Numerical approximation of the semi-classical Schrödinger equation in the electromagnetic field with Hagedorn wave packets

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Outline

1. Introduction
   - The Schrödinger equation with vector potential
   - Challenges and previous work

2. Hagedorn wave packets and leading order approximation
   - Hagedorn wave packets
   - Leading order approximation

3. Higher Order Approximation

4. Numerical Examples

5. Conclusions and final remarks
Many problems of solid state physics require the solution of the Schrödinger equation in the electromagnetic field with a small (scaled) Planck constant $\varepsilon$. ($\varepsilon \ll 1$)

\[ i\varepsilon \partial_t u = \frac{1}{2} (-i\varepsilon \nabla_x - A)^2 u + Vu, \quad t \in \mathbb{R}, \quad x \in \mathbb{R}^3; \quad (1) \]

\[ u(x, 0) = u_0(x), \quad x \in \mathbb{R}^3 \quad (2) \]

Mathematically, the electromagnetic field, or respectively, electric field $E(x) \in \mathbb{R}^3$ and magnetic field $B(x) \in \mathbb{R}^3$ are described by the scalar potential $V(x) \in \mathbb{R}$ and the vector potential $A(x, t) \in \mathbb{R}^3$ as

\[ E = -\nabla V(x), \quad B = \nabla \times A. \quad (3) \]
Schrödinger equation in the electromagnetic field

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The semi-classical Schrödinger propagates $O(\varepsilon)$ oscillations in space and time. So the wave function does not converge in the strong sense.

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*W. Bao, S. Jin, and P. A. Markowich (2002).*
*S. Jin, and Z. Zhou (2013).*
Other approximate approaches

- **Geometric optics and WKB methods**
  \[
  u = a^\varepsilon(t, x) e^{iS(t,x)/\varepsilon} = (a_0(t, x) + \varepsilon a_1(t, x) + \cdots) e^{iS(t,x)/\varepsilon}.
  \]

- **Wigner transform**
  \[
  W^\varepsilon(t, x, k) = \int \frac{dy}{(2\pi)^d} e^{ik \cdot y} u\left(t, x - \frac{\varepsilon}{2} y\right) \overline{u\left(x + \frac{\varepsilon}{2} y\right)}.
  \]

- **Gaussian beam approach**
  \[
  u = a(t; y) e^{iT(t;x;y)/\varepsilon},
  \]
  \[
  T(t, x; y) = S(t; y) + p(t; y) \cdot (x - y) + \frac{1}{2} (x - y) \cdot M(t; y)(x - y).
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More comments on Gaussian beams

- **Leading order approximation**: error $O(\sqrt{\epsilon})$.
- **Higher order approximation**: error $O(\epsilon^{k/2})$

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\]

\[
a^\epsilon(t, x; y) = a_0(t; y) + O(\epsilon) + \cdots.
\]

Drawback: non-constant cut-off functions needed to maintain Gaussian profile.

Alternative: Hagedorn wave packets approach.
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Drawback: non-constant cut-off functions needed to maintain Gaussian profile.

Alternative: Hagedorn wave packets approach.
Hagedorn proposed a way to parametrize an $N$-dimensional Gaussian wave packets with parameters $q$, $p$, $Q$, $P$:

$$\Phi_0 [q, p, Q, P] = \left(\pi \varepsilon\right)^{-\frac{N}{4}} \left(\det Q\right)^{-\frac{1}{2}} \exp \left(\frac{i}{2\varepsilon} (x - q) \cdot PQ^{-1} (x - q) + \frac{i}{\varepsilon} p \cdot (x - q)\right),$$

where $q \in \mathbb{R}^N$ and $p \in \mathbb{R}^N$ represents the position and momentum of the beam, and $Q$, $P$ are complex $N \times N$ matrices satisfying

$$Q^T P - P^T Q = 0,$$  \hspace{1cm} (4)

