmann equation (cf. [9, 8]). A "Wigner Monte Carlo method" has been developed for the numerical treatment of the equation. We refer to [4] for a recent description of the method, to [13] for more details (including a list of early references), and to the monograph [15] for an overview of the field. Deterministic numerical methods for the Wigner equation were studied, e.g., in [19, 1]. A comparison of deterministic and stochastic methods was given in [20].

The purpose of this paper is to introduce a class of stochastic algorithms for the numerical treatment of the Wigner equation (1.1). The algorithms are derived using the theory of pure jump processes with a general state space. The class contains several new algorithms as well as some of the algorithms previously considered in the literature. The approximation error and the efficiency of the algorithms are analyzed. Numerical experiments are performed in a benchmark test case, where certain advantages of the new class of algorithms are demonstrated.

The paper is organized as follows. The class of algorithms is introduced in Section 2. A detailed description is given and the connection with the Wigner equation is established. The results of numerical experiments are presented in Section 3. The approximation error with respect to several parameters is analyzed and various efficiency issues are studied. Finally, some comments are given in Section 4.

2 A class of stochastic algorithms

In this section we introduce a class of algorithms for the numerical treatment of the Wigner equation (1.1).

2.1 Description of the algorithms

The algorithms are based on a system of particles

$$\Big(u_j(t), x_j(t), k_j(t)\Big), \qquad j = 1, \ldots, N(t)\,, \qquad t \geq 0\,, \tag{2.1}$$

with a random time evolution. Each particle is characterized by a real-valued weight $u_j(t)$, a position $x_j(t) \in \mathbb{R}^d$ and a wave-vector $k_j(t) \in \mathbb{R}^d$.

Initial state

The initial state of the system (2.1) is chosen in such a way that it approximates the function $f_0 \in L^1(\mathbb{R}^d \times \mathbb{R}^d)$ in the initial condition (1.2). Let $N(0) = N_{\rm ini}$, with probability 1, where $N_{\rm ini}$ is the initial number of particles. The first particle is constructed as follows. Consider a probability density p on $\mathbb{R}^d \times \mathbb{R}^d$, which is strictly positive on the support of f_0. Generate $x_1(0)$ and $k_1(0)$ according to p. Under the conditions $x_1(0) = x$ and $k_1(0) = k$, define $u_1(0) = \frac{f_0(x,k)}{p(x,k)}$. Then one obtains

$$\mathbb{E}\Big(u_1(0)\,\varphi(x_1(0), k_1(0))\Big) \;=\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \varphi(x,k)\, f_0(x,k)\, dk\, dx\,, \tag{2.2}$$

where $\mathbb{E}$ denotes mathematical expectation and φ is an arbitrary bounded measurable function. The simplest choice is

$$p(x,k) \;=\; \frac{|f_0(x,k)|}{\|f_0\|_1}\,, \tag{2.3}$$

where $\|.\|_1$ denotes the L^1-norm. In this case, one obtains

$$u_1(0) \;=\; \|f_0\|_1 \,\mathrm{sign}\, f_0(x,k)\,. \tag{2.4}$$

If $\|f_0\|_1 = 1$, then the weight $u_1(0)$ (taking values $+1$ and -1) is called sign. Finally, particles with indices $j = 2, \ldots, N_{\rm ini}$ are independent copies of the first particle.

Time evolution

The time evolution of the system (2.1) contains both a continuous component (movement in the position space) and a jump component (creation of new particles). In addition, the total number of particles is controlled by a certain reduction procedure. A splitting time step Δt is used in order to separate the transport and the creation processes. The system (2.1) evolves from t to $t + \Delta t$ according to the following steps:

1. transport step

   All particles (u_j, x_j, k_j) move according to

$$x_j \quad \to \quad x_j + v(k_j)\,\Delta t\,, \tag{2.5}$$

   where (cf. (1.1))

$$v(k) \quad = \quad \frac{\hbar}{m}\,k\,, \qquad\qquad k \in \mathbb{R}^d\,. \tag{2.6}$$

   The components u_j and k_j do not change.

2. creation step

   According to probabilistic rules, all particles (u_j, x_j, k_j) create new particles that are added to the system (cf. Section 2.1.1).

3. cancellation step

   If the total number of particles exceeds a certain bound N_{canc} , then pairs of particles with similar positions and wave-vectors, but with opposite signs, are removed from the system (cf. Section 2.1.2).

Functionals

Functionals of the solution of the Wigner equation (1.1) are expressed in terms of the particle system (2.1) using the representation

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \varphi(x,k)\,f(t,x,k)\,dk\,dx \quad = \quad \frac{1}{N_{\mathrm{ini}}}\,\mathbb{E}\left(\sum_{j=1}^{N(t)} u_j(t)\,\varphi(x_j(t),k_j(t))\right), \tag{2.7}$$

where $t \geq 0$ and φ is an appropriate test function. Property (2.7) will be derived in Section 2.2. The case $t = 0$ follows from (2.2). Averaging over a number of independent repetitions is used to approximate the expectation on the right-hand side of (2.7) and to construct confidence intervals. Particular functionals of interest are the mean density

$$\varrho(t,x) \quad = \quad \int_{\mathbb{R}^d} f(t,x,k)\,dk\,, \tag{2.8}$$

the mean velocity (cf. (2.6))

$$\bar{v}(t,x) \quad = \quad \frac{1}{\varrho(t,x)}\int_{\mathbb{R}^d} v(k)\,f(t,x,k)\,dk \tag{2.9}$$

and the mean energy

$$\bar{\varepsilon}(t,x) \quad = \quad \frac{1}{\varrho(t,x)}\int_{\mathbb{R}^d} \varepsilon(k)\,f(t,x,k)\,dk\,, \tag{2.10}$$

where $\varepsilon(k) = \frac{m}{2}\,|v(k)|^2\,,\ k \in \mathbb{R}^d$. According to (2.7), the functionals (2.8)–(2.10) are approximated as

$$\int_{\mathbb{R}^d} g(k)\, f(t,x,k)\, dk \quad \sim \quad \frac{1}{|D(x)|\, N_{\rm ini}}\, \mathbb{E}\left(\sum_{j:\, x_j(t) \in D(x)} u_j(t)\, g(k_j(t)) \right),$$

where $g = 1, v, \varepsilon$ and $D(x)$ is a spatial cell containing x , with volume $|D(x)|$.

2.1.1 Creation procedures

Here we introduce two procedures for performing the creation step. One of them uses explicitly the Wigner kernel V_W , while the other needs only the expression for the potential energy V . A rigorous derivation of these procedures will be given in Section 2.2. Both procedures depend on some cutoff parameter $c > 0$, which assures finiteness of certain integrals with respect to the wave-vector. We introduce the notations

$$\mathbb{B}_d(c) = \{k \in \mathbb{R}^d \,:\, \|k\| \le c\} \qquad \text{and} \qquad C_d = \frac{1}{\hbar\, \pi^d}\,. \tag{2.11}$$

We assume that the potential energy is integrable,

$$I(V) := \int_{\mathbb{R}^d} |V(x)|\, dx \quad < \quad \infty\,. \tag{2.12}$$

The state of the particle system at the start of the creation step is denoted by

$$(u_j, x_j, k_j)\,, \qquad j = 1, \ldots, N\,. \tag{2.13}$$

Creation according to V_W

Let $\hat{V}_W$ be a function such that

$$|V_W(x,k)| \quad \le \quad \hat{V}_W(x,k) \qquad \forall\, x, k \in \mathbb{R}^d \tag{2.14}$$

and

$$\sup_{x \in \mathbb{R}^d} \hat{\gamma}(x,c) \quad < \quad \infty \qquad \forall\, c > 0\,, \tag{2.15}$$

where

$$\hat{\gamma}(x,c) \quad = \quad \frac{1}{2} \int_{\mathbb{B}_d(c)} \hat{V}_W(x,k)\, dk\,. \tag{2.16}$$

The splitting time step is assumed to satisfy

$$\Delta t \quad < \quad \left(\sup_{x \in \mathbb{R}^d} \hat{\gamma}(x,c) \right)^{-1}. \tag{2.17}$$

The creation step is performed (independently for each j) as follows:

2.1. With probability

$$1 - \hat{\gamma}(x_j, c)\,\Delta t\,, \tag{2.18}$$

do not create anything.

2.2. Otherwise, generate a random parameter $\tilde{k}$ according to the density

$$\frac{1}{2\,\hat{\gamma}(x_j, c)}\,\hat{V}_W(x_j, k)\,, \qquad k \in \mathbb{B}_d(c)\,. \tag{2.19}$$

2.3. With probability

$$1 - \frac{|V_W(x_j, \tilde{k})|}{\hat{V}_W(x_j, \tilde{k})}\,, \tag{2.20}$$

do not create anything.

