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

Zhennan Zhou[1]
joint work with Prof. Shi Jin.

[1]Department of Mathematics
University of Wisconsin-Madison

Mathematical and Numerical Methods for
Complex Quantum Systems, March 2014

Outline

Schrödinger equation in the electromagnetic field

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

$$i\varepsilon\partial_t u = \frac{1}{2}\left(-i\varepsilon\nabla_{\mathbf{x}} - \mathbf{A}\right)^2 u + Vu, \quad t \in \mathbb{R}, \quad x \in \mathbb{R}^3; \tag{1}$$

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3 \tag{2}$$

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

$$\mathbf{E} = -\nabla V(\mathbf{x}), \qquad \mathbf{B} = \nabla \times \mathbf{A}. \tag{3}$$

Schrödinger equation in the electromagnetic field

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

$$i\varepsilon\partial_t u = \frac{1}{2}\left(-i\varepsilon\nabla_{\mathbf{x}} - \mathbf{A}\right)^2 u + Vu, \quad t \in \mathbb{R}, \quad x \in \mathbb{R}^3; \tag{1}$$

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3 \tag{2}$$

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

$$\mathbf{E} = -\nabla V(\mathbf{x}), \qquad \mathbf{B} = \nabla \times \mathbf{A}. \tag{3}$$

Challenges and previous work

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

Numerically, if the wave function is simulated directly, one needs to resolve the oscillations. The constraint that $\Delta x \sim O(\varepsilon)$ cannot be removed.

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

Challenges and previous work

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

Numerically, if the wave function is simulated directly, one needs to resolve the oscillations. The constraint that $\Delta x \sim O(\varepsilon)$ cannot be removed.

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

Other approximate approaches

- Geometric optics and WKB methods

$$u = a^\varepsilon(t,x)e^{iS(t,x)/\varepsilon} = \left(a_0(t,x) + \varepsilon a_1(t,x) + \cdots\right) e^{iS(t,x)/\varepsilon}.$$

- 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

$$u = a(t;y)e^{iT(t,x;y)/\varepsilon},$$

$$T(t,x;y) = S(t;y) + p(t;y)\cdot(x-y) + \frac{1}{2}(x-y)\cdot M(t;y)(x-y).$$

Other approximate approaches

- Geometric optics and WKB methods

$$u = a^\varepsilon(t,x)e^{iS(t,x)/\varepsilon} = \left(a_0(t,x) + \varepsilon a_1(t,x) + \cdots\right) e^{iS(t,x)/\varepsilon}.$$

- 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

$$u = a(t;y)e^{iT(t,x;y)/\varepsilon},$$

$$T(t,x;y) = S(t;y) + p(t;y)\cdot(x-y) + \frac{1}{2}(x-y)\cdot M(t;y)(x-y).$$

Other approximate approaches

- Geometric optics and WKB methods

$$u = a^\varepsilon(t,x)e^{iS(t,x)/\varepsilon} = \left(a_0(t,x) + \varepsilon a_1(t,x) + \cdots\right) e^{iS(t,x)/\varepsilon}.$$

- 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

$$u = a(t;y)e^{iT(t,x;y)/\varepsilon},$$

$$T(t,x;y) = S(t;y) + p(t;y)\cdot(x-y) + \frac{1}{2}(x-y)\cdot M(t;y)(x-y).$$

More comments on Gaussian beams

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

$$u = a^{\varepsilon}(t,x;y)e^{iT(t,x;y)/\varepsilon},$$

$$T(t,x;y) = S(y)+p\cdot(x-y)+\frac{1}{2}(x-y)\cdot M(x-y)+O\left((x-y)^3\right)+\cdots,$$

$$a^{\varepsilon}(t,x;y) = a_0(t;y)+O(\varepsilon)+\cdots.$$

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

Alternative: Hagedorn wave packets approach.

