Numerical Methods for the Nonlinear Schrödinger Equation with Low-regularity Potential & Nonlinearity

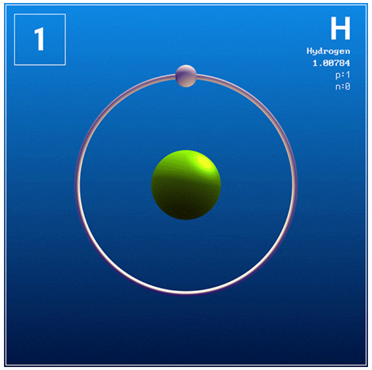
Weizhu Bao

Department of Mathematics

National University of Singapore

Email: matbaowz@nus.edu.sg

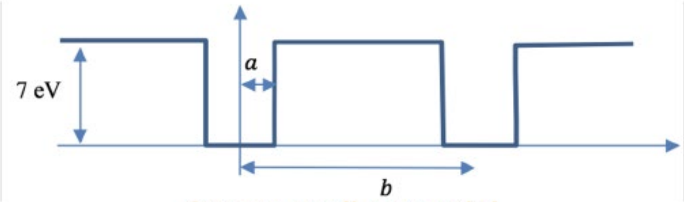
URL: http://blog.nus.edu.sg/matbwz/



Collaborators: Yue Feng (XJTU), Bo Lin (Huairou Lab), Ying Ma (Beijing Univ Tech.)
Chushan Wang (Univ Chicago), Yifei Wu (Nanjing Normal Univ)

Outline

- (Nonlinear) Schrödinger equation
  - Background, properties & different applications
  - Review of existing numerical methods & error bounds under `smooth' solutions
- For low-regularity potential & nonlinearity
  - Time-splitting methods
  - Exponential wave integrator (EWI)
  - A novel explicit & symmetric EWI (sEWI)



Square-well potential

- Extensions to
  - Singular potential & nonlinearity
  - Other dispersive PDEs, ….
- Conclusions

Coulomb potential

$$V(\vec{x}) = \sum_{j=1}^{N} \frac{Z_j}{|\vec{x} - \vec{x}_j|}$$

The Schrödinger equation

- Written by Ewin Schrödinger in 1925 —Nobel prize in 1933

$$i\hbar\,\partial_t\psi(\vec{x},t)=\left(-\frac{\hbar^2}{2m}\nabla^2+V(\vec{x})\right)\psi(\vec{x},t)\quad\underset{\vec{p}\to -i\hbar\nabla}{\overset{E\to i\hbar\partial_t}{\Leftarrow}}\quad E=\frac{\vec{p}^{\,2}}{2m}+V(\vec{x})$$

  - It describes the evolution over time of a physical system in which quantum effects, such as wave–particle duality, are significant in quantum mechanics.

- Physical observables
  - With probability density and current

$$\rho=|\psi|^2=\psi^*\psi,\qquad j=\frac{\hbar}{m}\mathrm{Im}\left(\psi^*\nabla\psi\right)$$

  - Continuity equation $\partial_t\rho+\nabla\bullet j=0$
  - Explain the spectrum of the Hydrogen atom

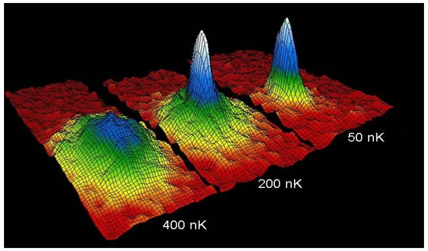
Ewin Schrödinger

The nonlinear Schrödinger equation (NLSE)

$$i\partial_t \psi = -\Delta \psi + V(\vec{x})\psi + f\left(|\psi|^2\right)\psi$$

- t : time & $\vec{x}\ (\in \mathbb{R}^d)$ with $d = 1,2,3$: spatial coordinate
- $\psi := \psi(\vec{x},t)$: complex-valued wave function or order parameter
- $V(\vec{x})$: real-valued external potential
- $f(\rho)$ with $\rho := |\psi|^2 \geq 0$: given nonlinearity
  - =0: linear;
  - >0: repulsive interaction (or defocusing nonlinearity)
  - <0: attractive interaction (or focusing nonlinearity)
- For dynamics, initial data is given as

$$\psi(\vec{x},t=0) = \psi_0(\vec{x}), \quad \vec{x} \in \mathbb{R}^d$$



BEC@ JILA, 1995

Numerical Methods for NLSE

$$i\partial_t \psi = -\Delta \psi + V(\vec{x})\psi + f\left(|\psi|^2\right)\psi$$