2.4. Otherwise, create a pair of particles

$$\Big(\tilde{u}(u_j, x_j, \tilde{k}), x_j, k_j + \tilde{k}\Big), \Big(-\tilde{u}(u_j, x_j, \tilde{k}), x_j, k_j - \tilde{k}\Big), \tag{2.21}$$

where

$$\tilde{u}(u, x, k) = u\,\mathrm{sign} V_W(x, k)\,. \tag{2.22}$$

Example 2.1 *It follows from (1.4) that (cf. (2.11))*

$$V_W(x, k) \;\; = \;\; 2\,C_d \int_{\mathbb{R}^d} \sin(2\,k \cdot y)\,V(x - y)\,dy\,. \tag{2.23}$$

According to (2.12) and (2.23), a universal majorant satisfying (2.14) and (2.15) is

$$\hat{V}_W(x, k) \;\; = \;\; 2\,C_d\,I(V)\,. \tag{2.24}$$

The rate function (2.16) takes the form

$$\hat{\gamma}(x, c) \;\; = \;\; C_d\,I(V)\,|\mathbb{B}_d(c)|\,, \tag{2.25}$$

and (2.19) is the uniform density. The probability (2.20) takes the form

$$1 - \frac{1}{I(V)}\,\left|\int_{\mathbb{R}^d} \sin(2\,\tilde{k} \cdot y)\,V(x_j - y)\,dy\right|.$$

Creation according to V

Let $\hat{V}$ be a function such that (cf. (2.23))

$$2\,C_d\left|\sin(2\,k\cdot y)\,V(x-y)\right| \;\leq\; \hat{V}(x,y,k) \qquad \forall\, x,y,k\in\mathbb{R}^d \tag{2.26}$$

and

$$\sup_{x\in\mathbb{R}^d}\hat{\gamma}_V(x,c) \;<\; \infty \qquad \forall\, c>0\,, \tag{2.27}$$

where

$$\hat{\gamma}_V(x,c) \;=\; \frac{1}{2}\int_{\mathbb{B}_d(c)} dk \int_{\mathbb{R}^d} dy\,\hat{V}(x,y,k)\,. \tag{2.28}$$

The splitting time step is assumed to satisfy

$$\Delta t \;<\; \left(\sup_{x\in\mathbb{R}^d}\hat{\gamma}_V(x,c)\right)^{-1}. \tag{2.29}$$

The creation step is performed (independently for each j) as follows:

2.1. With probability

$$1-\hat{\gamma}_V(x_j,c)\,\Delta t\,, \tag{2.30}$$

do not create anything.

2.2. Otherwise, generate two random parameters $\tilde{x}$ and $\tilde{k}$ according to the density

$$\frac{1}{2\,\hat{\gamma}_V(x_j,c)}\,\hat{V}(x_j,y,k)\,, \qquad y\in\mathbb{R}^d\,, \quad k\in\mathbb{B}_d(c)\,. \tag{2.31}$$

2.3. With probability

$$1-\frac{2\,C_d\left|\sin(2\,\tilde{k}\cdot\tilde{x})\,V(x_j-\tilde{x})\right|}{\hat{V}(x_j,\tilde{x},\tilde{k})}\,, \tag{2.32}$$

do not create anything.

2.4. Otherwise, create a pair of particles

$$\Big(u'(u_j,x_j,\tilde{k},\tilde{x}),x_j,k_j+\tilde{k}\Big),\Big(-u'(u_j,x_j,\tilde{k},\tilde{x}),x_j,k_j-\tilde{k}\Big), \tag{2.33}$$

where

$$u'(u,x,k,y)=u\,\mathrm{sign}\Big[\sin(2\,k\cdot y)\,V(x-y)\Big]. \tag{2.34}$$

Example 2.2 *According to (2.12), a universal majorant satisfying (2.26) and (2.27) is*

$$\hat{V}(x,y,k) \;=\; 2\,C_d\,|V(x-y)|\,. \tag{2.35}$$

The rate function (2.28) takes the form

$$\hat{\gamma}_V(x,c) \;=\; C_d\,I(V)\,|\mathbb{B}_d(c)|\,, \tag{2.36}$$

which is identical to (2.25). It follows from (2.31) that $\tilde{k}$ is distributed uniformly on $\mathbb{B}_d(c)$, while $\tilde{x}$ is distributed according to the density $\frac{1}{I(V)}\,V(x_j-y)\,,\ y\in\mathbb{R}^d$ (cf. (2.12)). The probability (2.32) takes the form $1-|\sin(2\,\tilde{k}\cdot\tilde{x})|$.

2.1.2 Cancellation procedure

Here we introduce a procedure for performing the cancellation step. This procedure depends on a partition

$$\mathbb{R}^d \times \mathbb{R}^d \;=\; \bigcup_{l=1}^{L} S_l\,, \tag{2.37}$$

where $(S_l\,,\, l=1,\ldots,L)$ is a finite collection of disjoint subsets (e.g., rectangular cells, some of them being infinite). The idea is to remove pairs of particles with opposite signs, which belong to the same element of the partition. Let (2.13) be the state of the particle system at the start of the cancellation step. The cancellation step is performed as follows:

3.1. The number and the sign of the particles to be obtained in each cell is determined by summing up the corresponding particle signs,

$$\sigma_l \;=\; \sum_{j=1}^{N} u_j\, \chi_{S_l}(x_j,k_j)\,, \qquad l=1,\ldots,L\,,$$

where χ denotes the indicator function. The number of particles after cancellation is $|\sigma_l|$. These particles are positive, if $\sigma_l > 0$, and negative , if $\sigma_l < 0$.

3.2. Going again through the list, one keeps or removes particles until the necessary number is achieved in each cell. Formally, for $j=1,\ldots,N$, the following steps are performed:

- Define $l(j)$ such that $(x_j,k_j) \in S_{l(j)}$.
- If $|\sigma_{l(j)}| > 0$ and $u_j \neq \operatorname{sign}\sigma_{l(j)}$, then remove particle (u_j,x_j,k_j).
- Otherwise, keep the particle and replace $\sigma_{l(j)}$ by $\sigma_{l(j)} - u_j$.

The procedure is based on two loops over the list of all particles. Its generalization to the case of arbitrary particle weights (instead of signs) is rather straightforward.

2.2 Derivation of the creation procedures

Consider a particle system $z_j(t)\,,\;\; j=1,\ldots,N(t)\,,\;\; t\geq 0$, with the time evolution of a pure Markov jump process. Independently of each other, the particles create new particles that are added to the system. The creation rate and the offspring distribution are determined by some kernel q. Then the measures

$$\nu(t,dz) = \mathbb{E}\left(\sum_{j=1}^{N(t)} \delta_{z_j(t)}(dz)\right)$$

satisfy the equation

$$\frac{d}{dt}\int_{\mathbb{Z}} \psi(z)\,\nu(t,dz) \;=\; \int_{\mathbb{Z}} \nu(t,dz) \int_{\mathcal{Z}} q(z,d\xi)\Big[\psi(\xi_1)+\ldots+\psi(\xi_k)\Big], \tag{2.38}$$

where $\mathbb{Z}$ is the single particle state space, $\mathcal{Z} = \bigcup_{k=0}^{\infty} \mathbb{Z}^k$ is the space of offspring vectors, and the test functions ψ are continuous with compact support. Equation (2.38) is a straightforward consequence of Dynkin's formula, but also a simple corollary of the general results obtained in [2].

Consider

$$\mathbb{Z} = \mathbb{U} \times \mathbb{R}^d \times \mathbb{R}^d\,, \qquad z = (u, x, k)\,, \qquad \psi(z) = u\,\varphi(x, k) \tag{2.39}$$

and

$$f(t, dx, dk) = \int_{\mathbb{U}} u\,\nu(t, du, dx, dk)\,, \tag{2.40}$$

where $\mathbb{U}$ is a bounded subset of $\mathbb{R}$ (for example, $\mathbb{U} = \{-1, +1\}$). Then one obtains

$$\int_{\mathbb{Z}} \psi(z)\,\nu(t, dz) = \tag{2.41}$$
$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \varphi(x, k)\,f(t, dx, dk) = \mathbb{E}\left(\sum_{j=1}^{N(t)} u_j(t)\,\varphi(x_j(t), k_j(t))\right).$$

If q is such that

$$\int_{\mathbb{Z}} \nu(t, dz) \int_{\mathcal{Z}} q(z, d\xi)\Big[\psi(\xi_1) + \ldots + \psi(\xi_k)\Big] = \tag{2.42}$$
$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(t, dx, dk) \int_{\mathbb{R}^d} V_W^{(c)}(x, k' - k)\,\varphi(x, k')\,dk'\,,$$

where

$$V_W^{(c)}(x, k) \;=\; \begin{cases} V_W(x, k)\,, & \text{if} \quad \|k\| \le c\,, \\ 0 \qquad\;, & \text{otherwise}\,, \end{cases} \tag{2.43}$$

and $c > 0$ is a cutoff parameter, then (2.38) takes the form

$$\frac{d}{dt}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \varphi(x, k)\,f(t, dx, dk) = \tag{2.44}$$
$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(t, dx, dk) \int_{\mathbb{R}^d} V_W^{(c)}(x, k' - k)\,\varphi(x, k')\,dk'\,.$$

Equation (2.44) is a weak form of the Wigner equation (1.1) (for measure-valued functions and with cutoff in the Wigner kernel). Note that transport and creation processes are separated. Property (2.7) is a consequence of (2.41).

