A multistep scheme for solving Wigner equation

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Abstract: In this paper, an explicit multistep scheme is proposed of solving the Wigner equation, which can be derived from the integral form of hyperbolic system via operator semi-group theory, and the pseudo-differential operator is tackled by the spectral collocation method. Since the hyperbolic operator is not approximated by any difference method, the multistep scheme is not restricted by CFL condition, thereby permitting the employment of explicit methods with a longer time step. It is also demonstrated that the calculation of Wigner potentials can be performed via two successive FFT procedures, thereby reducing the computational complexity dramatically. Numerical examples illustrating the accuracy are presented.

Keywords: Wigner equation; spectral collocation method; Adams multistep scheme; quantum transport.

1 Introduction

The progressive miniaturization of semiconductor devices, and the use of bulk materials other than silicon, necessitates the use of a wide variety of model in semiconductor device simulation [1]. Among various of quantum mechanical models, the Wigner representation [2] is a useful tool to describe the quantum transport of charged particles in a solid state medium. Although it is not a real probability function due to possible negative values, the Wigner function serves the role of a distribution [3], thereby facilitating the prediction of macroscopically measurable quantities, such as currents and heat fluxes. Recently, the Wigner function is also widely applied in non-equilibrium quantum statistical mechanics, optics and information theory [3,4].

Various of numerical methods are proposed to solve Wigner equation. Frensley proposed the inflow boundary condition for open quantum system and simulated the resonant tunneling diode (RTD) using a first-order upwind finite difference method (FDM) [20]. Afterwards Ringhofer adapted FDMs by using spectral collocation method to discretize the pseudo-differential operator, termed mixed finite-difference-spectral-collocation scheme [6]. Another class of scheme, termed operator splitting scheme, was performed in [7] to study Landau damping of quantum system and generalized by Arnold and Ringhofer to study Wigner-Poisson problem [8]. Monte Carlo techniques were employed in the simulation of RTDs to account for scattering effects [9]. Several advanced techniques, like adaptive mesh and conservative spectral element methods, were also adapted in solving Wigner equation while preserving the mass conservation [4].

However, solving Wigner equation in three dimension is still problematic due to the dramatic growth of sampling points in full phase space [10]. Besides, it’s difficult to find a sparse matrix representation of the nonlocal pseudo-differential operator, thereby making a stable explicit scheme much more advantageous. The boundary condition in three dimension is also an open problem since the inflow boundary condition has been
reported to cause spurious numerical reflections of outgoing wave packets [11], which can be resolved by absorbing boundary condition [12]. It should be noticed that the Wigner equation is a Cauchy problem, therefore one should handle unphysical phenomena carefully when introducing an artificial boundary condition.

The main objective of this paper is to derive an explicit multistep scheme for solving Wigner equation combining with spectral collocation method. The intuition comes from the fact that the Wigner equation can be represented as an abstract ODE via operator semi-group theory, therefore several multistep ODE solvers might be adapted to tackle quantum transport equation by tracking the characteristic in $x$–direction. It is demonstrated that the cost of computing Wigner function can be reduced dramatically via Fast Fourier transformation, thereby facilitating the simulation in high-dimensional case. And an explicit scheme allows an easier strategy for parallel computing. The accuracy of the multistep scheme is illustrated by simulating motions of a Gaussian wave packet in several potential barriers, that have been studied in [4].

The rest of the paper is organized as follows. In Section 2, the Wigner equation and modeling of quantum plasma are introduced. The multistep scheme is derived in Section 3, with a brief review of spectral collocation method. Numerical examples are demonstrated in Section 4. Concluding remarks are given in Section 5.

2 An introduction to Wigner equation

In this section we briefly review the Wigner equation and several models of quantum plasma. For convenience, the author uses the same notation as [1]. The Wigner function $w(x, k, t)$ is defined by using the Weyl-Wigner transformation of the density matrix for mixed states [1, 3],

$$w(x, k, t) = \frac{(2\pi)^{-d}}{\int \cdots \int} \rho(x + \eta \frac{1}{2}, x - \eta \frac{1}{2}, t) e^{-i \eta \cdot k},$$

which satisfies the Fourier transformed quantum Liouville equation, referred to as the (collisionless) Wigner equation

$$\partial_t w + \frac{\hbar}{m} k \cdot \nabla_x w + \theta[V] w = 0,$$

$$\theta[V] = \delta V \left( x, \gamma \right), \quad \delta V \left( x, \gamma \frac{1}{2} \right) = V \left( x + \gamma \frac{1}{2} \right) - V \left( x - \gamma \frac{1}{2} \right),$$

where $\theta[V]$ is termed pseudo-differential operator.

