Solving the Time-Dependent Schrödinger Equation on the Real Line

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Workshop on Numerical Analysis and Approximation Theory,
Vasyl Stefanyk Precarpathian National University (online),
12 May 2026

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The equation of interest

Time-Dependent Schrödinger Equation (TDSE)

$$\mathrm{i}\varepsilon\frac{\partial u}{\partial t} = -\varepsilon^2\frac{\partial^2 u}{\partial x^2} + V(x)u, \quad x \in \mathbb{R}, \quad t \geq 0,$$

where $0 < \varepsilon \ll 1$ (*semiclassical* parameter), $u(x,0) = u_0(x) \in \mathrm{L}_2(\mathbb{R})$ (initial condition), $V\colon \mathbb{R} \to \mathbb{R}$ (interaction potential, smooth).

The system is required to satisfy

$$\int_{\mathbb{R}} |u(x,t)|^2 \,\mathrm{d}x \equiv 1 \quad \text{for all } t,$$

and any numerical solution must be consistent with this **conservation law**.

Existence of dynamics

Assume that $\widehat{H}$ is a **self-adjoint operator** on a Hilbert space $\mathscr{H}$. Then, there is a unique family of unitary operators $\mathrm{e}^{-\mathrm{i}t\widehat{H}}$, $t \in \mathbb{R}$, with the following properties:

- Group property:
$$\mathrm{e}^{-\mathrm{i}(t+s)\widehat{H}} = \mathrm{e}^{-\mathrm{i}t\widehat{H}}\mathrm{e}^{-\mathrm{i}s\widehat{H}}, \quad \text{for all } t, s \in \mathbb{R}.$$
- Strong continuity: For all $u_0 \in \mathscr{H}$,
$$\mathrm{e}^{-\mathrm{i}t\widehat{H}}u_0 \to u_0 \quad \text{in the } \mathscr{H}\text{-norm as } t \to 0.$$
- **Solution of the TDSE**:
$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{-\mathrm{i}t\widehat{H}}u_0 = \widehat{H}\mathrm{e}^{-\mathrm{i}t\widehat{H}}u_0, \quad u_0 \in \mathscr{D}(\widehat{H}).$$

Free evolution

The solution of the Free Schrödinger Equation (FSE), that is, $V \equiv 0$, can be written in terms of the Fourier transform (FT), as

$$u(x,t) = \mathrm{e}^{-\mathrm{i}t\widehat{T}}u_0 = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\widehat{u}_0(\xi)\mathrm{e}^{-\mathrm{i}\xi^2\varepsilon t+\mathrm{i}x\xi}\mathrm{d}\xi,$$

where the FT is defined as

$$\widehat{u}_0(\xi) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}u_0(x)\mathrm{e}^{-\mathrm{i}\xi x}\mathrm{d}x.$$

Splittings

Suppose that $\widehat{T}$, $\widehat{V}$, and $\widehat{H} = \widehat{T} + \widehat{V}$ are self-adjoint operators on a Hilbert space $\mathscr{H}$. Then, for every $t \in \mathbb{R}$ and $u_0 \in \mathscr{H}$,

$$\mathrm{e}^{-\mathrm{i}t\widehat{H}} u_0 = \lim_{n\to\infty} \left(\mathrm{e}^{-\mathrm{i}t\widehat{T}/n} \mathrm{e}^{-\mathrm{i}t\widehat{V}/n} \right)^n u_0. \qquad \text{“Lie–Trotter”}$$

In view of the strong continuity of $\mathrm{e}^{-\mathrm{i}t\widehat{V}}$, an equivalent statement is

$$\mathrm{e}^{-\mathrm{i}t\widehat{H}} u_0 = \lim_{n\to\infty} \left(\mathrm{e}^{-\mathrm{i}t\widehat{V}/(2n)} \mathrm{e}^{-\mathrm{i}t\widehat{T}/n} \mathrm{e}^{-\mathrm{i}t\widehat{V}/(2n)} \right)^n u_0. \qquad \text{“Strang”}$$

Note that in general the operators $\widehat{T}$ and $\widehat{V}$ **do not commute**.