More comments on Gaussian beams

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

$$u = a^{\varepsilon}(t,x;y)e^{iT(t,x;y)/\varepsilon},$$

$$T(t,x;y) = S(y)+p\cdot(x-y)+\frac{1}{2}(x-y)\cdot M(x-y)+O\left((x-y)^3\right)+\cdots,$$

$$a^{\varepsilon}(t,x;y) = a_0(t;y)+O(\varepsilon)+\cdots.$$

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

Alternative: Hagedorn wave packets approach.

More comments on Gaussian beams

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

$$u = a^{\varepsilon}(t,x;y)e^{iT(t,x;y)/\varepsilon},$$

$$T(t,x;y) = S(y)+p\cdot(x-y)+\frac{1}{2}(x-y)\cdot M(x-y)+O\left((x-y)^3\right)+\cdots,$$

$$a^{\varepsilon}(t,x;y) = a_0(t;y)+O(\varepsilon)+\cdots.$$

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

Alternative: Hagedorn wave packets approach.

Ground state Hagedorn wave packet

Hagedorn proposed a way to parametrize an N-dimensional Gaussian wave packets with parameters $\mathbf{q}$, $\mathbf{p}$, $\mathbf{Q}$, $\mathbf{P}$:

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

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

$$\mathbf{Q}^T\mathbf{P}-\mathbf{P}^T\mathbf{Q}=0, \tag{4}$$

$$\mathbf{Q}^*\mathbf{P}-\mathbf{P}^*\mathbf{Q}=2i\mathbf{I}. \tag{5}$$

Hagedorn wave packets

The Hagedorn wave packets are connected by the raising and lowering operators $\mathcal{R}$ and $\mathcal{L}$, which are defined as follows:

$$\mathcal{R} = (\mathcal{R}_j) = -\frac{i}{\sqrt{2\varepsilon}} \left(\mathbf{P}^* \left(\mathbf{x} - \mathbf{q} \right) + \mathbf{Q}^* \left(-i\varepsilon \nabla_{\mathbf{x}} - \mathbf{p} \right) \right); \tag{6}$$

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

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

$$\Phi_{\mathbf{k}+\langle j \rangle} = \frac{1}{\sqrt{k_j + 1}} \mathcal{R}_j \Phi_{\mathbf{k}}, \quad \Phi_{\mathbf{k}-\langle j \rangle} = \frac{1}{\sqrt{k_j}} \mathcal{L}_j \Phi_{\mathbf{k}}.$$

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

Hagedorn wave packets

The Hagedorn wave packets are connected by the raising and lowering operators $\mathcal{R}$ and $\mathcal{L}$, which are defined as follows:

$$\mathcal{R} = (\mathcal{R}_j) = -\frac{i}{\sqrt{2\varepsilon}} \left(\mathbf{P}^* \left(\mathbf{x} - \mathbf{q} \right) + \mathbf{Q}^* \left(-i\varepsilon \nabla_{\mathbf{x}} - \mathbf{p} \right) \right); \tag{6}$$

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

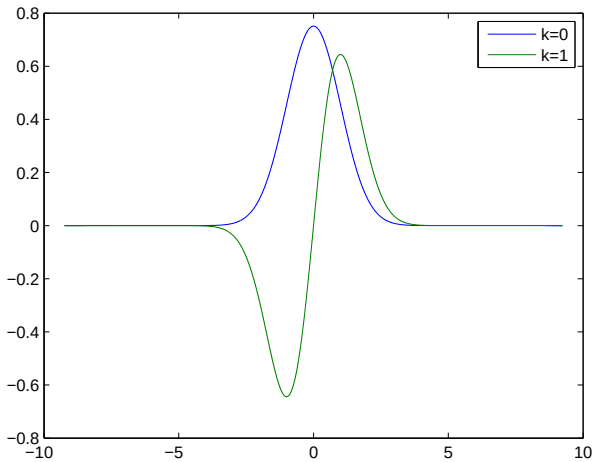
Define $\langle j \rangle = \hat{e}_j$ to be the j^{th} unit vector, we have