It is easy to derive the spectral representation of pseudo-differential operator via Eq.(2), while an equivalent formula for $\theta[V]$ is given by

$$\theta[V] w(x, k, t) = (2\pi)^{-d} \int \cdots \int \left( \delta \left( \frac{\hbar}{2}, t \right) \right) \left( x, \gamma \frac{1}{2} \right) w \left( x, \gamma \right) \exp \left( i \eta \cdot (k - \gamma) \right),$$

where $\hbar$ is the reduced Planck constant. Eq.(3) can be computed via the numerical integration techniques in simulation.
In modeling the electron plasma in metal, however, it is necessary to consider the scattering processes of electrons with phonons quantum mechanically [13]. In practice, there are two approaches to formulating the scattering effect, namely, the relaxation time model and the Fokker-Planck term. The relaxation time model is

\[ Q(w) = \frac{1}{\tau} \left( \frac{n}{n_0} w_0 - w \right), \]

and Fokker-Planck term model is given by

\[ Q(w) = \frac{1}{\tau} \text{div}_k \left( \frac{mT_0}{\hbar^2} \nabla_k w + kw \right), \]

where \( T_0 \) denote the lattice temperature.

Finally, it is reasonable to consider the self-consistent electrostatic potential in simulating RTDs, which be achieved by coupling Eq.(2) with a Poisson equation

\[ \Delta_x V(x, t) = \int_{\mathbb{R}^d} dk \ w(x, k, t) - D(x), \]

where \( D(x) \) denotes the Doping concentration.

After changing the time scale (let \( \frac{\hbar}{m} = 1 \)), we arrive at the reduced collisional Wigner-Poisson equation, which is a quantum analogue to its classical counterpart, the Vlasov-Poisson equation [14],

\[
\partial_t w + k \cdot \nabla_x w + \theta [V] w = Q(w), \quad \theta [V] = V \left( x + \frac{1}{2i} \nabla_k \right) - V \left( x - \frac{1}{2i} \nabla_k \right),
\]

\[ \Delta_x V(x, t) = \int_{\mathbb{R}^d} dk \ w(x, k, t) - D(x), \quad Q(w) = \frac{1}{\tau} \left( \frac{n}{n_0} w_0 - w \right), \]

\[ w(x, k, 0) = w_0(x, k). \]

The existence and uniqueness of a global classical solution of collisionless Wigner-Poisson equation is given by Brezzi and Markowich [15], via the reformulation of the quantum transport problem as a system of countably many Schrödinger equations coupled to a Poisson equation. For more details of Wigner function, one can refer to [3].

3 Numerical scheme

In this section, we mainly discuss the numerical scheme of solving Eq.(7). It is observed that the operator \( k \cdot \nabla_x \) in the second term is a hyperbolic one, and the third term does not possess classical characteristics. Therefore, traditional numerical scheme can be roughly summarized as three procedures:

1. Transform Eq.(7) into a hyperbolic system through discretization in \( k \)-direction.
2. Use finite difference method to discretize the hyperbolic operator \( k \cdot \nabla_x \),
3. Use ODE solver to tackle the large ODE system.

As the computational scale may change rapidly in the ODE system, it’s better to use an implicit ODE solver, which is much more stable in stiff problems. However, the real problem is that the matrix representation of pseudo-differential operator \( \theta [V] \) is always dense, thereby undermining the efficiency of matrix inverted
method or iterative method. This can be partially resolved by spectral method, since the computational complexity can be reduced via Fast Fourier Transformation or Fast Cosine Transformation [1, 2].

In addition, implicit methods seem impractical in high-dimensional case due to the increasing of grid points. As the result, the simulation of Wigner equation is still restricted to one dimensional case even using modern computers. An explicit method is much more preferable in solving the high dimensional problem, like Wigner Monte Carlo method, owing to its lower computational complexity.

An alternative way to solve Eq.(7) is to treat the reduced hyperbolic system as an abstract ODE system, thus the numerical schemes can be derived via operator semigroup theory, which track the drift along the characteristic in x-direction properly. Before discussing the multistep scheme, we need to transformed Eq.(7) into a hyperbolic system, through the spectral collocation method.