- Different numerical methods
  - Finite difference time domain (FDTD) --Sanz-Serna, '84; Chan & Shen, '86; Glassey, 92'; Karakashian, Akrivis & Dougalis, '93; Akrivis, '93; Chan, '94; Chan, Guo & Jiang, 94'; Chang & Sun, '03; Bao & Cai, '13; Wang, '14; Henning & Peterseim, '17; ...
  - Time-splitting (pseudo)spectral (TSSP) method -- Hardin & Tarppent, '73; Taha & Ablowitz, 84'; Weideman & Herbst, 86'; Pathria & Moris, 90'; Jahnke & Lubich, '00; Besse, Bid´egaray & Descombes, '02; Bao, Jaksch & Markowich,'03; Lubich, '08; Antoine, Bao & Besse, '13; Eilinghoff, Schnaubelt & Schratz, '16; Ostermann, Rousset & Schratz, '22; Bao, Cai & Feng, '23; Carles & Su, '23; Ji & Ostermann, '23; Ji, Ostermann, Rousset & Schratz, '24; ...
  - Exponential wave integrator (EWI) --Berland, Owren and Skaflestad, '06; Celledoni,Cohen & Owren,'08; Hochbruck & Ostermann,'10; Bao & Cai, '14; Alama Bronsard, Bruned & Schratz,'22; Bao & Wang, 24',...
- Optimal error estimates under `smooth' solution!!
  - TSSP method is most popular in practical computation: due to stability, accuracy, efficiency, structure-preserving properties in full discrete level & optimal resolution in semiclassical regime!!

[1] X. Antoine, W. Bao and C. Besse, Computational methods for the dynamics of the nonlinear Schrödinger/Gross-Pitaevskii equations, Comput. Phys. Commun., Vol. 84, pp. 2621-2633, 2013.
[2]. W. Bao and Y. Cai, Mathematical theory and numerical methods for Bose-Einstein condensation, Kinet. Relat. Mod., Vol. 6, pp. 1-135, 2013.

Review on Error Estimates

$$i\partial_t \psi = -\Delta\psi + V(\vec{x})\psi + f\left(|\psi|^2\right)\psi$$

- Regularity on solution for different numerical methods $I := [0,T]$

	first-order in L^2	second-order in L^2
FDTD	$\psi \in C^2(I;L^2) \sim H^4$	$\psi \in C^3(I;L^2) \sim H^6$
Splitting	$\psi \in C(I;H^2)$	$\psi \in C(I;H^4)$
EWI	$\psi \in C^1(I;L^2) \sim H^2$	$\psi \in C^2(I;L^2) \sim H^4$

$$\psi \in H^4 \Leftrightarrow \partial_{tt} \in L^2$$

$$\Uparrow$$

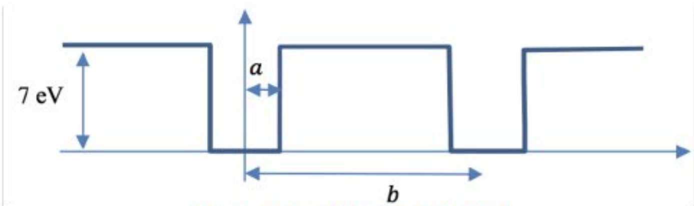
$$\psi_0 \in H^4 \ \& V \in H^2$$

$$f(\rho) = \rho^\sigma, \sigma \ge 1$$

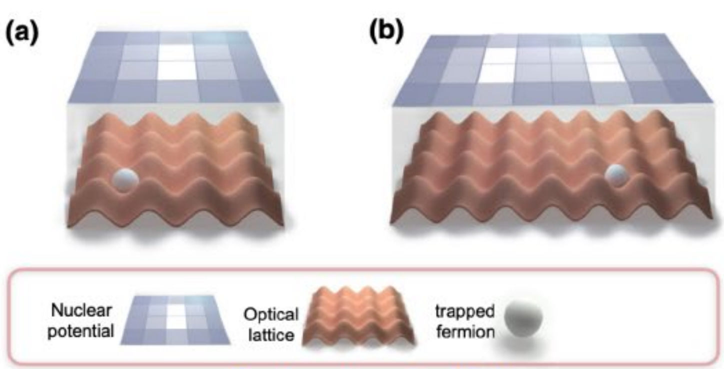
- Observations
  - FDTD methods require stronger regularity than others!!
  - Time-splitting methods and EWIs require the same regularity on solution
- How to handle the solution is low-regularity-- due to low-regularity of initial data, potential, nonlinearity???? – error estimates & new numerical methods with optimal error bounds ???
  - For low-regularity initial data $\quad \psi_0 \in H^2$ or $V \in L^\infty$ or $0 < \sigma < 1$???
    - Low-regularity integrators --Ostermann & Schratz, '18; Knoller, Ostermann & Schratz, '19; Zhao, '21; Li & Wu, '21; Alama Bronsard, Bruned & Schratz, '22; Alama Bronsard,'23; Ostermann, Rousset & Schratz; Feng, Maierhofer & Schratz, '23; Schratz & Rousset, '24; Feng, Maierhofer & Wang, '24; ...
  - Focus on NLSE with low-regularity (or even singular) potential & nonlinearity