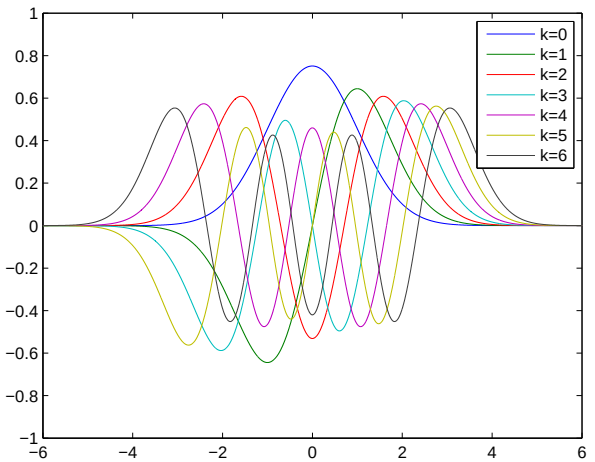
$$\Phi_{\mathbf{k}+\langle j \rangle} = \frac{1}{\sqrt{k_j + 1}} \mathcal{R}_j \Phi_{\mathbf{k}}, \quad \Phi_{\mathbf{k}-\langle j \rangle} = \frac{1}{\sqrt{k_j}} \mathcal{L}_j \Phi_{\mathbf{k}}.$$

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

Plots of Hagedorn wave packets

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 α, β and γ are continuous real $N \times N$ matrix-valued functions, and in addition, α and γ are symmetric; δ and ϵ are continuous, real vector-valued functions; and ζ is a continuous real scalar function. Consider the following Hamiltonian

$$H = \frac{1}{2} \begin{pmatrix} -i\varepsilon\nabla_{\mathbf{x}} \\ \mathbf{x} \end{pmatrix} \cdot \begin{pmatrix} \alpha & \beta \\ \beta^T & \gamma \end{pmatrix} \begin{pmatrix} -i\varepsilon\nabla_{\mathbf{x}} \\ \mathbf{x} \end{pmatrix} + \delta \cdot (-i\varepsilon\nabla_{\mathbf{x}}) + \epsilon \cdot \mathbf{x} + \zeta. \quad (8)$$

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

$$\begin{cases} \dot{\mathbf{q}} &= \beta \cdot \mathbf{q} + \alpha \cdot \mathbf{p} + \delta \\ \dot{\mathbf{p}} &= -\gamma \cdot \mathbf{q} - \beta^T \cdot \mathbf{p} - \epsilon \\ \dot{\mathbf{Q}} &= \beta \cdot \mathbf{Q} + \alpha \cdot \mathbf{P} \\ \dot{\mathbf{P}} &= -\gamma \cdot \mathbf{Q} - \beta^T \cdot \mathbf{P} \\ \dot{S} &= \frac{\alpha}{2} |\mathbf{p}|^2 - \frac{\gamma}{2} |\mathbf{q}|^2 - \epsilon \cdot \mathbf{q} - \zeta. \end{cases} \quad (9)$$

Properties of Hagedorn wave packets

Suppose α, β and γ are continuous real $N \times N$ matrix-valued functions, and in addition, α and γ are symmetric; δ and ϵ are continuous, real vector-valued functions; and ζ is a continuous real scalar function. Consider the following Hamiltonian

$$H = \frac{1}{2} \begin{pmatrix} -i\varepsilon\nabla_{\mathbf{x}} \\ \mathbf{x} \end{pmatrix} \cdot \begin{pmatrix} \alpha & \beta \\ \beta^T & \gamma \end{pmatrix} \begin{pmatrix} -i\varepsilon\nabla_{\mathbf{x}} \\ \mathbf{x} \end{pmatrix} + \delta \cdot (-i\varepsilon\nabla_{\mathbf{x}}) + \epsilon \cdot \mathbf{x} + \zeta. \quad (8)$$