### A. Spectral collocation method

The spectral collocation method, derived by Ringhofer [1, 6], is based on the fact that the plane waves are the eigenfunctions of the pseudo-differential operator associated with the Wigner potentials. Under the assumption that \( V(x) \) is smoothly defined and \( w(x, k, t) \) has a compact support, the author has showed this method is well-posed and convergent [6].

Following Ringhofer, assume that \( w(x, k, t) \) has a compact support in \( k \in [-\frac{\pi}{N}, \frac{\pi}{N}] \), then we approximate the Wigner function by trigonometric polynomial of the form

\[
w \approx w_N(x, k, t) = \sum_{n \in \mathbb{N}} c(x, n, t) \phi_n(k) \cdot \mathbb{N} = \{-N, \cdots, N\}, \quad N = 2^m
\]

The plane wave basis

\[
\phi_n(k) = \left( \frac{\alpha}{2\pi} \right)^{d/2} \exp(i\alpha \cdot k)
\]

satisfies

\[
\int_{[-\frac{\pi}{N}, \frac{\pi}{N}]} \phi_m^* \phi_n = \delta(m-n), \quad (\Delta k)^d \sum_{n \in \mathbb{N}} \phi_m(k_s)^* \phi_n(k_s) = \delta_N(m-n),
\]

where \( \delta_N \) is a Kronecker \( \delta \) with period \( N \), \( \Delta k = \frac{\pi}{Na} \) and \( k_s = \frac{s\pi}{Na} \).

Since

\[
c(x, n, t) = (\Delta k)^d \sum_{s \in \mathbb{N}} \phi_n^*(k_s) w_N(x, k_s, t),
\]

then \( \theta[V]w \) can be approximated by

\[
B(x, k_m, t) = \theta[V]w_N(x, k_m, t) = i \frac{(\Delta k)^d}{\hbar} \sum_{n \in \mathbb{N}} \sum_{s \in \mathbb{N}} \delta V \left( x, \frac{\alpha h}{2}, n, t \right) w_N(x, k_s, t) \phi_n^*(k_s) \phi_n(k_m),
\]

where \( B \) is a tensor matrix.

When an explicit scheme is used, namely, \( w_N(x, k, t) \) is known, the computation of tensor matrix \( B \) can be performed by two successive FFT procedures, since

\[
B(x, k_m, t) = \theta[V]w_N(x, k_m, t) = i \frac{(\Delta k)^d}{\hbar} \sum_{n \in \mathbb{N}} \sum_{s \in \mathbb{N}} w_N(x, k_s, t) \phi_n^*(k_s) \delta V \left( x, \frac{\alpha h}{2}, n, t \right) \phi_n(k_m).
\]
For simplicity, we assume \( d = 1 \). Denote by
\[
H_n = \sum_{x=-N}^{N} w(x, k_x, t) e^{-in k_x} = \sum_{s=-N}^{N} w(x, k_x, t) e^{-2\pi nk_s}, \quad n = -N + 1, \ldots, N
\]
\[
H_{-N} = \sum_{s=-N}^{N} w(x, k_x, t) e^{\pi s i}.
\]
(14)

A simple calculation yields
\[
H_n = \sum_{s=0}^{2N-1} w(x, k_x, t) e^{-2\pi ns} + w(x, k_{-N}, t) e^{i \pi n},
\]
(15)
where \( k_s = k_{s-2N} (s = N + 1, \ldots, 2N - 1) \). Thus, the first term in the right-hand side can be performed by standard FFT program.

It remains to calculate
\[
B(x, k_m, t) = \sum_{n=-N}^{N} \left[ H_n \delta \psi(x, an, t) \right] e^{2\pi nk_m}, \quad m = -N + 1, \ldots, N
\]
\[
B(x, k_{-N}, t) = \sum_{n=-N}^{N} \left[ H_n \delta \psi(x, an, t) \right] e^{-in \pi}.
\]
(16)

via inverse FFT program as
\[
B(x, k_m, t) = \sum_{n=0}^{2N-1} S_n e^{2\pi nk_m} + H_{-N} \delta \psi(x, an, t) e^{-i \pi m}, \quad m = -N + 1, \ldots, N,
\]
(17)
where \( S_n = H_n \delta \psi(x, an, t) \) and \( S_n = S_{n-2N} (n = N + 1, \ldots, 2N - 1) \).