$$Q^* P - P^* Q = 2i I.$$  \hspace{1cm} (5)
The Hagedorn wave packets are connected by the raising and lowering operators $\mathcal{R}$ and $\mathcal{L}$, which are defined as follows:

\begin{align}
\mathcal{R} = (\mathcal{R}_j) &= -\frac{i}{\sqrt{2\epsilon}} \left( P^* (x - q) + Q^* (-i\epsilon \nabla_x - p) \right); \\
\mathcal{L} = (\mathcal{L}_j) &= \frac{i}{\sqrt{2\epsilon}} \left( P^T (x - q) + Q^T (-i\epsilon \nabla_x - p) \right). 
\end{align}

Define $\langle j \rangle = \hat{e}_j$ to be the $j^{th}$ unit vector, we have

\begin{align*}
\Phi_{k+\langle j \rangle} &= \frac{1}{\sqrt{k_j + 1}} \mathcal{R}_j \Phi_k, \\
\Phi_{k-\langle j \rangle} &= \frac{1}{\sqrt{k_j}} \mathcal{L}_j \Phi_k.
\end{align*}

An orthonormal basis for the $L^2(\mathbb{R}^N)$ space.
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$$\mathcal{R} = (\mathcal{R}_j) = -\frac{i}{\sqrt{2\varepsilon}} \left( \mathbf{P}^* (\mathbf{x} - \mathbf{q}) + \mathbf{Q}^* (-i\varepsilon \nabla_{\mathbf{x}} - \mathbf{p}) \right);$$

$$\mathcal{L} = (\mathcal{L}_j) = \frac{i}{\sqrt{2\varepsilon}} \left( \mathbf{P}^T (\mathbf{x} - \mathbf{q}) + \mathbf{Q}^T (-i\varepsilon \nabla_{\mathbf{x}} - \mathbf{p}) \right).$$ (6) (7)

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An orthonormal basis for the $L^2 (\mathbb{R}^N)$ space.

Z. Zhou

Hagedorn wave packets in the electromagnetic field
In one dimensional cases, the Hagedorn wave packets are Hermite polynomials multiplied by a complex Gaussian. For example, when $q = p = 0$, $Q = P = 1$, we plot the first 6 Hagedorn wave packets in the following.
Properties of Hagedorn wave packets

Suppose $\alpha$, $\beta$ and $\gamma$ are continuous real $N \times N$ matrix-valued functions, and in addition, $\alpha$ and $\gamma$ are symmetric; $\delta$ and $\epsilon$ are continuous, real vector-valued functions; and $\zeta$ is a continuous real scalar function. Consider the following Hamiltonian

$$H = \frac{1}{2} \left( \begin{array}{ccc} -i\epsilon \nabla_x & \alpha & \beta \\ \beta^T & -i\epsilon \nabla_x & \gamma \\ \end{array} \right) + \delta \cdot (-i\epsilon \nabla_x) + \epsilon \cdot x + \zeta. \quad (8)$$

Given any initial condition $[q(0), p(0), Q(0), P(0), S(0)]$, there exists a unique solution $[q(t), p(t), Q(t), P(t), S(t)]$ to the system

$$\begin{cases}
\dot{q} = \beta \cdot q + \alpha \cdot p + \delta \\
\dot{p} = -\gamma \cdot q - \beta^T \cdot p - \epsilon \\
\dot{Q} = \beta \cdot Q + \alpha \cdot P \\
\dot{P} = -\gamma \cdot Q - \beta^T \cdot P \\
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\end{cases} \quad (9)$$
Properties (continued)

Let \([q(t), p(t), Q(t), P(t), S(t)]\) be any solution to the system (9). Then for every \(k\),

\[
\Psi = e^{iS(t)/\epsilon} \Phi_k [q(t), p(t), Q(t), P(t)](t, x)
\]

satisfies the Schrödinger equation \(i\epsilon \frac{\partial \Psi}{\partial t} = H(t)\Psi\), where \(H(t)\) is of the form (8).