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

$$\begin{cases} \dot{\mathbf{q}} &= \beta \cdot \mathbf{q} + \alpha \cdot \mathbf{p} + \delta \\ \dot{\mathbf{p}} &= -\gamma \cdot \mathbf{q} - \beta^T \cdot \mathbf{p} - \epsilon \\ \dot{\mathbf{Q}} &= \beta \cdot \mathbf{Q} + \alpha \cdot \mathbf{P} \\ \dot{\mathbf{P}} &= -\gamma \cdot \mathbf{Q} - \beta^T \cdot \mathbf{P} \\ \dot{S} &= \frac{\alpha}{2} |\mathbf{p}|^2 - \frac{\gamma}{2} |\mathbf{q}|^2 - \epsilon \cdot \mathbf{q} - \zeta. \end{cases} \quad (9)$$

Properties (continued)

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

$$\Psi = e^{iS(t)/\varepsilon} \Phi_{\mathbf{k}} \left[\mathbf{q}(t), \mathbf{p}(t), \mathbf{Q}(t), \mathbf{P}(t)\right](t, x)$$

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

This theorem means, as long as

- the scalar potential is at most quadratic in $\mathbf{x}$,
- the vector potential is at most linear in $\mathbf{x}$,

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

Properties (continued)

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

$$\Psi = e^{iS(t)/\varepsilon} \Phi_{\mathbf{k}} \left[\mathbf{q}(t), \mathbf{p}(t), \mathbf{Q}(t), \mathbf{P}(t)\right](t, x)$$

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

This theorem means, as long as

- the scalar potential is at most quadratic in $\mathbf{x}$,
- the vector potential is at most linear in $\mathbf{x}$,

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

Magical lemma

Theorem

Suppose $H(\varepsilon)$ is a family of self-adjoint operators for $\varepsilon > 0$. Suppose Ψ 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

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

Then,

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

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

Then, $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$, implies that $\Psi(t)$ gives asymptotic solutions to the Schrödinger equation with error $O\left(\varepsilon^{1/2}\right)$ 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;
- $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$, if Ψ is a Hagedorn wave packet.

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

Then, $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$, implies that $\Psi(t)$ gives asymptotic solutions to the Schrödinger equation with error $O\left(\varepsilon^{1/2}\right)$ 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;
- $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$, if Ψ is a Hagedorn wave packet.

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

Then, $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$, implies that $\Psi(t)$ gives asymptotic solutions to the Schrödinger equation with error $O\left(\varepsilon^{1/2}\right)$ 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;
- $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$, if Ψ is a Hagedorn wave packet.

More properties of Hagedorn wave packets

Effective width in position and momentum space:

$$x - q = \sqrt{\frac{\varepsilon}{2}} \left(Q\mathcal{R} + \bar{Q}\mathcal{L} \right); \tag{10}$$

$$-i\varepsilon\partial_x - p = \sqrt{\frac{\varepsilon}{2}} \left(P\mathcal{R} + \bar{P}\mathcal{L} \right). \tag{11}$$

Therefore, if Ψ is a Hagedorn wave packet, for $m, n \in \mathbb{N}$,

$$\left\| (x-q)^m \left(-i\varepsilon\partial_x - p \right)^n \Psi \right\| = O\left(\varepsilon^{\frac{m+n}{2}} \right).$$

More properties of Hagedorn wave packets

Effective width in position and momentum space:

$$x - q = \sqrt{\frac{\varepsilon}{2}} \left(Q\mathcal{R} + \bar{Q}\mathcal{L} \right); \tag{10}$$

$$-i\varepsilon\partial_x - p = \sqrt{\frac{\varepsilon}{2}} \left(P\mathcal{R} + \bar{P}\mathcal{L} \right). \tag{11}$$

Therefore, if Ψ is a Hagedorn wave packet, for $m, n \in \mathbb{N}$,

$$\left\| (x-q)^m \left(-i\varepsilon\partial_x - p\right)^n \Psi \right\| = O\left(\varepsilon^{\frac{m+n}{2}}\right).$$

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.

Hagedorn(1998) *E. Faou, V. Gradinaru, C. Lubich (2009)*

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.

Hagedorn(1998) *E. Faou, V. Gradinaru, C. Lubich (2009)*

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.