Finally, we provide two examples of creation kernels q satisfying (2.42).

Creation according to V_W

Consider the creation kernel (cf. (2.11))

$$\hat{q}(z, d\xi) = \frac{1}{2}\int_{\mathbb{B}_d(c)} dk'\,\hat{V}_W(x, k')\times \tag{2.45}$$
$$\left[\frac{|V_W(x, k')|}{\hat{V}_W(x, k')}\,\delta_{((\tilde{u}, x, k+k'), (-\tilde{u}, x, k-k'))}(d\xi) + \left(1 - \frac{|V_W(x, k')|}{\hat{V}_W(x, k')}\right)\delta_{\emptyset}(d\xi)\right],$$

where $z = (u, x, k)$, the function $\hat{V}_W$ satisfies (2.14), $\tilde{u} = \tilde{u}(u, x, k')$ is defined in (2.22), and $\emptyset$ denotes the empty vector. It follows from (1.4) that

$$V_W(x, -k) \;=\; -V_W(x, k) \qquad \forall\, x, k \in \mathbb{R}^d\,. \tag{2.46}$$

According to (2.39), (2.40) and (2.46), one obtains

$$\begin{aligned}
&\int_{\mathbb{Z}} \nu(t, dz) \int_{\mathcal{Z}} \hat{q}(z, d\xi) \Big[\psi(\xi_1) + \ldots + \psi(\xi_k)\Big] = \\
&\qquad \frac{1}{2} \int_{\mathbb{U}} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \nu(t, du, dx, dk) \int_{\mathbb{B}_d(c)} |V_W(x, k')|\, \tilde{u} \Big[\varphi(x, k + k') - \varphi(x, k - k')\Big] dk' \\
&= \; \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(t, dx, dk) \int_{\mathbb{B}_d(c)} V_W(x, k') \Big[\varphi(x, k + k') - \varphi(x, k - k')\Big] dk' \\
&= \; \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(t, dx, dk) \int_{\mathbb{R}^d} V_W^{(c)}(x, k' - k)\, \varphi(x, k')\, dk'
\end{aligned}$$

so that $\hat{q}$ satisfies (2.42). The procedure (2.18)–(2.22) is based on the kernel $\hat{q}$. Note that the creation rate (2.16) satisfies $\hat{\gamma}(x, c) = \hat{q}(z, \mathcal{Z})$.

Creation according to V

Consider the creation kernel (cf. (2.11))

$$\begin{aligned}
\hat{q}_V(z, d\xi) = \frac{1}{2} \int_{\mathbb{B}_d(c)} dk' \int_{\mathbb{R}^d} dy\, \hat{V}(x, y, k') \times \qquad\qquad (2.47)\\
\left[\frac{2\, C_d \Big| \sin(2\, k' \cdot y)\, V(x - y) \Big|}{\hat{V}(x, y, k')}\, \delta_{((u', x, k + k')(-u', x, k - k'))}(d\xi) + \right.\\
\left. \left(1 - \frac{2\, C_d \Big| \sin(2\, k' \cdot y)\, V(x - y) \Big|}{\hat{V}(x, y, k')} \right) \delta_{\emptyset}(d\xi) \right],
\end{aligned}$$

where $z = (u, x, k)$, the function $\hat{V}$ satisfies (2.26), $u' = u'(u, x, k', y)$ is defined in (2.34), and $\emptyset$ denotes the empty vector. According to (2.23), (2.39), (2.40) and (2.46), one obtains

$$\begin{aligned}
&\int_{\mathbb{Z}} \nu(t, dz) \int_{\mathcal{Z}} \hat{q}_V(z, d\xi) \Big[\psi(\xi_1) + \ldots + \psi(\xi_k)\Big] = \\
&\qquad C_d \int_{\mathbb{U}} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \nu(t, du, dx, dk) \int_{\mathbb{B}_d(c)} dk' \int_{\mathbb{R}^d} dy \times \\
&\qquad \Big| \sin(2\, k' \cdot y)\, V(x - y) \Big|\, u' \Big[\varphi(x, k + k') - \varphi(x, k - k')\Big] \\
&= \; C_d \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(t, dx, dk) \int_{\mathbb{B}_d(c)} dk' \int_{\mathbb{R}^d} dy \times \\
&\qquad \sin(2\, k' \cdot y)\, V(x - y) \Big[\varphi(x, k + k') - \varphi(x, k - k')\Big]
\end{aligned}$$

$$= \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(t,dx,dk)\int_{\mathbb{B}_d(c)} dk'\, V_W(x,k')\Big[\varphi(x,k+k')-\varphi(x,k-k')\Big]$$
$$= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(t,dx,dk)\int_{\mathbb{R}^d} V_W^{(c)}(x,k'-k)\,\varphi(x,k')\,dk'$$

so that $\hat{q}_V$ satisfies (2.42). The procedure (2.30)–(2.34) is based on the kernel (2.47). Note that the creation rate (2.28) satisfies $\hat{\gamma}_V(x,c) = \hat{q}_V(z,\mathcal{Z})$.

Remark 2.3 *It follows from (2.44) and the anti-symmetry of $V_W^{(c)}$ (cf. (2.43)) that the total mean density is constant,*

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(t,x,k)\,dk\,dx \;=\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f_0(x,k)\,dk\,dx \qquad \forall\, t\geq 0\,. \tag{2.48}$$

This conservation property is exactly reproduced by the algorithms, since always pairs of particles with opposite signs are created or cancelled.

2.3 Properties of the creation procedures

We study the average number of creations on a time step, as well as the average number of generations of auxiliary random parameters on a time step. The creation rate determines the number of particles and, thus, the number of cancellations. The generation rate determines the number of fictitious creation events (or, rejections) and influences the effort per creation event.

Creation according to V_W

Consider the creation procedure (2.18)–(2.22) with initial state (2.13). Let ξ_j be random variables taking the value 1, if a creation event took place for the particle with index $j = 1,\ldots,N$, and the value 0, otherwise. Let η_j be random variables taking the value 1, if a random parameter $\tilde{k}$ was generated, and the value 0, otherwise. One obtains

$$\mathbb{P}(\eta_j = 0) \;=\; 1-\hat{\gamma}(x_j,c)\,\Delta t \tag{2.49}$$

and

$$\mathbb{P}(\xi_j = 0\,|\,\eta_j = 1) = \tag{2.50}$$
$$\frac{1}{2\,\hat{\gamma}(x_j,c)}\int_{\mathbb{B}_d(c)} \hat{V}_W(x_j,k)\left[1-\frac{|V_W(x_j,k)|}{\hat{V}_W(x_j,k)}\right]dk = 1-\frac{\gamma(x_j,c)}{\hat{\gamma}(x_j,c)}\,,$$

where

$$\gamma(x,c) \;=\; \frac{1}{2}\int_{\mathbb{B}_d(c)} |V_W(x,k)|\,dk\,. \tag{2.51}$$

It follows from (2.49) and (2.50) that

$$\mathbb{P}(\xi_j = 1) = \mathbb{P}(\xi_j = 1\,|\,\eta_j = 1)\,\mathbb{P}(\eta_j = 1) \;=\; \gamma(x_j,c)\,\Delta t\,. \tag{2.52}$$

According to (2.49) and (2.52), one obtains

$$\mathbb{E}\left(\sum_{j=1}^{N}\varphi(x_j)\,\xi_j\right) \;=\; \Delta t\sum_{j=1}^{N}\varphi(x_j)\,\gamma(x_j,c) \tag{2.53}$$

and

$$\mathbb{E}\left(\sum_{j=1}^{N}\varphi(x_j)\,\eta_j\right) \;=\; \Delta t\sum_{j=1}^{N}\varphi(x_j)\,\hat{\gamma}(x_j,c)\,, \tag{2.54}$$

respectively, where φ is some test function.

Let $D(x)$ be a spatial cell containing $x\in\mathbb{R}^d$. Then (2.53), with $\varphi=\chi_{D(x)}$, where χ denotes the indicator function, implies

$$\mathbb{E}\left(\sum_{j=1}^{N}\chi_{D(x)}(x_j)\,\xi_j\right) \;\sim\; \gamma(x,c)\,\Delta t\sum_{j=1}^{N}\chi_{D(x)}(x_j) \tag{2.55}$$

so that $\gamma(x,c)$ determines the average number of creations per particle and per unit time in the cell $D(x)$. Analogously, (2.54) implies

$$\mathbb{E}\left(\sum_{j=1}^{N}\chi_{D(x)}(x_j)\,\eta_j\right) \;\sim\; \hat{\gamma}(x,c)\,\Delta t\sum_{j=1}^{N}\chi_{D(x)}(x_j) \tag{2.56}$$

so that $\hat{\gamma}(x,c)$ determines the average number of $\tilde{k}$-generations per particle and per unit time in the cell $D(x)$. According to (2.55) and (2.56), the quantity

$$\frac{\hat{\gamma}(x,c)}{\gamma(x,c)} \;\sim\; \frac{\mathbb{E}\left(\sum_{j=1}^{N}\chi_{D(x)}(x_j)\,\eta_j\right)}{\mathbb{E}\left(\sum_{j=1}^{N}\chi_{D(x)}(x_j)\,\xi_j\right)} \tag{2.57}$$

determines the average number of $\tilde{k}$-generations per creation event in the cell $D(x)$.