This theorem means, as long as

- the scalar potential is at most quadratic in \(x\),
- the vector potential is at most linear in \(x\),

the Hagedorn wave packets are the exact solutions to the Schrödinger equation.
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Magical lemma

**Theorem**

Suppose $H(\varepsilon)$ is a family of self-adjoint operators for $\varepsilon > 0$. Suppose $\Psi$ belongs to the domain of $H(\varepsilon)$, is continuously differentiable in $t$ and approximately solves the Schrödinger equation in the sense that

$$i\varepsilon \frac{\partial \Psi}{\partial t} = H(\varepsilon)\Psi + R(t, \varepsilon),$$

where $R(t, \varepsilon)$ satisfies

$$\|R(t, \varepsilon)\| \leq \mu(t, \varepsilon).$$

Then,

$$\left\| e^{-itH(\varepsilon)/\varepsilon} \Psi(0) - \Psi(t) \right\| \leq \varepsilon^{-1} \int_0^t \mu(s, \varepsilon) ds.$$
Magical lemma (continued)

According to this Lemma, if

- $\Psi(t)$ is the exact solution to the Schrödinger equation with some modified Hamiltonian $H_0$, with $H_r = H(\epsilon) - H_0$;
- $H(\epsilon)$ is the original Hamiltonian, $e^{-iH(\epsilon)t/\epsilon} \Psi(0)$ stands for the exact solution to the original Schrödinger equation.

Then, $\|H_r \Psi\| = O\left(\epsilon^{3/2}\right)$, implies that $\Psi(t)$ gives asymptotic solutions to the Schrödinger equation with error $O\left(\epsilon^{1/2}\right)$ within finite time.

Especially, for the Hagedorn wave packet approach, want to choose $H_0$ such that:

- the Hagedorn wave packets give exact solution to the $H_0$ part;
- $\|H_r \Psi\| = O\left(\epsilon^{3/2}\right)$, if $\Psi$ is a Hagedorn wave packet.
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More properties of Hagedorn wave packets

Effective width in position and momentum space:

\[ x - q = \sqrt{\frac{\varepsilon}{2}} (QR + \bar{Q}L) ; \quad (10) \]

\[ -i\varepsilon \partial_x - p = \sqrt{\frac{\varepsilon}{2}} (PR + \bar{P}L) . \quad (11) \]

Therefore, if \( \Psi \) is a Hagedorn wave packet, for \( m, n \in \mathbb{N} \),

\[ \| (x - q)^m (-i\varepsilon \partial_x - p)^n \Psi \| = O \left( \varepsilon^{\frac{m+n}{2}} \right) . \]
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Vanishing vector potential case

When the vector potential $A \equiv 0$, namely $H = -\frac{\varepsilon^2}{2} \Delta + U(x)$, Hagedorn has shown that, one can take

$$H_0 = -\frac{\varepsilon^2}{2} \Delta + U_2(x),$$

$$U_2(x) = U(q) + U'(q)(x - q) + \frac{1}{2} U''(q)(x - q)^2.$$  

Then,

$$H_r = \frac{1}{6} U'''(q)(x - q)^3 + o \left( (x - q)^3 \right).$$

This implies $\|H_r \psi\| = O(\varepsilon^{3/2})$, which is the desired estimate for the leading order approximation.

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Reformulate the model

We consider the one-dimensional Schrödinger equation in the electromagnetic field

\[ i\varepsilon \partial_t \varphi = H\varphi = \frac{1}{2} \left( -i\varepsilon \nabla_x - A \right)^2 \varphi + V\varphi. \]

The right hand side can be reformulated as

\[ H\varphi = -\frac{\varepsilon^2}{2} \Delta_x \varphi + \frac{1}{2} \left( \left( -i\varepsilon \nabla_x \right) \cdot (-A) + (-A) \cdot \left( -i\varepsilon \nabla_x \right) \right) \varphi + U(x)\varphi, \]

where \( U(x) = V(x) + \frac{1}{2} |A(x)|^2. \)
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Consider the Hamiltonian

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- \( A_1 = A(q) + \partial_x A(q)(x - q) \),
- \( A_q = \frac{1}{2} \partial_{xx} A(x)(x - q)^2 \),
- \( A_r = A - A_1 - A_q, \quad A - A_1 = A_q + A_r \).