Hagedorn(1998) *E. Faou, V. Gradinaru, C. Lubich (2009)*

Reformulate the model

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

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

The right hand side can be reformulated as

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

where $U(x) = V(x) + \frac{1}{2}|\mathbf{A}(x)|^2$.

Reformulate the model

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

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

The right hand side can be reformulated as

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

where $U(x) = V(x) + \frac{1}{2}\left|\mathbf{A}(x)\right|^2$.

Treatment for vector potentials

Consider the Hamiltonian

$$H = -\frac{\varepsilon^2}{2}\Delta + \frac{1}{2}\left((-i\varepsilon\partial_x)(-A) + (-A)(-i\varepsilon\partial_x)\right). \tag{12}$$

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

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

$$H = -\frac{\varepsilon^2}{2}\Delta + \frac{1}{2}\left((-i\varepsilon\partial_x)(-A) + (-A)(-i\varepsilon\partial_x)\right). \tag{12}$$

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

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 (continued)

We simplify the residual Hamiltonian,

$$\begin{aligned} H_r\varphi &= (H - H_0)\,\varphi \\ &= \frac{1}{2}\,(-i\varepsilon\partial_x)\,(-A_q - A_r)\,\varphi + \frac{1}{2}\,(-A_q - A_r)\,(-i\varepsilon\partial_x)\,\varphi \\ &\quad + pA_q\varphi + pA_r\varphi - pA_r\varphi \\ &= \frac{1}{2}\,(-A_q - A_r)\,(-i\varepsilon\partial_x - p)\,\varphi \\ &\quad \frac{1}{2}\,(-i\varepsilon\partial_x - p)\,(-A_q - A_r)\,\varphi \\ &\quad - pA_r\varphi. \end{aligned}$$

This implies $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$!!!

Treatment for vector potentials (continued)

We simplify the residual Hamiltonian,

$$\begin{aligned} H_r\varphi &= (H - H_0)\,\varphi \\ &= \frac{1}{2}\,(-i\varepsilon\partial_x)\,(-A_q - A_r)\,\varphi + \frac{1}{2}\,(-A_q - A_r)\,(-i\varepsilon\partial_x)\,\varphi \\ &\quad + pA_q\varphi + pA_r\varphi - pA_r\varphi \\ &= \frac{1}{2}\,(-A_q - A_r)\,(-i\varepsilon\partial_x - p)\,\varphi \\ &\quad \frac{1}{2}\,(-i\varepsilon\partial_x - p)\,(-A_q - A_r)\,\varphi \\ &\quad - pA_r\varphi. \end{aligned}$$

This implies $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$!!!

Treatment for vector potentials (continued)

We simplify the residual Hamiltonian,

$$\begin{aligned} H_r\varphi &= (H - H_0)\,\varphi \\ &= \frac{1}{2}\,(-i\varepsilon\partial_x)\,(-A_q - A_r)\,\varphi + \frac{1}{2}\,(-A_q - A_r)\,(-i\varepsilon\partial_x)\,\varphi \\ &\quad + pA_q\varphi + pA_r\varphi - pA_r\varphi \\ &= \frac{1}{2}\,(-A_q - A_r)\,(-i\varepsilon\partial_x - p)\,\varphi \\ &\quad \frac{1}{2}\,(-i\varepsilon\partial_x - p)\,(-A_q - A_r)\,\varphi \\ &\quad - pA_r\varphi. \end{aligned}$$

This implies $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$!!!

Treatment for vector potentials (continued)

We simplify the residual Hamiltonian,

$$\begin{aligned} H_r\varphi &= (H - H_0)\,\varphi \\ &= \frac{1}{2}\,(-i\varepsilon\partial_x)\,(-A_q - A_r)\,\varphi + \frac{1}{2}\,(-A_q - A_r)\,(-i\varepsilon\partial_x)\,\varphi \\ &\quad + pA_q\varphi + pA_r\varphi - pA_r\varphi \\ &= \frac{1}{2}\,(-A_q - A_r)\,(-i\varepsilon\partial_x - p)\,\varphi \\ &\quad \frac{1}{2}\,(-i\varepsilon\partial_x - p)\,(-A_q - A_r)\,\varphi \\ &\quad - pA_r\varphi. \end{aligned}$$

This implies $\|H_r\Psi\| = O\left(\varepsilon^{3/2}\right)$!!!