Creation according to V

Consider the creation procedure (2.30)–(2.34) with initial state (2.13). In analogy with (2.49) and (2.52), one obtains $\mathbb{P}(\eta_j=1)=\hat{\gamma}_V(x_j,c)\,\Delta t$ and $\mathbb{P}(\xi_j=1)=\gamma_V(x_j,c)\,\Delta t$, where

$$\gamma_V(x,c) \;=\; C_d\int_{\mathbb{B}_d(c)}dk\int_{\mathbb{R}^d}dy\,\Big|\sin(2\,k\cdot y)\,V(x-y)\Big|. \tag{2.58}$$

Note that (cf. (2.23), (2.51))

$$\gamma(x,c)=C_d\int_{\mathbb{B}_d(c)}dk\left|\int_{\mathbb{R}^d}dy\,\sin(2\,k\cdot y)\,V(x-y)\right| \;\le\; \gamma_V(x,c)\,. \tag{2.59}$$

Remark 2.4 *Here we discuss the effect of using an acceptance-rejection technique in the creation procedure (2.18)–(2.22). With the trivial majorant*

$$\hat{V}_W(x,k) \;=\; |V_W(x,k)|\,, \tag{2.60}$$

the procedure simplifies as follows:

2.1. With probability (cf. (2.51))

$$1-\gamma(x_j,c)\,\Delta t\,, \tag{2.61}$$

do not create anything.

2.2. Otherwise, generate a random parameter $\tilde{k}$ according to the density

$$\frac{1}{2\,\gamma(x_j,c)}\,|V_W(x_j,k)|\,, \qquad k\in\mathbb{B}_d(c)\,. \tag{2.62}$$

2.3. Create a pair of particles (2.21).

In order to generate a sample according to the density (2.62), the acceptance-rejection method can be applied. When using a majorant $\hat{V}_W$ satisfying (2.14), then $\tilde{k}$ is generated according to the density (2.19) and accepted with probability

$$\frac{|V_W(x_j,\tilde{k})|}{\hat{V}_W(x_j,\tilde{k})}\,. \tag{2.63}$$

According to (2.61), the creation rate is γ . According to (2.19) and (2.63), the total acceptance probability is

$$\frac{1}{2\,\hat{\gamma}(x_j,c)}\int_{\mathbb{B}_d(c)}|V_W(x_j,k)|\,dk \;=\; \frac{\gamma(x_j,c)}{\hat{\gamma}(x_j,c)}\,. \tag{2.64}$$

Since the number of trials to get one success has geometric distribution with parameter (2.64), the average number of $\tilde{k}$-generations per creation event is determined by the function

$$\frac{\hat{\gamma}(x,c)}{\gamma(x,c)}\,. \tag{2.65}$$

Thus, according to (2.57) and (2.65), the creation effort remains the same, when an acceptance-rejection technique is used instead of fictitious creation events.

Remark 2.5 *Here we discuss the effect of using the positive part of the Wigner kernel V_W in the creation procedure (2.18)–(2.22). With the majorant (2.60), the creation kernel (2.45) takes the form*

$$q(z,d\xi) \;=\; \frac{1}{2}\int_{\mathbb{B}_d(c)} dk'\,|V_W(x,k')|\,\delta_{((\tilde{u},x,k+k'),(-\tilde{u},x,k-k'))}(d\xi)$$

$$
\begin{aligned}
&= \frac{1}{2}\int_{\mathbb{B}_d(c)} dk' \Big[V_W^+(x,k') + V_W^-(x,k')\Big]\,\delta_{((\tilde{u},x,k+k'),(-\tilde{u},x,k-k'))}(d\xi) \\
&= \frac{1}{2}\int_{\mathbb{B}_d(c)} dk'\, V_W^+(x,k')\,\delta_{((u,x,k+k'),(-u,x,k-k'))}(d\xi) + \\
&\quad \frac{1}{2}\int_{\mathbb{B}_d(c)} dk'\, V_W^-(x,k')\,\delta_{((-u,x,k+k'),(u,x,k-k'))}(d\xi) \\
&= \int_{\mathbb{B}_d(c)} dk'\, V_W^+(x,k')\,\delta_{((u,x,k+k'),(-u,x,k-k'))}(d\xi)\,, \qquad (2.66)
\end{aligned}
$$

where V_W^+ and V_W^- denote the positive and the negative part of V_W . Note that (cf. (2.46))

$$V_W^+(x,k) \;=\; V_W^-(x,-k) \qquad \forall\, x,k \in \mathbb{R}^d$$

and (cf. (2.51))

$$\int_{\mathbb{B}_d(c)} V_W^+(x,k)\,dk = \int_{\mathbb{B}_d(c)} V_W^-(x,k)\,dk \;=\; \gamma(x,c)\,.$$

The representation (2.66) of the creation kernel suggests the following procedure:

2.1. With probability (2.61), do not create anything.

2.2. Otherwise, generate a random parameter $\tilde{k}$ according to the density

$$\frac{1}{\gamma(x_j,c)}\,V_W^+(x_j,k)\,, \qquad k \in \mathbb{B}_d(c)\,.$$

2.3. Create a pair of particles $(u,x,k+\tilde{k})\,,\ (-u,x,k-\tilde{k})\,.$

When using an acceptance-rejection technique with a majorant $\hat{V}_W$ satisfying (2.14), then $\tilde{k}$ is generated according to the density (2.19) and accepted with probability

$$\frac{V_W^+(x_j,\tilde{k})}{\hat{V}_W(x_j,\tilde{k})}\,. \qquad (2.67)$$

According to (2.61), the creation rate remains γ . According to (2.19) and (2.67), the total acceptance probability takes the form

$$\frac{1}{2\,\hat{\gamma}(x_j,c)}\int_{\mathbb{B}_d(c)} V_W^+(x_j,k)\,dk \;=\; \frac{\gamma(x_j,c)}{2\,\hat{\gamma}(x_j,c)}\,,$$

which is half of the quantity (2.64). The average number of $\tilde{k}$-generations per creation event is determined by the function

$$\frac{2\,\hat{\gamma}(x,c)}{\gamma(x,c)}\,. \qquad (2.68)$$

Thus, according to (2.65) and (2.68), the creation effort doubles, when using the function V_W^+ instead of $|V_W|$.

3 Numerical studies

In this section we consider a benchmark test case. Several of the algorithms introduced in Section 2 are used to estimate functionals of the solution of the Wigner equation (1.1).

3.1 Test case

We consider the example of a one-dimensional potential barrier, where $d = 1$ and

$$V(x) \;=\; a\,\chi_{[-b/2,b/2]}(x)\,, \qquad x \in \mathbb{R}\,, \qquad \text{for some} \quad a, b > 0\,. \tag{3.1}$$

In this case, an explicit expression of the Wigner kernel is available,

$$V_W(x,k) \;=\; \frac{2\,a}{\hbar\,\pi\,k}\sin(2\,k\,x)\,\sin(k\,b)\,, \qquad x, k \in \mathbb{R}\,. \tag{3.2}$$

Moreover, there exists an analytic solution for the corresponding Schrödinger equation [10] so that benchmark curves can be obtained via (1.3). We describe three algorithms for the creation step that are adapted to the test case (3.1). Note that both the transport step (cf. (2.5)) and the cancellation step are independent of the specific form of V .

Algorithm 1

This algorithm is based on Example 2.1. According to (2.11) and (2.12), one obtains

$$|\mathbb{B}_d(c)| = 2\,c\,, \qquad I(V) = a\,b\,, \qquad C_d = \frac{1}{\hbar\,\pi}\,. \tag{3.3}$$

The majorant (2.24) takes the form $\hat{V}_W(x,k) = \frac{2\,a\,b}{\hbar\,\pi}$ and the rate function (2.25) is

$$\hat{\gamma}(x,c) \;=\; \frac{2\,a\,b\,c}{\hbar\,\pi}\,. \tag{3.4}$$

The condition (2.17) on the splitting time step is

$$\Delta t \;<\; \frac{\hbar\,\pi}{2\,a\,b\,c}\,. \tag{3.5}$$

The algorithm (2.18)–(2.22) takes the form:

2.1. With probability

$$1 - \frac{2\,a\,b\,c}{\hbar\,\pi}\;\Delta t\,, \tag{3.6}$$

do not create anything.