Now the Wigner equation (7) is simply approximated by collocation at the appropriate equally space nodes, namely,
\[
\partial_t w_N(x, k_m, t) + k_m \cdot \nabla_x w_N(x, k_m, t) + B(x, k_m, t) = Q(w_N(x, k_m, t)), \quad m = -N, \ldots, N,
\]
(18)

This section ends with some discussion about numerical methods for scattering term and discontinuous potential. In general, the relaxation time model can be handled by numerical integration, while the Fokker-Planck model handled by Monte Carlo method or any numerical solver for parabolic equation.

In real simulation of RTDs, the potential may have some gaps due to the barriers in semiconductor [17]. As smoothness of \( w \) and \( V \) is strongly related to the aliasing error and the convergence of spectral collocation method [6,16], the barrier potential cannot be tackled by spectral methods. This problem can be partially resolved by splitting the potential into two parts, namely, \( V = V_{\text{barrier}} + V_{\text{self-consistent}} \), where \( V_{\text{barrier}} \) is the barrier potential, and \( V_{\text{self-consistent}} \) is the self-consistent electrostatic field [9]. Thus, the smooth \( V_{\text{self-consistent}} \) can be tackled by spectral collocation method, while the non-smooth barrier potential tackled by numerical integration.
B. Multistep scheme for solving hyperbolic system

The remaining part is to find a numerical solver for the hyperbolic system (18). The multistep scheme is derived by observing that (18) can be represented as an abstract ODE or a mild solution via operator semigroup theory.

Denote by \( A = k_m \cdot \nabla_x \) and \( T(t) = e^{-tA} \) the operator semigroup generated by \( A \). As \( A \) is a symmetric operator, \( T(t) \) is a \( C_0 \) semigroup [13].

Now we rewrite (18) in integral form

\[
w_N(x, k_m, t) = T(t)w_N(x, k_m, 0) - \int_0^t dtT(t-s)[B(x, k_m, s) + Q(w_N(x, k_m, s))],
\]

since \( T(t) x = x - k_m t \), it yields

\[
w_N(x, k_m, t + \Delta t) = w_N(x - k_m \Delta t, k_m, t) - \int_t^{t+\Delta t} dt\left[B + Qw_N\right](x - k_m(t + \Delta t - s), k_m, s).
\]

To derive a numerical scheme for (20), a direct choice is to use interpolation or extrapolation polynomials to estimate the integral, using the same idea as Adams methods in solving ODEs [19].

Denote by \( g_m(x, s) = T(t_{n+1} - s)[B(x, k_m, s) + Q(w_N(x, k_m, s))] \), then \( g_m(x, t_{n+1}) \) can be approximated by extrapolation polynomial \( p(x, k_m, t) \) on nodes \( t_n, t_{n-1}, \ldots, t_{n-p} \), which can be expressed in terms of backward differences,

\[
\nabla^0 g_m(x, t_n) = g_m(x, t_n), \quad \nabla^{j+1} g_m(x, t_n) = \nabla^j g_m(x, t_n) - \nabla^{j} g_m(x, t_{n-1}),
\]

as follows:

\[
p(x, k_m, t) = p(x, k_m, t_n + s\Delta t) = \sum_{j=0}^{k-1} (-1)^j \binom{s-1}{j} \nabla^j g_m(x, t_n),
\]

Inserting (22) into (20), we arrive at the generalized Adams methods for solving hyperbolic system (18).

We denote \( \tilde{w}_N \) the numerical solution of \( w \).

**Algorithm 3.1** Explicit Adams methods

\[
p = 1: \quad \tilde{w}_N(x, k_m, t_{n+1}) = \tilde{w}_N(x - k_m \Delta t, k_m, t_n) - \frac{3}{2} \Delta t \left[ \tilde{B} + Q\tilde{w}_N \right](x - k_m \Delta t, k_m, t_n)
\]

\[
+ \frac{1}{2} \Delta t \left[ \tilde{B} + Q\tilde{w}_N \right](x - 2k_m \Delta t, k_m, t_{n-1}),
\]

\[
p = 2: \quad \tilde{w}_N(x, k_m, t_{n+1}) = \tilde{w}_N(x - k_m \Delta t, k_m, t_n) - \frac{23}{12} \Delta t \left[ \tilde{B} + Q\tilde{w}_N \right](x - k_m \Delta t, k_m, t_n)
\]

\[
+ \frac{16}{12} \Delta t \left[ \tilde{B} + Q\tilde{w}_N \right](x - 2k_m \Delta t, k_m, t_{n-1}) - \frac{5}{12} \Delta t \left[ \tilde{B} + Q\tilde{w}_N \right](x - 3k_m \Delta t, k_m, t_{n-2})
\]