We will look at the speed of convergence later.

Real line versus periodic boundary conditions

- The TDSE is naturally defined on the **real line** because quantum particles move in **unbounded physical space** rather than on a periodic domain; localized wave packets decay at infinity, whereas periodic boundary conditions introduce nonphysical self-interactions.
- Many papers address the treatment of splitting techniques in both the semiclassical regime, $0 < \varepsilon \ll 1$, and the atomistic regime, $\varepsilon = 1$. However, they typically consider the equation on a torus with **periodic boundary conditions**.

$\longrightarrow$ Main reason: The TDSE with periodic boundary conditions can be approximated efficiently by means of the **Fast Fourier Transform** (FFT).

The Split Operator Fourier Transform (SOFT) method

Consider the TDSE

$$\mathrm{i}\frac{\partial u}{\partial t} = \widehat{H}u = -\frac{\partial^2 u}{\partial x^2} + V(x)u, \quad x \in [-\pi, \pi], \quad t \geq 0,$$

with **periodic boundary conditions** $u(-\pi, t) = u(\pi, t)$ for all t.

Galerkin method: Consider a finite-dimensional approximation space $\mathscr{V}_K$ spanned by $K \geq 1$ basis functions $\varphi_0, \ldots, \varphi_{K-1}$. We determine an approximate wave function $\psi_K(t) \in \mathscr{V}_K$ by the condition that, at every instant t,

$$\frac{\mathrm{d}\psi_K}{\mathrm{d}t} \in \mathscr{V}_K \quad \text{such that} \quad \left\langle \varphi, \mathrm{i}\frac{\mathrm{d}\psi_K}{\mathrm{d}t} - \widehat{H}\psi_K \right\rangle = 0 \quad \text{for all } \varphi \in \mathscr{V}_K.$$

$\langle \cdot, \cdot \rangle$ denotes the inner product on $\mathrm{L}_2([-\pi, \pi])$.

Upon writing

$$\psi_K(t) = \sum_{k=0}^{K-1} c_k(t)\varphi_k$$

and inserting this into the **Galerkin condition**, we find

$$\mathrm{i} M_K \dot{c} = H_K c, \quad c \in \mathbb{C}^K,$$

with matrices $(M_K)_{j,k} = \langle \varphi_j, \varphi_k \rangle$, $(H_K)_{j,k} = \langle \varphi_j, \widehat{H}\varphi_k \rangle$.

For the **Fourier basis functions**

$$\varphi_k(x) = \mathrm{e}^{\mathrm{i}kx}/\sqrt{2\pi}, \quad k = -K/2, \ldots, K/2-1,$$

we obtain $M_K = \mathrm{Id}$ as well as

$$(H_K)_{j,k} = (D_K)_{j,k} + (V_K)_{j,k} := k^2\delta_{j,k} + \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}jx} V(x) \mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}x.$$

Using the FFT, the **matrix elements of V_K** can be approximated by

$$V_K \approx \mathscr{F}_K D_V \mathscr{F}_K^{-1}, \qquad D_V = \mathrm{diag}(V(x_0), \ldots, V(x_{K-1})),$$

where $\mathscr{F}_K \colon \mathbb{C}^K \to \mathbb{C}^K$ denotes the (unitary) **discrete Fourier transform** (DFT).

The integral is approximated via the trapezoidal rule.