2.2. Otherwise, generate a random parameter $\tilde{k}$ uniformly on the interval $[-c, c]$.

2.3. With probability

$$1 - \left| \sin(2\,\tilde{k}\,x_j)\,\frac{\sin(\tilde{k}\,b)}{\tilde{k}\,b} \right|,$$

do not create anything.

2.4. Otherwise, create a pair of particles

$$\Big(\tilde{u}, x_j, k_j + \tilde{k}\Big), \Big(-\tilde{u}, x_j, k_j - \tilde{k}\Big)\,, \tag{3.7}$$

where

$$\tilde{u} = u_j\,\mathrm{sign}\left[\frac{\sin(2\,\tilde{k}\,x_j)\,\sin(\tilde{k}\,b)}{\tilde{k}}\right].$$

Algorithm 2

This algorithm is based on a more sophisticated choice of the majorant $\hat{V}_W$ in (2.14), which takes into account the specific form (3.2) of the Wigner kernel V_W . Namely, we consider

$$\hat{V}_W(x,k) \;\;=\;\; \frac{2\,a}{\pi\,\hbar}\,\min\left(b, \frac{1}{|k|}\right). \tag{3.8}$$

We assume $b\,c > 1$, since otherwise algorithm 2 would be identical to algorithm 1. The rate function (2.16) takes the form

$$\hat{\gamma}(x,c) = \int_0^c \hat{V}_W(x,k)\,dk = \tag{3.9}$$
$$\frac{2\,a}{\pi\,\hbar}\left[\int_0^{1/b} b\,dk + \int_{1/b}^{c}\frac{1}{k}\,dk\right] = \frac{2\,a}{\pi\,\hbar}\,[1+\log(b\,c)]\,.$$

The condition (2.17) on the splitting time step is $\Delta t < \frac{\hbar\,\pi}{2\,a\,[1+\log(b\,c)]}$, which is less restrictive than (3.5). The algorithm (2.18)–(2.22) takes the form:

2.1. With probability

$$1 - \frac{2\,a}{\pi\,\hbar}\,[1+\log(b\,c)]\,\Delta t\,,$$

do not create anything.

2.2. Otherwise, generate a random parameter $\tilde{k}$ according to the density

$$\frac{1}{2\,[1+\log(b\,c)]}\,\min\left(b, \frac{1}{|k|}\right), \qquad k \in [-c, c]\,. \tag{3.10}$$

2.3. With probability

$$1 - \frac{|\sin(2\,\tilde{k}\,x_j)\,\sin(\tilde{k}\,b)|}{\min\Big(|\tilde{k}|\,b, 1\Big)}\,,$$

do not create anything.

2.4. Otherwise, create a pair of particles (3.7).

The generation according to the density (3.10) is performed using the inverse transform method. Due to the symmetry of the function (3.8), one first obtains some $k' \in [0, c]$ by solving the equation

$$\frac{1}{1+\log(b\,c)} \int_0^{k'} \min\left(b, \frac{1}{|k|}\right) dk \;\; = \;\; r\,, \tag{3.11}$$

where r is a uniform random number from $[0, 1]$, and then defines $\tilde{k} = \pm\, k'$, where the sign plus or minus is chosen with equal probability. Since

$$\int_0^{k'} \min\left(b, \frac{1}{|k|}\right) dk \;\; = \;\; \left\{ \begin{array}{rl} b\,k'\,, & \text{if} \quad b\,k' \le 1\,, \\ 1+\log(b\,k')\,, & \text{if} \quad b\,k' > 1\,, \end{array} \right.$$

equation (3.11) implies

$$k' = \frac{r\,[1+\log(b\,c)]}{b}\,, \qquad \text{if} \qquad r \;\le\; \frac{1}{1+\log(b\,c)}\,,$$

and

$$k' = \frac{\exp\Big(r\,[1+\log(b\,c)]-1\Big)}{b}\,, \qquad \text{if} \qquad r \;>\; \frac{1}{1+\log(b\,c)}\,.$$

Algorithm 3

This algorithm is based on Example 2.2. According to (3.3), the majorant (2.35) takes the form

$$\hat{V}(x, y, k) \;\; = \;\; \frac{2\,a}{\hbar\,\pi}\,\chi_{[-b/2,b/2]}(x-y)\,.$$

The rate function (2.36) is identical to (3.4) so that the condition (2.29) on the splitting time step is (3.5). The algorithm (2.30)–(2.34) takes the form:

2.1. With probability (3.6), do not create anything.

2.2. Otherwise, generate two uniformly distributed parameters

$$\tilde{k} \in [-c, c] \qquad \text{and} \qquad \tilde{x} \in [x_j - b/2, x_j + b/2]\,.$$

2.3. With probability $1 - |\sin(2\,\tilde{k}\,\tilde{x})|$, do not create anything.

2.4. Otherwise, create a pair of particles

$$\Big(u', x_j, k_j + \tilde{k}\Big), \Big(-u', x_j, k_j - \tilde{k}\Big), \quad \text{where} \quad u' = u_j\,\text{sign}\Big[\sin(2\,\tilde{k}\,\tilde{x})\Big].$$

Initial state

We consider (cf. (1.2))

$$f_0(x,k) \;=\; \frac{1}{\pi\,\sigma_1\,\sigma_2}\,\exp\left(-\frac{(x-x_0)^2}{\sigma_1^2}\right)\,\exp\left(-\frac{(k-k_0)^2}{\sigma_2^2}\right), \tag{3.12}$$

where $x_0, k_0 \in \mathbb{R}$ and $\sigma_1, \sigma_2 > 0$. According to (2.8)–(2.10), one obtains the initial mean density

$$\varrho(0,x) \;=\; \frac{1}{\sqrt{\pi}\,\sigma_1}\,\exp\left(-\frac{(x-x_0)^2}{\sigma_1^2}\right), \qquad x \in \mathbb{R}\,,$$

and the (constant) initial mean velocity and energy

$$\bar{v}(0,x) = v(k_0)\,, \qquad \bar{\varepsilon}(0,x) = \frac{\hbar^2}{2\,m}\left(\frac{\sigma_2^2}{2} + k_0^2\right) = \varepsilon(k_0) + \frac{\hbar^2\,\sigma_2^2}{4\,m}\,. \tag{3.13}$$

Asymptotic values of the creation rates

According to (3.2), the creation rate (2.51) (related to creation according to V_W) takes the form

$$\gamma(x,c) \;=\; \frac{2\,a}{\hbar\,\pi}\int_0^c \frac{1}{k}\,|\sin(2\,k\,x)\,\sin(k\,b)|\,dk\,. \tag{3.14}$$

According to (3.1) and (3.3), the creation rate (2.58) (related to creation according to V) takes the form

$$\gamma_V(x,c) \;=\; \frac{2\,a}{\hbar\,\pi}\int_0^c dk \int_{x-b/2}^{x+b/2} dy\,|\sin(2\,k\,y)|\,. \tag{3.15}$$

Note that

$$\lim_{x\to\infty}\int_\alpha^\beta |\sin(k\,x)|\,g(k)\,dk \;=\; \frac{2}{\pi}\int_\alpha^\beta g(k)\,dk \qquad \forall\,\alpha<\beta\in\mathbb{R}\,, \tag{3.16}$$

for any continuous function g. Indeed, one obtains

$$\begin{aligned}\int_\alpha^\beta |\sin(k\,x)|\,dk \;&\sim\; \int_0^{\beta-\alpha} |\sin(k\,x)|\,dk \;=\; \frac{1}{x}\int_0^{(\beta-\alpha)\,x} |\sin(k)|\,dk \\ &\sim\; \frac{1}{\pi\,x}\int_0^{(\beta-\alpha)\,\pi\,x} |\sin(k)|\,dk \;\sim\; \frac{(\beta-\alpha)\,x}{\pi\,x}\int_0^{\pi} |\sin(k)|\,dk\,,\end{aligned}$$

which implies (3.16) with $g=1$. The general case is a consequence of

$$\begin{aligned}\lim_{x\to\infty}\int_\alpha^\beta |\sin(k\,x)|\,g(k)\,dk \;&\sim\; \sum_j g(k_j)\left(\lim_{x\to\infty}\int_{k_j}^{k_{j+1}} |\sin(k\,x)|\,dk\right) \\ &=\; \frac{2}{\pi}\sum_j g(k_j)\,(k_{j+1}-k_j)\,.\end{aligned}$$

It follows from (3.14)–(3.16) that

$$\gamma(\infty, c) := \lim_{x\to\infty} \gamma(x, c) = \frac{4\,a}{\hbar\,\pi^2} \int_0^c \frac{1}{k}\,|\sin(k\,b)|\,dk = \frac{4\,a}{\hbar\,\pi^2} \int_0^{b\,c} \frac{1}{k}\,|\sin k|\,dk \tag{3.17}$$

and

$$\gamma_V(\infty, c) := \lim_{x\to\infty} \gamma_V(x, c) \;=\; \frac{4\,a\,b\,c}{\hbar\,\pi^2}\,. \tag{3.18}$$

3.2 Approximation error

Here we study the approximation error of the algorithms described in Section 3.1. There is an error depending on the time step Δt, which is used to separate transport and creation processes. Another source of error is the cutoff parameter c, which makes the creation rate finite. The main approximation parameter related to the cancellation step is the partition (2.37). For simplicity, we use symmetric domains $[-x_{\max}, x_{\max}]$ and $[-k_{\max}, k_{\max}]$, which are divided into N_x and N_k equal subintervals. The total cancellation error also depends on the initial number of particles N_{ini} and on the cancellation bound N_{canc}, which influence the frequency of cancellations. Note that, due to cancellation, there is no longer independence with respect to the initial particles.