Leading order approximation

Theorem

Suppose $A(x) \in C^3(\mathbb{R})$ *satisfies* $C_1 \leqslant A(x) \leqslant C_2 e^{Mx^2}$ *and* $C_1 \leqslant \partial_x A(x) \leqslant C_2 e^{Mx^2}$ *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*

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

Let the Hamiltonian $H = -\frac{\varepsilon^2}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\left((-i\varepsilon\partial_x)(-A) + (-A)(-i\varepsilon\partial_x)\right) + U$, *and suppose* $\Psi(t) = e^{iS(t)/\varepsilon}\Phi_k(\cdot, q(t), p(t), Q(t), P(t))$ ....

Theorem

Then, there exists a constant $C(k,\, t)$, such that

$$\left\| e^{itH/\varepsilon}\Psi(0) - \Psi(t) \right\| \leqslant C(k,\, t)\varepsilon^{\frac{1}{2}}. \tag{13}$$

Galerkin approximation I

Is $O(\varepsilon^{1/2})$ satisfactory? Maybe not...

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

$$i\varepsilon\frac{\partial\varphi}{\partial t} = H\varphi = (H_0 + H_r)\,\varphi,$$

where the H_0 part is taken care of by the ODE system, we aim to use a Galerkin method to handle the equation of the residual Hamiltonian

$$i\varepsilon\frac{\partial\varphi}{\partial t} = H_r\varphi.$$

Galerkin approximation I

Is $O(\varepsilon^{1/2})$ satisfactory? Maybe not...

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

$$i\varepsilon \frac{\partial \varphi}{\partial t} = H\varphi = (H_0 + H_r)\,\varphi,$$

where the H_0 part is taken care of by the ODE system, we aim to use a Galerkin method to handle the equation of the residual Hamiltonian

$$i\varepsilon \frac{\partial \varphi}{\partial t} = H_r \varphi.$$

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

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

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

$$\left\langle i\varepsilon \frac{\partial \varphi_M}{\partial t} - H_r \varphi_M, \Phi_k \right\rangle = 0, \quad \forall k \in \Lambda. \tag{14}$$

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

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

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

$$\left\langle i\varepsilon \frac{\partial \varphi_M}{\partial t} - H_r \varphi_M, \Phi_k \right\rangle = 0, \quad \forall k \in \Lambda. \tag{14}$$

Galerkin Approximation III

The Galerkin approximation (14) is equivalent to the system of ordinary differential equations

$$i\varepsilon \frac{dc_k}{dt} = \sum_{l \in \Lambda} f_{kl} c_l, \quad k \in \Lambda, \tag{15}$$

where

$$f_{kl} = \int_R \overline{\Phi_k} H_r \Phi_l dx.$$

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

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

High order asymptotic solution

Theorem

Given $c_k(0) = c'_k$ *for* $0 \leqslant k \leqslant K$, *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

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

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

$$\left\|\Psi(t) - e^{iS(t)/\varepsilon}\sum_{k=0}^{K+3N-3} c_k(t)\Phi_k\left(\cdot,\, q(t),\, p(t),\, Q(t),\, P(t)\right)\right\| \leqslant C_2(T)\varepsilon^{\frac{N}{2}}.$$

Remarks

- 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

- 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

- 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

- 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.

the set up

- 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 $c_{\mathbf{k}}$ is solved analytically where Gauss-Hermite quadrature is applied to numerically evaluate the integrals.