The **SOFT method** is now obtained by computing the solution

$$c(t) = \mathrm{e}^{-\mathrm{i}t(D_K + \mathscr{F}_K D_V \mathscr{F}_K^{-1})} c_0$$

using, for example, the Lie–Trotter splitting:

$$\begin{aligned} c(t) &= \mathrm{e}^{-\mathrm{i}t(D_K + \mathscr{F}_K D_V \mathscr{F}_K^{-1})} c_0 \approx \left(\mathrm{e}^{-\mathrm{i}tD_K/n} \mathrm{e}^{-\mathrm{i}t\mathscr{F}_K D_V \mathscr{F}_K^{-1}/n} \right)^n c_0 \\ &= \left(\mathrm{e}^{-\mathrm{i}tD_K/n} \mathscr{F}_K \mathrm{e}^{-\mathrm{i}tD_V/n} \mathscr{F}_K^{-1} \right)^n c_0. \end{aligned}$$

The DFT is executed via the FFT with complexity $\mathscr{O}(K \log K)$.

SOFT is the gold standard

(in moderate dimensions)

The **periodic setting imposes unwelcome limitations** on the solution. Provided the equation is solved for sufficiently long time, the wave function can reach the boundary. Periodicity then becomes a problem since the wave function "pops out" at the other end.

SOFT has also been implemented for high-dimensional systems.

See numerical experiments (1 and 2) for harmonic potential!

- $\varepsilon = 1$
- $V(x) = \frac{1}{2}x^2$
- $u_0 = \pi^{-1/4} \exp\left(-x^2/2 + \mathrm{i}x\right)$

Splittings via the sBCH formula

Goal: Determine the **effective exponent of the Strang splitting**

$$\mathrm{e}^{\frac{t}{2}A}\mathrm{e}^{tB}\mathrm{e}^{\frac{t}{2}A} = \mathrm{e}^{S(A,B;t)}, \qquad S(A,B;t) = tS_1 + t^3S_3 + t^5S_5 + \cdots$$

$\rightarrow$ A direct expansion yields the first coefficients:

$$S_1 = A + B, \qquad S_3 = -\frac{1}{24}[[B,A],A] - \frac{1}{12}[[B,A],B].$$

Remark:

A general formula for $S(A,B;t)$ can be obtained in a much more elegant way!

Here A and B are assumed **bounded**. Extending $S(A,B;t)$ to unbounded operators is nontrivial.

Order of the Strang splitting in semiclassical scaling

From the sBCH expansion we obtain the (local) error estimate

$$\begin{aligned} \mathrm{e}^{\frac{t}{2}A}\mathrm{e}^{tB}\mathrm{e}^{\frac{t}{2}A} - \mathrm{e}^{t(A+B)} &= \mathrm{e}^{t(A+B)+\mathscr{O}(h^3)} - \mathrm{e}^{t(A+B)} \\ &= \mathrm{e}^{t(A+B)} + \mathscr{O}(h^3) - \mathrm{e}^{t(A+B)} = \mathscr{O}(t^3), \end{aligned}$$

where the leading error term is determined by triple commutators

$$[[B,A],A], \qquad [[B,A],B].$$

Question: What changes when we **apply the splitting to the semiclassical TDSE**?

Consider $\partial_t u(\tau) = (A+B)u(\tau)$ with $A = -\varepsilon^{-1}V$ and $B = \varepsilon\partial_x^2$. Then,

$$[[B,A],B] = -\varepsilon[[\partial_x^2, V], \partial_x^2] = \varepsilon\left(V^{(4)} + 4V^{(3)}\partial_x + 4V^{(2)}\partial_x^2\right)$$

$$[[B,A],A] = \varepsilon^{-1}[[\partial_x^2, V], V] = \varepsilon^{-1}2(V^{(1)})^2.$$

Thus, setting $\tau = ih$, the leading local error term satisfies

$$\mathrm{e}^{h(A+B)} - \mathrm{e}^{\frac{h}{2}A}\mathrm{e}^{hB}\mathrm{e}^{\frac{h}{2}A} = \mathscr{O}(h^3\varepsilon^{-1}).$$

Consequently, the **effective order** depends on the relation between h and ε:

$$\text{e.g.} \quad h \sim \varepsilon \;\Rightarrow\; \mathscr{O}(h^2), \qquad h \sim \sqrt{\varepsilon} \;\Rightarrow\; \mathscr{O}(h).$$

Remarks

- Unless the time step is unacceptably reduced, the **effective error is larger** than that suggested by an analysis which ignores the smallness of ε.
- The order reduction for Hamiltonians in a semiclassical setting motivates the search for **higher-order splittings**.