In the figures we illustrate the approximation error by comparing the numerical results with the analytic solution for the density (2.8) (cf. (1.3) and [10]). The illustrations are provided for algorithm 2. The results obtained by algorithms 1 and 3 are quite similar. These algorithms differ mostly with respect to their efficiency, which will be studied in Section 3.3.

Specification of the parameters

The parameters of the initial state (3.12) are

$$x_0 = -6\,\text{nm}\,, \qquad k_0 = 0.46\,\text{nm}^{-1}\,, \qquad \sigma_1 = 1\,\text{nm}\,, \qquad \sigma_2 = 1\,\text{nm}^{-1}\,. \tag{3.19}$$

The choice of k_0 is motivated by the assumption of an initial Maxwellian velocity distribution with temperature $T = 300\,\text{K}$, since $v(k_0) = \sqrt{\frac{2\,k_B\,T}{m}}$ (cf. (2.6)). Note that

$$\begin{aligned} &\hbar = 6.58 \times 10^{-16}\,\text{eV s}\,, \qquad k_B = 1.38 \times 10^{-23}\,\text{kg m}^2\,\text{s}^{-2}\,\text{K}^{-1}\,, \\ &m = 0.32\,m_e\,, \qquad m_e = 9.11 \times 10^{-31}\,\text{kg}\,, \\ &1\,\text{eV} = 1.60 \times 10^{-19}\,\text{kg m}^2\,\text{s}^{-2}\,, \qquad 1\,\text{nm} = 10^{-9}\,\text{m}\,, \qquad 1\,\text{fs} = 10^{-15}\,\text{s}\,. \end{aligned} \tag{3.20}$$

According to (3.19), the quantities (3.13) take the values

$$\begin{aligned} \bar v(0,x) &= 0.36\,\text{nm/fs} \times k_0 = 0.166\,\text{nm/fs} \\ \bar\varepsilon(0,x) &= 0.119\,\text{eV nm}^2 \times \left(\frac{\sigma_2^2}{2} + k_0^2\right) = 0.085\,\text{eV}\,. \end{aligned} \tag{3.21}$$

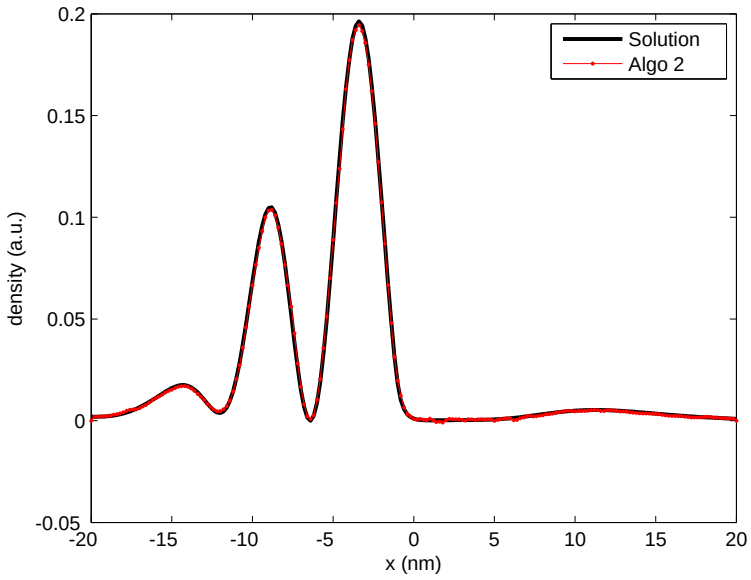

Figure 1: Mean density (2.8) for $t = 30\,\mathrm{fs}$, calculated with parameters (3.23)

The height and the width of the potential barrier (3.1) are

$$a = 0.3\,\mathrm{eV}\,, \qquad b = 2.14\,\mathrm{nm}\,. \tag{3.22}$$

The parameters of the algorithms are

$$\begin{aligned} &\Delta t = 0.05\,\mathrm{fs}\,, \quad c = 7.68\,\mathrm{nm}^{-1}\,, \quad N_{\mathrm{ini}} = 160000\,, \quad N_{\mathrm{canc}} = 480000\,, \\ &x_{\max} = 20\,\mathrm{nm}\,, \quad N_x = 200\,, \quad k_{\max} = 7.78\,\mathrm{nm}^{-1}\,, \quad N_k = 256\,. \end{aligned} \tag{3.23}$$

The final time is $t = 30\,\mathrm{fs}$ so that a particle starting at x_0 with velocity (3.21) reaches the barrier (cf. (3.19), (3.22)). The number of repetitions is $N_{\mathrm{rep}} = 100$. The results for this set of parameters, with $N_{x,\mathrm{obs}} = 201$ observation points in the x-direction, are shown in **Figure 1**. There is no visible deviation of the numerical approximation from the analytic curve.

Time step error

Numerical results have been obtained for $\Delta t = 0.2\,\mathrm{fs}$ and $\Delta t = 0.1\,\mathrm{fs}$, with all other parameters given in (3.23). The corresponding figure is not shown, since there is almost no visible deviation of the numerical approximations from the analytic solution. Note that the upper bound for the splitting time step in (3.5) takes the form (cf. (3.20), (3.22))

$$\Delta t_{\max}(c) = \frac{\hbar\,\pi}{2\,a\,b\,c} = \frac{3.45}{b\,c}\,\mathrm{fs} \quad = \quad 0.21\,\mathrm{fs}\,. \tag{3.24}$$

Taking the limit $\Delta t \to 0$ is possible without any restriction on the other parameters.

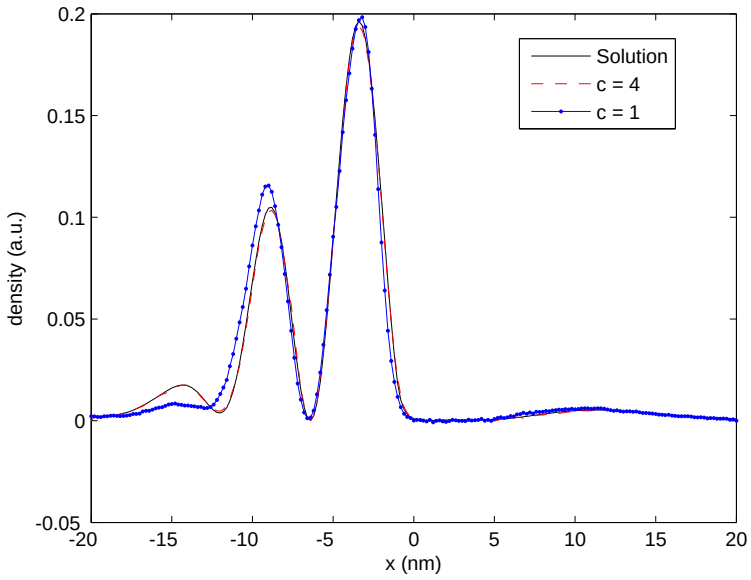

Figure 2: Mean density (2.8) for $t = 30\,\mathrm{fs}$, calculated with parameters (3.23) and different cutoffs

Cutoff error

Numerical results for $c = 1\,\mathrm{nm}^{-1}$ and $c = 4\,\mathrm{nm}^{-1}$, with all other parameters given in (3.23), are shown in **Figure 2**. There is a visible deviation of the first curve from the analytic solution, while the other curve is quite close. Note that taking the limit $c \to \infty$ separately from the other parameters is not possible. In particular, the upper bound on the splitting time step in condition (3.24) goes to zero. Moreover, with increasing c, the number of particles grows rapidly. Thus, even with an infinitesimally small time step, one would get more and more cancellations.

Cancellation error

We do not present numerical results concerning the dependence of the approximation error on the cancellation grid. Note that taking the limits $x_{\max}, k_{\max}, N_x, N_k \to \infty$ does not make sense. If the grid is too fine, the effect of cancellation will vanish, which leads to a blow-up of the particle system. On the other hand, if the grid is too coarse, then the error will become big. While the general picture is clear, a detailed study of the influence of the cancellation grid on the approximation error would be rather involved and might be the subject of a separate paper. The behaviour of the total k-density can be measured in order to determine an appropriate asymmetric domain $[k_{\min}, k_{\max}]$. A non-uniform grid can be used and adapted to the behaviour of the solution.