We take

\[ H_0 = -\frac{\varepsilon^2}{2} \Delta + \frac{1}{2} \left( (-i\varepsilon \partial_x) (-A_1) + (-A_1) (-i\varepsilon \partial_x) \right) - pA_q, \]

in which \(-pA_q\) is quadratic in \(x\) and \(A_1\) is linear in \(x\).
Treatment for vector potentials

Consider the Hamiltonian

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Treatment for vector potentials (continued)

We simplify the residual Hamiltonian,

\[
H_r \psi = (H - H_0) \psi = \frac{1}{2} (-i \varepsilon \partial_x)(-A_q - A_r) \psi + \frac{1}{2} (-A_q - A_r)(-i \varepsilon \partial_x) \psi + pA_q \psi + pA_r \psi - pA_r \psi
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This implies \( \|H_r \psi\| = O(\varepsilon^{3/2}) \) !!!
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\[ \frac{1}{2} (-i\varepsilon \partial_x - p) (-A_q - A_r) \varphi \]

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Suppose $A(x) \in C^3(\mathbb{R})$ satisfies $C_1 \leq A(x) \leq C_2 e^{Mx^2}$ and $C_1 \leq \partial_x A(x) \leq C_2 e^{Mx^2}$ for some $C_1$, $C_2$ and $M$. Let $(q(t), p(t), Q(t), P(t), S(t))$ be the solution to the system

$$
\begin{align*}
\dot{q}(t) &= -A(q(t)) + p(t) \\
\dot{p}(t) &= -U'(q) + A'(q)p \\
\dot{Q}(t) &= -A'(q)Q + P \\
\dot{P}(t) &= (pA''(q) - U''(q))Q + A'(q)P \\
\dot{S}(t) &= \frac{1}{2}p^2 - U(q).
\end{align*}
$$

Let the Hamiltonian $H = -\frac{\varepsilon}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} ((-i\varepsilon \partial_x)(-A) + (-A)(-i\varepsilon \partial_x)) + U$, and suppose $\Psi(t) = e^{iS(t)/\varepsilon} \Phi_k (\cdot, q(t), p(t), Q(t), P(t))$. ...
Then, there exists a constant $C(k, t)$, such that

$$
\left\| e^{itH/\varepsilon} \Psi(0) - \Psi(t) \right\| \leq C(k, t)\varepsilon^{\frac{1}{2}}.
$$

(13)
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We aim to improve the approximation so that the model error is $O(\varepsilon^{\alpha})$, where $\alpha > \frac{1}{2}$.

Consider the Schrödinger equation

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Galerkin approximation II

For fixed parameters \([q, p, Q, P]\), and some index set \(\Lambda = \{0, \cdots, L\}\), we define the following linear space spanned by Hagedorn wave packets

\[
M[q, p, Q, P] = \left\{ v(x) \in L^2(\mathbb{R}) : v(x) = \sum_{k \in \Lambda} c_k \Phi^q[p, Q, P], c_k \in \mathbb{C} \right\}.
\]

The variational approximation on the subspace \(M[q, p, Q, P]\) can be written as:

For any \(t\), determine \(\varphi_M \in M[q, p, Q, P]\), such that

\[
\left\langle i\varepsilon \frac{\partial \varphi_M}{\partial t} - H_r \varphi_M, \Phi_k \right\rangle = 0, \quad \forall k \in \Lambda.
\] (14)
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(14)
The Galerkin approximation (14) is equivalent to the system of ordinary differential equations

\[ i\varepsilon \frac{dc_k}{dt} = \sum_{l \in \Lambda} f_{kl} c_l, \quad k \in \Lambda, \]  