$\rightarrow$ **Symmetric Zassenhaus splittings**

Obtaining higher orders via symmetric Zassenhaus

$$\mathrm{e}^{\frac{t}{2}A}\mathrm{e}^{tB}\mathrm{e}^{\frac{t}{2}A} = \mathrm{e}^{S(A,B;t)} \quad \Leftrightarrow \quad \mathrm{e}^{tB} = \mathrm{e}^{-tA/2}\mathrm{e}^{S(A,B;t)}\mathrm{e}^{-tA/2}$$

Step 1, via the substitution $A \leftarrow -A,\ B \leftarrow A+B,\ S(-A,A+B;t) = tB + \mathscr{O}(t^3)$

$$\mathrm{e}^{t(A+B)} = \mathrm{e}^{tA/2}\mathrm{e}^{S(-A,A+B;t)}\mathrm{e}^{tA/2}$$

Step 2, via the substitution $A \leftarrow -B,\ B \leftarrow S(-A,A+B;t)$

$$\mathrm{e}^{-tB/2}\mathrm{e}^{S(-A,A+B;t)}\mathrm{e}^{-tB/2} = \mathrm{e}^{S(-B,S(-A,A+B;t);t)}$$

Hence,

$$\mathrm{e}^{t(A+B)} = \mathrm{e}^{tA/2}\mathrm{e}^{tB/2}\mathrm{e}^{S(-B,S(-A,A+B;t);t)}\mathrm{e}^{tB/2}\mathrm{e}^{tA/2}$$

Further iterations lead to splittings of the form $\mathscr{O}(h^{2n-1}\varepsilon^{-1})$ for $n = 3,4,\ldots$

Example for the TDSE ($n = 3$):

$$u(x,h) = \mathrm{e}^{\mathscr{R}_{-1}}\mathrm{e}^{\mathscr{R}_1}\mathrm{e}^{2\mathscr{R}_3}\mathrm{e}^{\mathscr{R}_1}\mathrm{e}^{\mathscr{R}_{-1}}u_0(x) + \mathscr{O}(h^5\varepsilon^{-1}),$$

where the Zassenhaus exponentials are given by

$$\mathscr{R}_{-1}(\tau) = -\frac{1}{2}\tau\varepsilon^{-1}V,$$

$$\mathscr{R}_1(\tau) = \frac{1}{2}\tau\varepsilon\partial_x^2,$$

$$\mathscr{R}_3(\tau) = \frac{1}{12}\tau^3\varepsilon\left\{\partial_x^2[V^{(2)}\cdot] + V^{(2)}\partial_x^2\right\} + \frac{1}{24}\tau^3\varepsilon^{-1}(V^{(1)})^2.$$

The exponential of the orange term can be computed e.g. with the *Hermitian Lanczos algorithm*.

An algorithm based on exact free Schrödinger evolutions

Recall the SOFT ansatz (on $[-\pi, \pi]$ with periodic boundary conditions):

$$\psi_K(t) = \sum_{k=0}^{K-1} c_k(t)\varphi_k$$

We now seek an analogue **on the real line** based on two ingredients:

1. A basis $\{\varphi_k\}$ for which expansion coefficients $\widehat{u}_k := \langle u_0, \varphi_k \rangle$ can be computed accurately and efficiently,
2. **Closed-form evolution** of the basis functions under the FSE,

$$\mathrm{e}^{-\mathrm{i}t\widehat{T}}\varphi_j(x) =: \psi_j(x,t)$$

A computational method based on Strang splitting:

Step Pre1: Compute the expansion coefficients for the initial wave function:

$$\widehat{u}_k = \langle u_0, \varphi_k \rangle, \quad k = 1, \dots K.$$

Step Pre2: Compute the **connection matrix** for the $\frac{1}{2}$-FSE action

$$\widehat{\psi}_{j,k} = \langle \mathrm{e}^{-\mathrm{i}\frac{h}{2}\widehat{T}} \varphi_k, \varphi_j \rangle = \langle \psi_k(\cdot, h/2), \varphi_j \rangle, \quad j, k = 1, \dots K.$$

Step Pre3: Compute the **connection matrix** for the potential action

$$\widehat{v}_{j,k} = \langle \mathrm{e}^{-\mathrm{i}h\widehat{V}} \varphi_k, \varphi_j \rangle, \quad j, k = 1, \dots K.$$

Step Iter: For $n = 1, 2, \ldots$, compute the coefficients of the evolved wave functions:

$$\widehat{u}_{j,1/2,-} = \sum_k \widehat{\psi}_{j,k} \widehat{u}_k$$
$$\widehat{u}_{j,1/2} = \sum_k \widehat{v}_{j,k} \widehat{u}_{k,1/2,-}$$
$$\widehat{u}_{j,1/2,+} = \sum_k \widehat{\psi}_{j,k} \widehat{u}_{k,1/2}$$
$$\widehat{u} \leftarrow \widehat{u}_{1/2,+}$$

- For the computation of the expansion coefficients, it is natural to use a quadrature rule adapted to the chosen basis functions (e.g. **Gaussian quadrature nodes**).
- In some situations, the connection matrix $\widehat{\psi}_{j,k}$ can even be computed analytically.
- The expansion coefficients and off-diagonal entries of $\widehat{\psi}_{j,k}$ typically **decay rapidly**. Hence the overall error is usually dominated by the splitting error.

Choice of the basis functions

What basis functions can be used to obtain a

closed formula under the FSE?

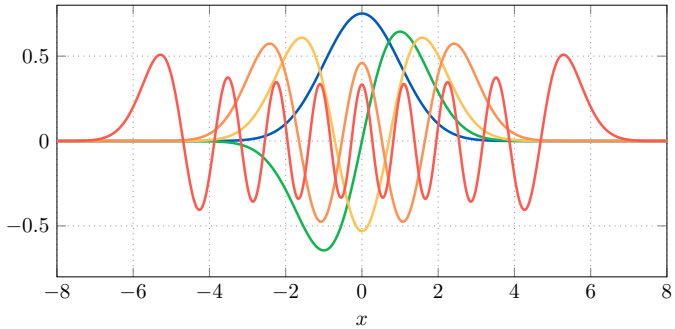
Hermite functions

The **Hermite functions** are given by

$$\varphi_n(x) = \frac{1}{\left(2^n n! \pi^{1/2}\right)^{1/2}} \mathrm{H}_n(x) \mathrm{e}^{-x^2/2}, \quad n \in \mathbb{Z}_+,$$

where H_n is the nth **Hermite polynomial**. They are eigenfunctions of the FT:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi_n(\xi) \mathrm{e}^{\mathrm{i}x\xi} \mathrm{d}\xi = \mathrm{i}^n \varphi_n(x), \quad x \in \mathbb{R}, \quad n \in \mathbb{Z}_+.$$



blue: $n = 0$, green: $n = 1$, yellow: $n = 2$, orange: $n = 4$, red: $n = 16$

Exact FSE dynamics

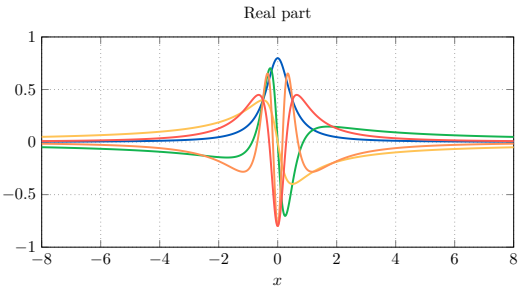
The explicit form of the Hermite FSE is given for all $x \in \mathbb{R}$ and all $t \geq 0$ by