An interesting observation concerns the influence of the initial particle number on the approximation error. A modification of the cancellation procedure, with uniform regeneration of particles, is used in the literature (cf. [4]). It turns out that this version creates an additional error. Numerical results for the parameters (3.23), as well as for $N_{\mathrm{ini}} = 32000$, are shown in

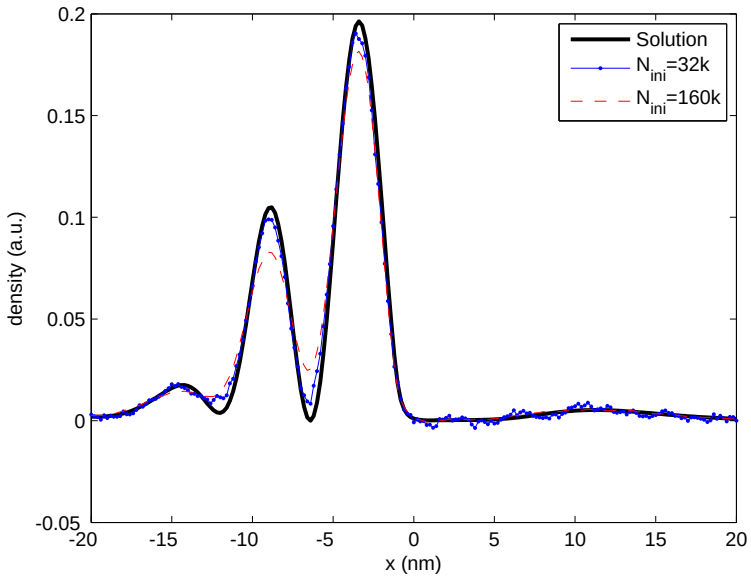

Figure 3: Mean density (2.8) for $t = 30\,\mathrm{fs}$, calculated with a modified cancellation procedure (uniform regeneration of particles), parameters (3.23) and a different initial particle number

Figure 3. There is a visible deviation of the numerical approximations from the analytic solution. Moreover, the error increases with increasing N_{ini}.

3.3 Efficiency issues

Here we study several issues related to the efficiency of the algorithms described in Section 3.1. Their effort (measured in terms of CPU time) depends on the various components (transport, creation, cancellation) and on the overhead (as, e.g., calculation of functionals). The part of the effort related to the transport step is inversely proportional to the splitting time step. The part of the effort related to creation and cancellation is asymptotically independent of the time step.

3.3.1 Creation effort

We obtain approximate expressions for several quantities related to the creation effort by using the asymptotic values (3.17), (3.18) of the creation rates. This approximation is justified by the fact that most of the particles are concentrated in the region, where the rate function is almost constant (cf. **Figure 4**). According to (2.53) (with $\varphi = 1$), the average number of creation events on Δt is

$$\Delta t \sum_{j=1}^{N} \gamma(x_j, c) \quad \sim \quad \Delta t\, N\, \gamma(\infty, c)\,. \tag{3.25}$$

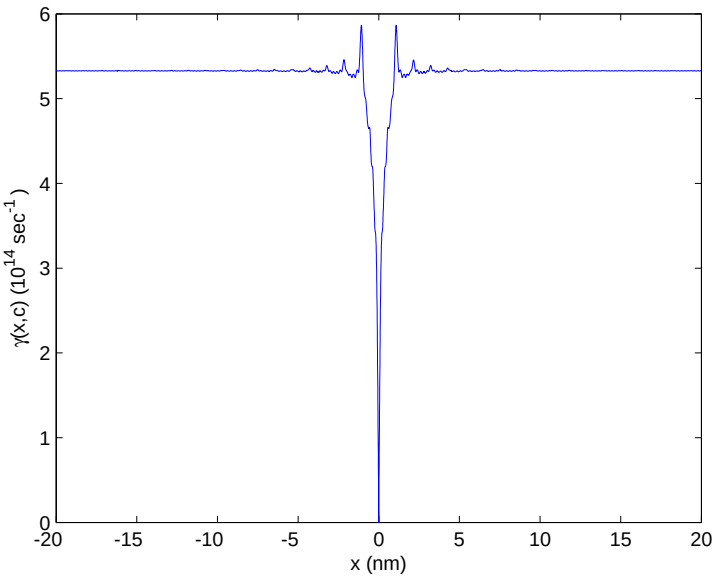

Figure 4: Rate function (3.14), with parameters (3.22) and (3.23)

Since the number of particles increases by 2 during each creation event, the average number of particles after Δt is

$$\mathbb{E}\, N(\Delta t, c) \;=\; N(0)\,(1 + 2\,\Delta t\,\gamma(\infty, c))\,.$$

With $\Delta t = t/K$, one obtains the average number of particles at time t ,

$$\mathbb{E}\, N(t, c) \;=\; \lim_{K\to\infty} N(0)\,(1 + 2\,\Delta t\,\gamma(\infty, c))^K = N(0)\,\exp(2\,t\,\gamma(\infty, c))\,, \quad (3.26)$$

and the average number of creation events up to time t (cf. (3.25)),

$$\begin{aligned} C(t, c) \;&=\; \gamma(\infty, c) \lim_{K\to\infty} \Big[\Delta t\; N(0) + \Delta t\; \mathbb{E}\, N(\Delta t, c) + \Delta t\; \mathbb{E}\, N(2\,\Delta t, c) + \ldots\Big] \\ &=\; \gamma(\infty, c) \int_0^t \mathbb{E}\, N(s, c)\, ds\,. \end{aligned} \quad (3.27)$$

It follows from (3.26) and (3.27) that

$$\int_0^t \mathbb{E}\, N(s, c)\, ds \;=\; \frac{N(0)}{2\,\gamma(\infty, c)}\Big(\exp(2\,\gamma(\infty, c)\,t) - 1\Big)$$

and

$$C(t, c) \;=\; \frac{N(0)}{2}\Big(\exp(2\,\gamma(\infty, c)\,t) - 1\Big). \quad (3.28)$$

Analogously, the average number of generation events up to time t is

$$\begin{aligned} &G(t, c) = \\ &\quad \hat\gamma(\infty, c) \int_0^t \mathbb{E}\, N(s, c)\, ds = \frac{N(0)}{2}\,\frac{\hat\gamma(\infty, c)}{\gamma(\infty, c)}\Big(\exp(2\,\gamma(\infty, c)\,t) - 1\Big). \end{aligned} \quad (3.29)$$

According to (3.28) and (3.29), the expression

$$\frac{G(t,c)}{C(t,c)} \;=\; \frac{\hat{\gamma}(\infty,c)}{\gamma(\infty,c)} \tag{3.30}$$

corresponds to the average number of generation events per creation event.

Now we specify expression (3.30) for the various algorithms. It follows from (3.4) and (3.9) that

$$\hat{\gamma}^{(1)}(\infty,c) = \hat{\gamma}_V(\infty,c) = \frac{2\,a\,b\,c}{\hbar\,\pi} \tag{3.31}$$

and

$$\hat{\gamma}^{(2)}(\infty,c) = \frac{2\,a\,(1+\log(b\,c))}{\hbar\,\pi}\,, \qquad \text{if} \quad b\,c \geq 1\,, \tag{3.32}$$

where the superscripts refer to the algorithms 1 and 2, respectively. According to (3.17), (3.18), (3.31) and (3.32), one obtains

$$\frac{\hat{\gamma}^{(1)}(\infty,c)}{\gamma(\infty,c)} = \frac{\pi\,b\,c}{2\,g(b\,c)}\,, \qquad \text{where} \quad g(x) = \int_0^x \frac{1}{k}\,|\sin k|\,dk\,, \tag{3.33}$$

$$\frac{\hat{\gamma}^{(2)}(\infty,c)}{\gamma(\infty,c)} = \frac{\pi\,(1+\log(b\,c))}{2\,g(b\,c)}\,, \qquad \text{if} \quad b\,c \geq 1\,, \tag{3.34}$$

and

$$\frac{\hat{\gamma}_V(\infty,c)}{\gamma_V(\infty,c)} \;=\; \frac{\pi}{2}\,. \tag{3.35}$$

Some measurements of the average number of generation events per creation event are shown in **Table 1**. The cutoff parameter c influences both the creation rate (i.e., the number of particles) and the generation rate (i.e., the effort per creation). For algorithms 1 and 3, the creation effort grows linearly with c . For algorithm 2, the creation effort grows logarithmically with c . The numbers obtained for the quantity G/C in Table 1 are consistent with the approximate expressions (3.33)-(3.35). Indeed, one obtains for algorithms 1 and 2, with parameters (3.22) and (3.23),

$$\frac{\hat{\gamma}^{(1)}(\infty,c)}{\gamma(\infty,c)} = 8.96\,, \qquad \frac{\hat{\gamma}^{(2)}(\infty,c)}{\gamma(\infty,c)} = 2.07\,,$$

and, with a different cutoff parameter,

$$\frac{\hat{\gamma}^{(1)}(\infty,15)}{\gamma(\infty,15)} = 15.2\,, \qquad \frac{\hat{\gamma}^{(2)}(\infty,15)}{\gamma(\infty,15)} = 2.12\,.$$

The value 1.57 for algorithm 3 does not depend on the parameters.