(15)

where

\[ f_{kl} = \int_{\mathbb{R}} \Phi_k \Phi_l H r \, dx. \]

If \( \mathbf{c}(t) \) denotes the vector with components \( c_k(t), \quad k \in \Lambda, \) and \( \mathbf{F} \) denotes the matrix with entries \( f_{kl} \), the solution to the equations (15) is thus given by

\[ \mathbf{c}(t) = \exp \left( -\frac{it}{\varepsilon} \mathbf{F} \right) \mathbf{c}(0). \]
Theorem

Given $c_k (0) = c'_k$ for $0 \leq k \leq K$, and $c_k (0) = 0$ for $k > K$, where $K$ is a non-negative integer.

If we denote the exact solution of the original Schrödinger equation by

$$\Psi(t) = e^{-itH/\epsilon} \left[ e^{iS(0)/\epsilon} \sum_{k=0}^{K} c'_k \phi_k (x, q(0), p(0), Q(0), P(0)) \right],$$

then, for any $T > 0$ there exists some constant $C_2$, such that $\forall t \in [0, T]$ implies,

$$\left\| \Psi(t) - e^{iS(t)/\epsilon} \sum_{k=0}^{K+3N-3} c_k(t) \phi_k (\cdot, q(t), p(t), Q(t), P(t)) \right\| \leq C_2(T) \epsilon^{N/2}.$$
operator splitting methods are available.

compared to high order Gaussian beam method, no cut-off function is needed.

can be easily extended to multidimensional cases.

If initialized properly, the wave packets will maintain the Gaussian profile.
Remarks

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If initialized properly, the wave packets will maintain the Gaussian profile.
The second order Strang splitting is applied to the modified Hamiltonian and the residual Hamiltonian.

The ODE system corresponding to the modified Hamiltonian is solved by the forth order Runge-Kutta method.

The ODE system for coefficients $c_k$ is solved analytically where Gauss-Hermite quadrature is applied to numerically evaluate the integrals.
Numerically, we have four kinds of error:

- the time splitting error — $O(\Delta t^2)$;
- the error in computing the parameter set $[q, p, Q, P] — O(\Delta t^4/\varepsilon)$;
- and the error in numerical evaluating the integrals — negligible.
- the approximation error in the Galerkin approximation — $O(\varepsilon^{k/2})$;
Example 1

- $U(x) = 1, A(x) = \cos(x)$.
- the reference solution by the SL-TSSP method, till $T = 0.5$.

The initial wave function

$$\psi_0 = e^{iS_0/\varepsilon} \Phi_0[q_0, p_0, Q_0, P_0]$$

$$= \exp(iS_0/\varepsilon) (\pi\varepsilon)^{-1/4} (\det Q_0)^{-1/2} \exp\left(\frac{i}{2\varepsilon} (x - q_0) \cdot P_0 Q_0^{-1} \cdot (x - q_0) + \frac{i}{\varepsilon} p_0 \cdot (x - q_0)\right),$$

with $q_0 = 0.1, p_0 = 1, Q_0 = 1, P = i, S_0 = 1$.

We approximate $\psi(t)$ by the first $K$ Hagedorn wave packets.

$$\psi(t) = e^{iS(t)/\varepsilon} \sum_{k=0}^{K-1} c_k(t) \Phi_k[q(t), p(t), Q(t), P(t)].$$
Example 1

- \( U(x) = 1, \ A(x) = \cos(x) \).
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\[
\psi_0 = e^{iS_0/\varepsilon} \Phi_0[q_0, p_0, Q_0, P_0]
\]

\[
= \exp \left( iS_0/\varepsilon \right) \left( \pi\varepsilon \right)^{-1/4} \left( \det Q_0 \right)^{-1/2} \exp \left( \frac{i}{2\varepsilon} (x - q_0) \cdot P_0 Q_0^{-1} \cdot (x - q_0) + \frac{i}{\varepsilon} p_0 \cdot (x - q_0) \right),
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\psi(t) = e^{iS(t)/\varepsilon} \sum_{k=0}^{K-1} c_k(t) \Phi_k[q(t), p(t), Q(t), P(t)].
\]
Example 1