The errors to observe

Numerically, we have four kinds of error:

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

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

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

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

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

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

The initial wave function

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

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

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

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

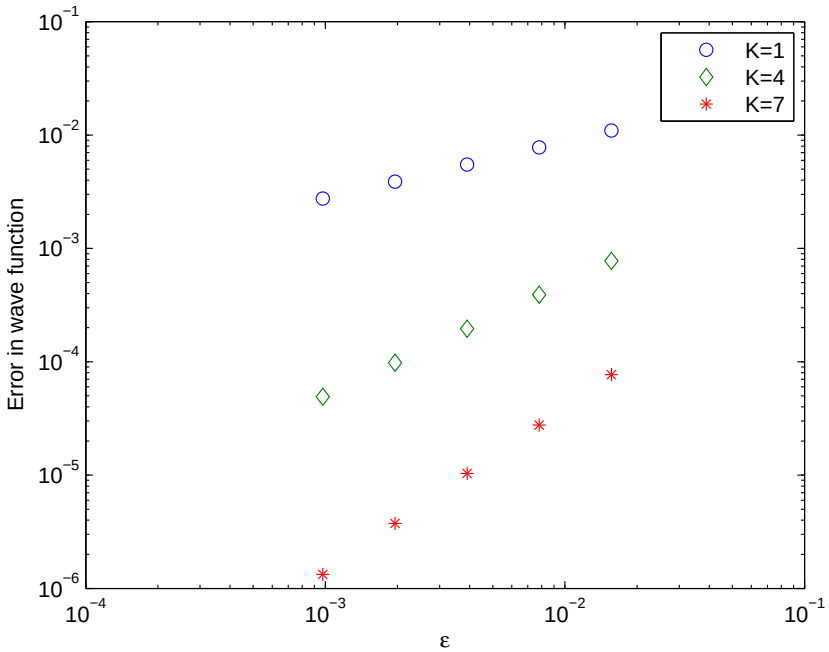


Figure: K=1, approximate error $O(\varepsilon^{1/2})$. K=4, approximate error $O(\varepsilon^{1})$. K=7, approximate error $O(\varepsilon^{3/2})$.

Example 1

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

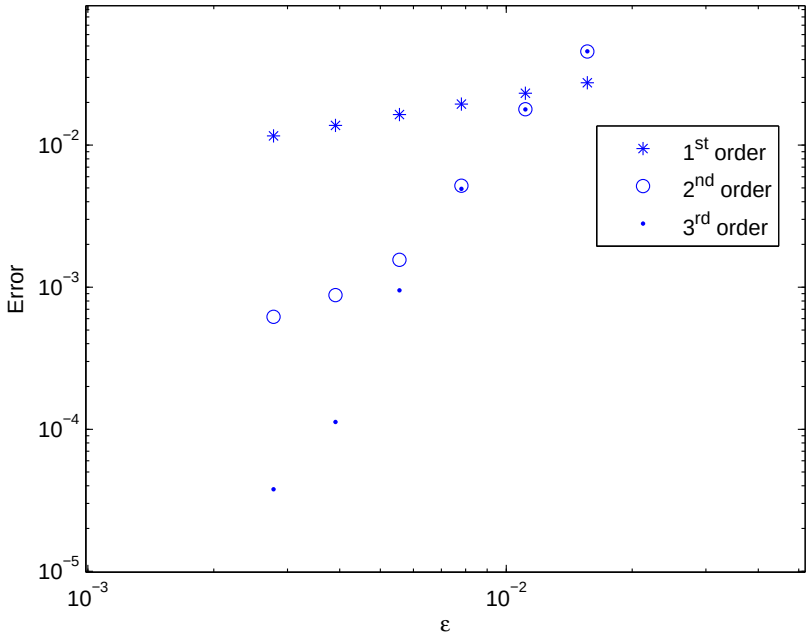


Figure: Approx. error: 1st order $O(\varepsilon^{1/2})$, 2nd order $O(\varepsilon^{1})$, 3rd order $O(\varepsilon^{3/2})$.

Agrees with results by Liu, Runborg and Tanushev (2013).

Example 2

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.