	G/C	CPU (sec.)	G/C ($c = 15$)	CPU ($c = 15$)
Algo 1	9.08	3119	15.4	4079
Algo 2	2.09	2261	2.14	2561
Algo 3	1.57	4741	1.57	7244

Table 1: Average number of generation events per creation event (3.30), calculated with parameters (3.23) and a different cutoff

Δt (fs)	$\mathbb{E}\,\tau(c)$ (fs)	$\mathbb{E}\,\tau_V(c)$ (fs)
0.05	1.10	0.25
0.02	1.05	0.20
0.01	1.04	0.19
0.005	1.03	0.18

Table 2: First cancellation time (3.36), calculated with parameters (3.23) and different time steps

3.3.2 Cancellation effort

The cancellation effort is determined by the effort per cancellation and by the number of cancellations.

The effort per cancellation is mainly determined by the average number N of particles at the cancellation times. The cancellation procedure described in Section 2.1.2 does not require any information about the specific pairs of particles to be cancelled. This leads to linear (with respect to N) effort. An efficient implementation of the cancellation procedure is not completely straightforward, since various "naive" versions will have quadratic effort. One may use separate lists of positive and negative particles in order to further improve efficiency. It would be possible to randomize the order in the list of particles, but no effect of ordering was observed in the numerical experiments.

The number of cancellations depends on the parameters N_{ini} and N_{canc} , as well as on the creation rate. It also depends on the cancellation grid, which influences the number of particles after cancellation. Using (3.26) one can approximate the mean first cancellation time, namely

$$\mathbb{E}\,N(t,c) = N_{\mathrm{canc}} \qquad \Rightarrow \qquad \mathbb{E}\,\tau(c) = \frac{1}{2\,\gamma(\infty,c)}\,\log(N_{\mathrm{canc}}/N_{\mathrm{ini}})\,. \tag{3.36}$$

With the parameters (3.22) and (3.23), it follows from (3.17), (3.18) and (3.36) that

$$\gamma(\infty,c) = 0.533\,\mathrm{fs}^{-1}\,, \qquad \mathbb{E}\,\tau(c) = 1.03\,\mathrm{fs} \tag{3.37}$$

and

$$\gamma_V(\infty,c) = 3.04\,\mathrm{fs}^{-1}\,, \qquad \mathbb{E}\,\tau_V(c) = 0.18\,\mathrm{fs}\,. \tag{3.38}$$

Measurements of the mean first cancellation time are provided in **Table 2**. They are consistent with the corresponding approximations obtained in (3.37), (3.38). Moreover, they illustrate the behaviour of the time step error.

Finally, we study the dependence of the effort on the initial number of particles. For large N_{ini} there are more cancellations (cf. (3.36)) so that the effort grows. Note that, due to the

N_{ini}	CPU (sec.)	max. stand. dev.
32k	2465	2.5 10^{-3}
160k	2768	6.7 10^{-4}

Table 3: Maximal standard deviations for the mean density (2.8), calculated with parameters (3.23) and a different initial particle number

conservation property (2.48), the number of particles is always bigger than N_{ini} provided that the initial particles are positive. On the other hand, it is intuitively clear that large N_{ini} lead to a smaller variance, which reduces the effort for reaching a given confidence level. **Table 3** shows the standard deviation (square root of the variance) and the CPU time, for $N_{\mathrm{ini}} = 32k$ and $N_{\mathrm{ini}} = 160k$. The variance reduction is much more significant compared to the increase in CPU time. In this particular example, the CPU time increases by 15 %, while the variance is reduced by a factor 4.

4 Comments

The main result of this paper is the introduction of a class of stochastic algorithms for the numerical treatment of the Wigner equation. The class provides certain degrees of freedom, which is of interest both from a practical and from a conceptual point of view. In particular, the procedure for the creation of particles is determined either by using the Wigner kernel V_W, or by using directly the potential energy V. In the literature on the Wigner Monte Carlo method (cf., e.g., [4]), this step is treated by using the positive part of the Wigner kernel.

Our derivation of the particle creation procedures is based on the Dynkin formula for pure jump processes with a general state space. This approach has certain advantages compared to the derivation via Neumann series (cf. [13]). In particular, it suggests a variety of algorithms and treats these different cases simultaneously.

The algorithms are based on random systems of positive and negative particles. This is a special case of the general approach via stochastic weighted particle systems, which has been studied in various other application areas in recent years. For example, positive variable weights were used for the Boltzmann equation (cf. [17, 18]) and for Smoluchowski's coagulation equation (cf. [14]). Positive and negative weights were used in the deviational particle approach for the Boltzmann equation (cf. [7, 16]) and in kinetic plasma simulations (cf. [21]). Complex-valued weights were used in the random cloud approach for the Schrödinger equation in [22].

First we provide some comments on specific results, which have been illustrated by the numerical experiments in Section 3.

- using V_W instead of V_W^+ in the particle creation procedure

  A gain factor 2 in the creation effort is obtained for the "V_W-method", compared to the "V_W^+-method". According to Remark 2.5, this effect is independent of the specific example. The relation of the CPU times for both methods indicates the distribution of effort between creation and other components. For the set of parameters (3.23) the reduction of CPU time is about 25 %.

- using an improved majorant in the particle creation procedure

  When using algorithms 1 and 2, the rate function γ is the same. According to (3.31) and (3.32), the relation of the average numbers of generation events per creation event is

$$\frac{\hat{\gamma}^{(1)}(\infty, c)}{\hat{\gamma}^{(2)}(\infty, c)} \quad = \quad \frac{b\,c}{1+\log(b\,c)}\,, \qquad \text{if} \quad b\,c > 1\,.$$

  Thus, there is always a gain factor in rejections (unsuccessful creation attempts). This factor improves with an increasing cutoff parameter c (cf. Table 1). However, the actual gain in CPU time also depends on the effort per creation attempt (the improved majorant should not be too complicated).

- reduction of the systematic error in the cancellation procedure

  The effect illustrated in Figures 1 and 3 is quite important. It is desirable to choose the initial number of particles rather big, since this significantly reduces the fluctuations (cf. Table 3). The issue of constructing regeneration algorithms, which perform better than uniform regeneration, has been addressed recently in [3].

Next we discuss several features of the class of algorithms that have not yet been studied in detail.

- using fictitious creation events in the particle creation procedure

  According to Remark 2.4, the approach via fictitious creation events has the same effort compared to the corresponding acceptance-rejection technique. It has the advantage that the calculation of the rate function γ is avoided. This is convenient, e.g., if the algorithms are used with different cutoff parameters.

- using V instead of V_W in the particle creation procedure

  The "V-method" has a higher creation rate (cf. (2.59)), but the same generation rate (cf. (2.25), (2.36)), compared to the "V_W-method". Thus, the number of particles grows more rapidly and one obtains more cancellations. The total effort is always bigger for the "V-method". In our test example, the increase in effort is between 50 % and 80 % , dependent on the cutoff parameter (cf. Table 1).

  The V-method does not need an explicit form of the Wigner kernel V_W . This might be a useful alternative to the numerical calculation of V_W , in particular, in higher dimensions. In the one-dimensional case there are explicit formulas for V_W , if V is a linear combination of indicator functions.

Finally, we comment on some issues that might be of relevance for future developments.

- avoiding the time step error

  In the literature on the Wigner Monte Carlo method there is usually no splitting of transport and particle creation. In our algorithms, the time step error can also be avoided. However, the rigorous derivation of the various creation procedures becomes technically more demanding, since the theory of piecewise deterministic Markov processes has to be

used. The corresponding algorithms are then special cases of the "random cloud model" introduced in [23]. Position-independent majorants (as, e.g., (3.8)) can be implemented as well.

Using a splitting time step provides several advantages from a methodological point of view. There is a clear separation of the three different ingredients of the evolution (transport, creation, cancellation). The derivation is much simpler, since it is based on pure jump processes.

Moreover, the splitting of creation and transport might be even useful for an extension towards the Wigner-Boltzmann equation, which includes various scattering mechanisms. Monte Carlo algorithms for electron transport in a self-consistent electric field always contain some splitting time step (cf., e.g., [11, 12]). Thus, once separated from transport, the particle creation mechanism can easily be attached to the existing codes. This applies as well to other extensions of the Wigner equation as, for example, the Wigner-Fokker-Planck equation (cf. [5] and references therein).

- using a continuous particle state space

  A discretization of the wave-vector is quite common in the literature (cf., e.g., [4]). This simplifies both the numerical approximation of V_W and the cancellation step. The error related to this discretization was studied in [6].

  In our algorithms, a discretization of the state space is used only in the cancellation step. This might be more appropriate for the anticipated extensions towards the Wigner-Boltzmann transport equation.

Acknowledgements

The authors are grateful to Omar Morandi for providing numerical data for a benchmark test at an early stage of the project. The first author acknowledges the support of the Università degli Studi di Catania, FIR 2014 "Charge Transport in Graphene and Low dimensional Structures: modeling and simulation".

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