Similarly, the integral can be approximated by interpolation polynomials, yielding
Algorithm 3.2 Implicit Adams methods

\[ p = 0 : \tilde{w}_N(x, k_m, t_{n+1}) = \tilde{w}_N(x - k_m\Delta t, k_m, t_n) - \frac{1}{2}\Delta t \left[ \tilde{B} + Q\tilde{w}_N \right](x, k_m, t_{n+1}) \]

\[ p = 1 : \tilde{w}_N(x, k_m, t_{n+1}) = \tilde{w}_N(x - k_m\Delta t, k_m, t_n) - \frac{5}{12}\Delta t \left[ \tilde{B} + Q\tilde{w}_N \right](x, k_m, t_{n+1}) \]

\[ - \frac{8}{12}\Delta t \left[ \tilde{B} + Q\tilde{w}_N \right](x - 2k_m\Delta t, k_m, t_{n-1}) \]

Implicit Adams methods are not so practical in solving hyperbolic system (17) directly, but they can be used to correct the predicted value of \( w \) through explicit methods, known as prediction-corrections scheme.

Numerical methods with higher order can be derived in a similar way. To guarantee the consistency and stability of numerical scheme, the coefficients should satisfy the root condition and certain algebraic relations [19].

A remarkable feature in generalized Adams methods is that grid points have drifts in \( x \)-direction, resulting from the operator \( T(t_{n+1} - t_n - p) \). Therefore these methods track the drift in characteristic direction in a more proper way. The drifted grid points may lie on the grid mesh, otherwise they can be approximated by interpolation functions.

It is also observed that the hyperbolic operator \( k_m \cdot \nabla_x \) is not approximated by any difference method. Thus the Adams scheme is free from the restriction of Courant number, thereby permitting the application of explicit methods with a reasonable time step. It is also observed that the generalized Adams methods can be used in arbitrary dimension, owing to the way of approximating an integral with respect to time variable.

The generalized Adams multistep methods seem quite cumbersome in solving a simple hyperbolic system, as the drift in characteristic direction may increase the computational complexity. Concretely speaking, the calculated data of \( \tilde{B} + Q\tilde{w}_N \) in \( n \)th step cannot be used in calculating \((n + 1)\)th step directly. A wise strategy is to sample grid points in \( x \)-direction along the characteristic line, thereby making the grid mesh to obtain as many drifted grid points as possible. Interpolation functions are unnecessary when the interval \( \Delta x \) is chosen as \( \Delta x = \Delta k \cdot \Delta t \), so that all the drifted points have already lied on the grid mesh, except those deviating from the computational domain.

A weakness of multistep scheme is requiring more initial values to start up. The missing starting points can be obtained from one-step methods, like FDMs and operator splitting scheme, with smaller step size. An alternative way is to use the idea of prediction-correction scheme, namely, we can use backward Euler method to predict the missing values and mid-point Euler method to correct them, with a smaller time step.

C. Boundary condition

So far we have not discussed the boundary condition. In general, no information of boundary condition is required in performing the multistep methods, since they are devised to tackle a Cauchy problem. In practice, however, the computation domain cannot be infinitely large and needs to be truncated. Therefore, we also need to handle the boundary condition.
Table 1: Units and parameters.

| Physical quantity | Unit | Value           |
|-------------------|------|-----------------|
| Time              | fs   | -               |
| Length            | nm   | -               |
| Energy            | eV   | -               |
| Temperature       | K    | -               |
| Electron mass $m_e$ | eV·fs²·nm⁻² | 5.68562966 |
| Planck constant $\hbar$ | eV·fs | 0.658211899 |
| Boltzmann constant $k_B$ | eV·K⁻¹ | $8.61734279 \times 10^5$ |

The boundary conditions in open quantum systems and corresponding mathematical concepts have been illustrated in [11, 20]. We only review the well-known inflow boundary condition, derived by Frensley,

$$w(x_L, k, t) = w_L(k, t), \quad k > 0,$$

$$w(x_R, k, t) = w_R(k, t), \quad k < 0,$$

where $w_L(k, t)$ and $w_R(k, t)$ can be approximated by Fermi-Dirac distribution.