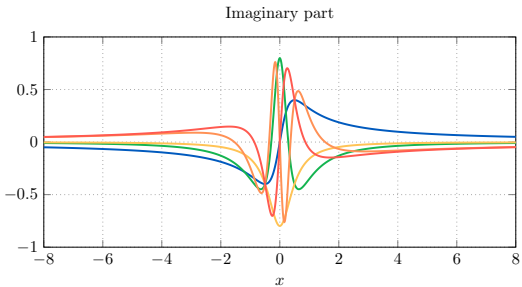
$$\psi_n(x,t) = \frac{(1+2i\varepsilon t)^{n/2}}{(1-2i\varepsilon t)^{(n+1)/2}} \exp\left(-\frac{it\varepsilon x^2}{1+4\varepsilon^2 t^2}\right) \varphi_n\left(\frac{x}{(1+4\varepsilon^2 t^2)^{1/2}}\right).$$

Malmquist–Takenaka functions

The **Malmquist–Takenaka functions** are given by

$$\varphi_n(x) = \sqrt{\frac{2}{\pi}}\mathrm{i}^n \frac{(1+2\mathrm{i}x)^n}{(1-2\mathrm{i}x)^{n+1}}, \quad n \in \mathbb{Z},$$





blue: $n = 0$, green: $n = 1$, yellow: $n = -1$, orange: $n = 2$, red: $n = -2$

FSE dynamics

The Malmquist–Takenaka system obeys the following recurrence for $n \geq 1$,

$$\psi_0(x,t) = \sqrt{\frac{\mathrm{i}}{8\varepsilon t}} \exp\left(\frac{(2x+\mathrm{i})^2}{16\mathrm{i}\varepsilon t}\right) \operatorname{erfc}\left(\frac{(2x+\mathrm{i})}{\sqrt{16\mathrm{i}\varepsilon t}}\right),$$

$$\psi_1(x,t) = -\mathrm{i}\psi_0 + (1-2\mathrm{i}x)\,\frac{\psi_0(x,t)-\psi_0(x,0)}{4\varepsilon t}$$

$$\mathrm{i}(n+1)\psi_{n+1} = \left(3n+1+\frac{2x+\mathrm{i}}{4\varepsilon t}\right)\psi_n + \mathrm{i}\left(3n-1+\frac{2x-\mathrm{i}}{4\varepsilon t}\right)\psi_{n-1} - (n-1)\psi_{n-2}.$$

→ **Clenshaw's algorithm** is most commonly applied to bases that satisfy three-term recurrence relations, and it can be used to compute the above FSE system.

See numerical experiment (3) for harmonic potential!

- $\varepsilon = 1$
- $V(x) = \frac{1}{2}x^2$
- $u_0 = \pi^{-1/4} \exp\left(-x^2/2 + \mathrm{i}x\right)$

See numerical experiment (4) for double-well potential!

- $\varepsilon = 1$
- $V(x) = \frac{1}{16\eta}x^4 - \frac{1}{2}x^2$, $\eta = 1.3544$
- $u_0 = \pi^{-1/4}\exp\left(-(x+2\sqrt{\eta})^2/2\right)$
- $K = 10$, $M = 64$
- SOFT with $M = 2048$ grid points

Further steps

- → Derivation of an **analytical connection matrix** in order to obtain a deeper structural understanding of the underlying evolution system.
- → Extension of the framework to **unbounded operators**. In particular, the symmetric Zassenhaus splitting appears to be applicable due to a rescaled semigroup property (ensuring that the expressions $\mathrm{e}^{\tau^{2n-1}\mathscr{R}_{2n-1}(1)}$ are well-defined).
- → Application of HFSE evolutions to **nonlinear Schrödinger equations**, especially to the *Gross–Pitaevskii equation*.

Thank you.