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

$$
\begin{aligned}
q_{x_i}(0) &= x_i \\
p_{x_i}(0) &= \partial_x S_0(x_i) \\
Q_{x_i}(0) &= 1 \\
P_{x_i}(0) &= \partial_{xx} S_0(x_i) + i \\
S_{x_i}(0) &= S_0(x_i) \\
c_0(0; x_i) &= A_0(x_i)(\pi\varepsilon)^{1/4} \\
c_k(0; x_i) &= 0, \quad k \geqslant 1.
\end{aligned}
$$

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.

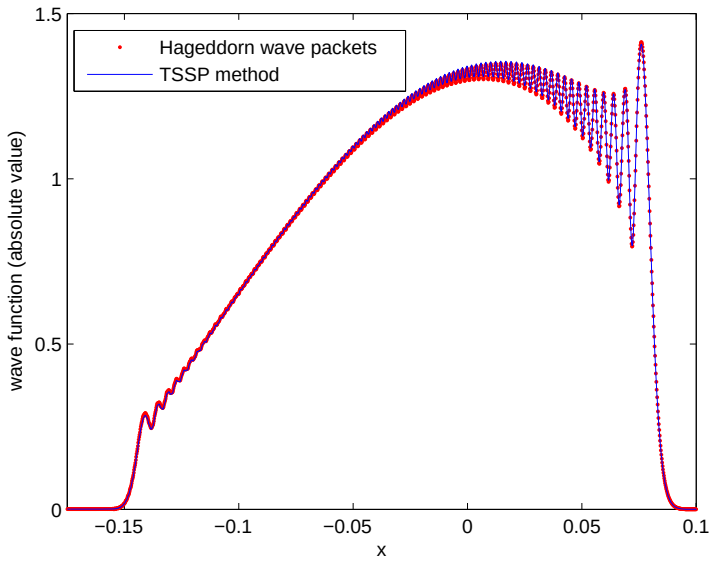
J. Qian and L. Ying, 2010

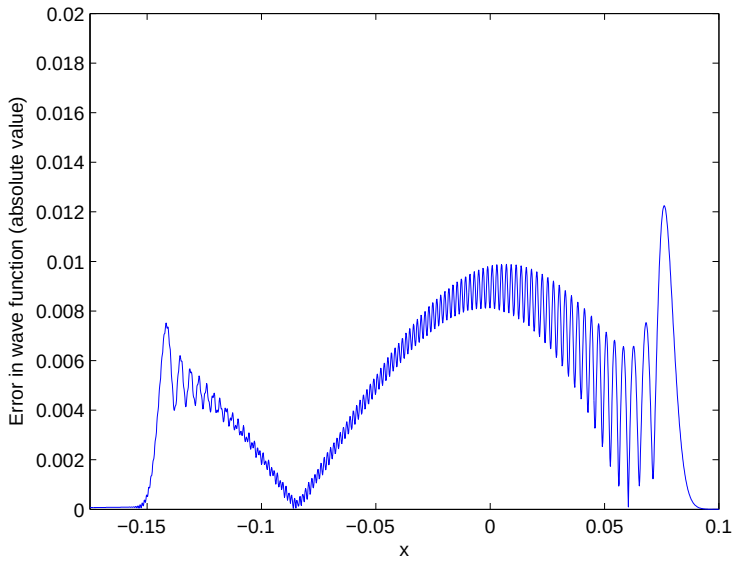
The so-called asymptotic decomposition method is to sample Gaussian beams on a uniform mesh $\{x_i\}$, with initial conditions

$$\begin{aligned} q_{x_i}(0) &= x_i \\ p_{x_i}(0) &= \partial_x S_0(x_i) \\ Q_{x_i}(0) &= 1 \\ P_{x_i}(0) &= \partial_{xx} S_0(x_i) + i \\ S_{x_i}(0) &= S_0(x_i) \\ c_0(0; x_i) &= A_0(x_i)(\pi\varepsilon)^{1/4} \\ c_k(0; x_i) &= 0, \quad k \geqslant 1. \end{aligned}$$

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 $t = 0.5$.





Summary

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 ε.

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 ε 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!

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!