Solving Wigner-Poisson equation is much more complicated due to the coupling self-consistent Poisson equation. Due to the non-locality of the pseudo-differential operator $\theta$, solving the Poisson equation with an improper boundary condition will cause severe unphysical effect. It is illustrated in [20] that the boundary conditions for (6) are chosen from the requirement that the system asymptotically approach charge neutrality. For simplicity, the Poisson equation is not included in subsequent numerical simulations.

4 Numerical results

A. Test problems

The numerical results are presented by simulating the motions of a Gaussian wave packet (GWP) in several barrier potentials, which have been studied in [4][10][21]. To facilitate the comparison, the author uses the same physical units and quantities as in [4][10], listed in Table 1. The rescaled Wigner-equation in one dimension is

$$\frac{\partial w}{\partial t} + \frac{hk}{m} \frac{\partial w}{\partial x} + \frac{1}{2\pi \hbar} \theta [V] w = 0. \quad (26)$$

The wave function of a GWP is

$$\psi(x, t) = \left[\frac{1}{2\pi \alpha^2 (1 + i\beta t)^2}\right]^{\frac{1}{2}} e^{i(k_0x - \omega_0 t)} \exp \left\{ \frac{(x - v_0 t)^2}{4\alpha^2 (1 + i\beta t)} \right\}, \quad (27)$$

where $v_0$ is the average velocity, $\alpha$ is the minimum position spread, and

$$\beta = \frac{\hbar}{2m\alpha^2}, \quad v_0 = \frac{\hbar k_0}{m} = \frac{2\omega_0}{k_0}. \quad (28)$$
The Wigner-function description of (27) is
\[
\omega (x, k, t) = 2 \exp \left\{ -\frac{(x - x_0 v_0 t)^2}{2a^2 (1 + \beta^2 r^2)} \right\} \exp \left\{ -2\alpha^2 \left( 1 + \beta^2 r^2 \right)^2 \left[ (k - k_0) - \beta t (x - x_0 - v_0 t) \right] \right\}.
\] (29)
which is an analytical solution of (26) when \( V = 0 \).

The initial condition \((t = 0)\) for the GWP simulation is
\[
\omega (x, k, 0) = 2 \exp \left\{ -\frac{(x - x_0)^2}{2a^2} \right\} \exp \left\{ -2\alpha^2 (k - k_0)^2 \right\}.
\] (30)

The quantum tunneling effect is investigated by simulating a GWP hitting a Gaussian barrier with three different heights. The Gaussian barrier with a width \( \omega \) is given
\[
V (x) = H \exp \left( \frac{x^2}{-\omega^2} \right),
\] (31)
where the self-consistent electrostatic potential is not included.

In all simulations, \( \alpha = 2.825 \), \( m = 0.0665m_e \), \( x_0 = -30 \) and \( k_0 = 1.4 \) so that the kinetic energy of GWP is \( E_0 \approx 1.12 \). The computational domain \( \mathbb{R} \times \mathbb{K} \) is chosen \( [-\frac{\pi h}{4m}, \frac{\pi h}{4m}] \times [-2\pi, 2\pi] \), with \( \Delta x = \frac{\pi h}{64m}, \Delta k = \frac{\pi}{64} \), \( \Delta t = 0.05 \) (the Courant number is \( \sigma = \frac{\Delta t}{\Delta x} = 1.02 \)). The explicit Adams three-step method is employed, and the missing starting points are obtained from first-order upwind finite difference method, with a smaller time step \( \delta t = 0.002 \) and inflow boundary condition
\[
\omega (x_L, k, t) = \omega (x_L, k, 0), \quad k > 0,
\]
\[
\omega (x_R, k, t) = \omega (x_R, k, 0), \quad k < 0,
\] (32)
In multistep scheme, the drifted grid points are interpolated by cubic spline if not lying on the grid mesh, and a simple nullification is made for the drifted grid points outside the computational domain.

The heights \( H \) of \( V (x) \) are chosen 0.3, 1.3 and 2.3, respectively, with \( \omega = 1 \).