With sufficiently fine time steps, the numerical error is dominated by the Galerkin approximation error $O(\varepsilon^\alpha)$.

\[
\begin{array}{cccc}
K=1 & K=4 & K=7 \\
\text{Error in wave function} & \varepsilon^{-1/2} & \varepsilon^1 & \varepsilon^{3/2}
\end{array}
\]

**Figure:** K=1, approximate error $O(\varepsilon^{1/2})$. K=4, approximate error $O(\varepsilon^1)$. K=7, approximate error $O(\varepsilon^{3/2})$. 
Example 1

Comparison with the Gaussian beam method: the approximation error $O(\varepsilon^\alpha)$, and the error introduced by cut-off functions.

Figure: Approx. error: 1st order $O(\varepsilon^{1/2})$, 2nd order $O(\varepsilon^1)$, 3rd order $O(\varepsilon^{3/2})$.

Agrees with results by Liu, Runborg and Tanushev (2013).
In this example, we want to test the Hagedorn wave packets after caustics formation. The initial condition is in the WKB form

\[ \varphi(x, t = 0) = \varphi_0(x) = A_0(x) e^{iS_0(x)/\varepsilon}, \]

where

\[ A_0(x) = e^{-25x^2}, \quad S_0(x) = \frac{1}{\pi} \cos(\pi x). \]

We choose the scalar potential \( U = 2x^3 \) and the vector potential \( A = \frac{1}{5} x^2 \). The strong scalar potential make the force one-directional. Two caustics form at around \( t = 0.5 \).
Example 2

Since the initial condition is not in a Gaussian wave packet form, one needs to firstly decompose the initial wave function into some Gaussian wave packet.

\[ c_0(0; x_i) = A_0(x_i)(\pi \varepsilon)^{1/4} \]
\[ c_k(0; x_i) = 0, \quad k \geq 1. \]

\[ J. Qian and L. Ying, 2010 \]
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\( J. \ Qian \ and \ L. \ Ying, \ 2010 \)

The so-called asymptotic decomposition method is to sample Gaussian beams on a uniform mesh \( \{ x_i \} \), with initial conditions

\[
q_{x_i}(0) = x_i \\
p_{x_i}(0) = \partial_x S_0(x_i) \\
Q_{x_i}(0) = 1 \\
P_{x_i}(0) = \partial_{xx} S_0(x_i) + i \\
S_{x_i}(0) = S_0(x_i) \\
c_0(0; x_i) = A_0(x_i)(\pi\epsilon)^{1/4} \\
c_k(0; x_i) = 0, \ \ k \geq 1.
\]
Example 2

We choose $\varepsilon = \frac{1}{4096}$, the computation interval $[a, b] = [-1.5, 1.5]$. We sample $N_x = 200$ Gaussian beams on this interval and compute by leading order Hagedorn wave packets ($K = 1$) till $t = 0.5$. 
In the project, we extended the Hagedorn wave packets approach to the non-vanishing vector potential cases.

- proved the Hagedorn wave packets dynamics corresponding to the modified Hamiltonian yields the leading order approximation,
- rigorously justified the Galerkin approximation for the residual Hamiltonian can improve the order of accuracy in $\varepsilon$.

This approach is similar to the Gaussian beam method...

However, this approach possesses the advantage that, it provided a uniform way to reduce approximation error, while higher order Gaussian beam method may not give an improved accuracy when $\varepsilon$ is not very small.
Future directions

In numerical implementation,

- what is the optimal way to choose time steps.

In analysis,

- if Hagedorn wave packets provide a better way to do initial condition decomposition.

and many fresh ideas...

Thanks for your attention and questions!
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