**B. Numerical results**

In order to test numerical accuracy, a comparison is made between the multistep scheme and the FDM by monitoring the error when simulating the time evolution of the GWP in the free space \((V = 0)\). The performance metric is \( L^2 \) error and \( L^\infty \) error [4],
\[
\varepsilon_2 (t) = \left[ \int_{\mathbb{R} \times \mathbb{K}} (\Delta \omega (x, k, t))^2 \, dx \, dk \right]^{\frac{1}{2}},
\]
\[
\varepsilon_{\infty} (t) = \max \{ \Delta \omega (x, k, t) \}, \quad (x, k) \in \mathbb{R} \times \mathbb{K},
\] (33)
where \( \Delta \omega (x, k, t) = \left| \omega^{\text{num}} (x, k, t) - \omega^{\text{exact}} (x, k, t) \right| \).

The evolution of a GWP in the free space \((V = 0)\) is simulated by both methods with the same time step \( \Delta t = 0.05 \). In this case, the multistep scheme reduces to
\[
\tilde{\omega}_{N} (x, k_m, t_{n+1}) = \tilde{\omega}_{N} \left( x - \frac{h}{m} k_m \Delta t, k_m, t_n \right),
\] (34)
which is the exact solution of \( \partial_t w + \frac{4}{m} k_m \nabla_x w = 0 \).

Since the missing initial values in multistep scheme should be gained via other one-step methods, the author chooses first-order upwind finite difference method, with inflow boundary condition and a smaller time step \( \delta t = 0.002 \), to compute the first two steps, thereby making the comparison more reasonable. As a result, the numerical error in multistep scheme comes from three sources, the error of interpolation functions, the error of first two steps and the artificial boundary condition. Numerical results are listed as follows.

\[ \frac{L^2}{L^\infty} \]

Figure 1: Numerical error of Wigner functions in the free space (\( V = 0 \))

It is demonstrated in Figure 1 that the Adams scheme is much more accurate than FDM, since it tracks the characteristic of hyperbolic system in a exact way. Actually, the maximum error in Adams scheme mainly results from the error of starting points and the inflow boundary condition.

Figure 2 illustrates the comparison between the exact evolution and numerical evolution of Wigner function in the free space. It is seen that the numerical error also propagates along the characteristic line, due to the construction of Adams scheme.

Figure 3 shows the Wigner functions for the GWP interacting with the Gaussian barrier \( V(x) = 0.3 e^{-\frac{x^2}{2}} \). The kinetic energy \( E_0 \) of GWP is about 1.12, which is much greater than the barrier height. Therefore, the GWP travels across the barrier.

When the height of barrier is comparable to \( E_0 \), as shown in Figure 4, the GWP is separated into two parts, one traveling across the barrier, another being reflected back. Due to the tunneling effect, some wave packets are able to overcome the barrier, although the height of barrier potential is greater than \( E_0 \).

For the barrier with higher height, like \( V(x) = 2.3 e^{-\frac{x^2}{2}} \), the GWP is reflected back almost completely, seen in Figure 5.
Figure 2: The Wigner functions for the GWP in the free space ($V = 0$)

5 Conclusion

In this paper we mainly discuss a multistep scheme to tackle the hyperbolic operator $k \cdot \nabla x$. It makes use of the property of operator semigroup generated by first-order differential operator, thereby tracking the characteristic more properly than finite difference method. And the size of time step in multistep scheme is not restricted by Courant-Friedrichs-Lévy condition, therefore explicit methods can be employed with a longer time step. Numerical simulations also validate the feasibility of an explicit method, with a sufficiently large time step $t = 0.05$. Moreover, the multistep scheme is devised to tackle a Cauchy problem, thereby giving more freedom of choosing a reasonable boundary condition.

The spectral collocation method is employed to discretize the pseudo-differential operator $\theta$ due to its simplicity. In principle, the cost of calculating $\theta$ via spectral representation is quite small owing to FFT, thus it is a practical way to solve the high-dimensional problem. The weakness of spectral method is that its convergence is strongly related to smoothness of $w$ and $V$. If the potential function can be artificially split into a
smooth part and a non-smooth part, then the calculation of smooth potential can be tackled in an efficient way. There are several alternatives, like numerical integration method, which is expected to be compatible with the multistep scheme.

The author omits the detailed discussion about self-consistent field and scattering term as it is quite difficult to find an appropriate boundary condition and a reasonable numerical example, which may be expected in subsequent paper.

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Figure 4: The Wigner functions for the GWP interacting with Gaussian barrier ($H = 1.3$)
Figure 5: The Wigner functions for the GWP interacting with Gaussian barrier ($H = 2.3$)