Examples of Low-Regularity/Singular Potential

$$i\partial_t \psi = -\Delta \psi + V(\vec{x})\psi + f\left(|\psi|^2\right)\psi$$

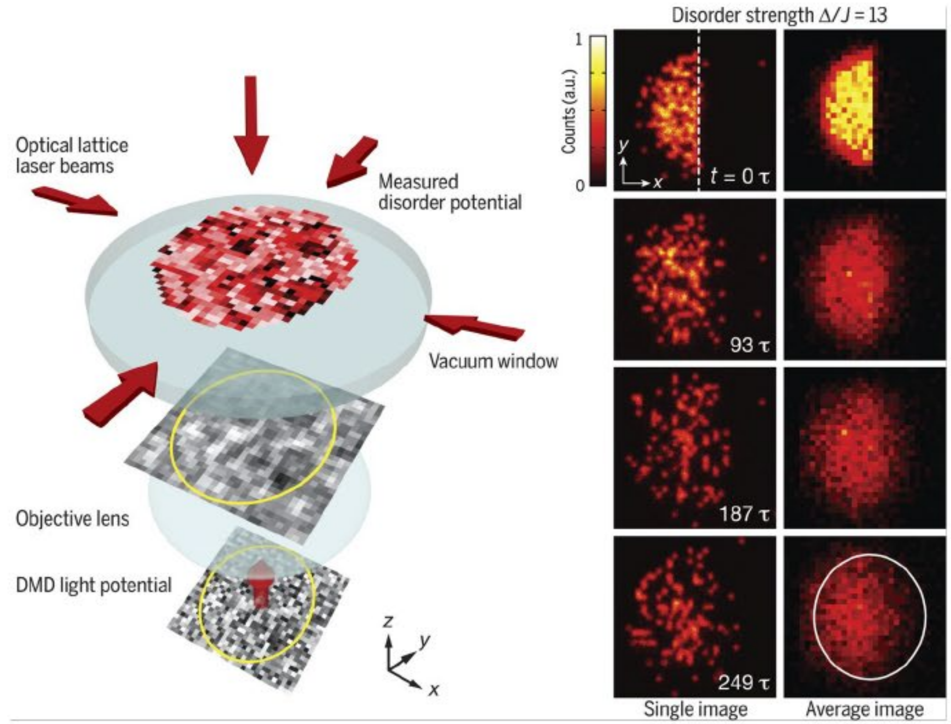


Square-well potential



Coulomb potential

$$V(\vec{x}) = \sum_{j=1}^{N} \frac{Z_j}{|\vec{x} - \vec{x}_j|}$$



Disorder potential

(Gross & Bloch, **Science**, 2017)

$$V(\vec{x}) = \sum_{\vec{l} \in \mathbb{Z}^d} \xi_{\vec{l}}\, e^{2\pi i \vec{l}\cdot\vec{x}/L}$$

The potential may be L^∞ (**low regularity**) or L^2 (even H^{-s}) (**singular**).

Examples of Low-Regularity/Singular Nonlinearity

$$i\partial_t\psi = -\Delta\psi + V(\vec{x})\psi + f\left(|\psi|^2\right)\psi$$

- **Non-integer power nonlinearity** (Schrödinger-Poisson-Xα model; Lee-Huang-Yang correction; Mean-field model for Bose-Fermi mixture; Non-Kerr media in nonlinear optics)

$$f(\rho) = \beta_1\rho^{\sigma_1} + \beta_2\rho^{\sigma_2}, \quad \rho \geq 0, \quad \beta_1, \beta_2 \in \mathbb{R}, \quad 0 < \sigma_1 < \sigma_2.$$

- **Logarithmic-power nonlinearity** (LHY correction in 2D)

$$f(\rho) = \beta\rho^\sigma \ln(\rho), \quad \rho \geq 0, \quad \beta \in \mathbb{R}, \quad \sigma > 0.$$

C^1-nonlinearity

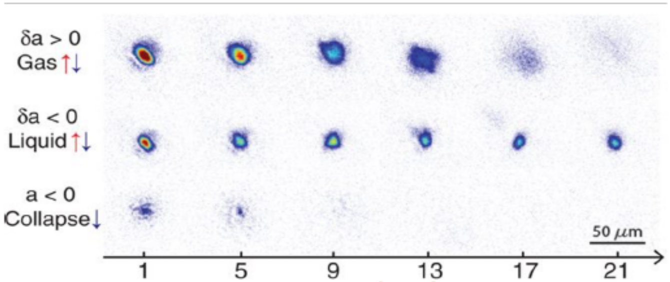
$f(|z|^2)z : \mathbb{C} \to \mathbb{C}$, $\mathbb{C} \leftrightarrow \mathbb{R}^2$

- **Logarithmic nonlinearity** (Optical Fiber; BEC;)

$$f(\rho) = \beta\ln(\rho), \quad \rho \geq 0, \quad \beta \in \mathbb{R}.$$

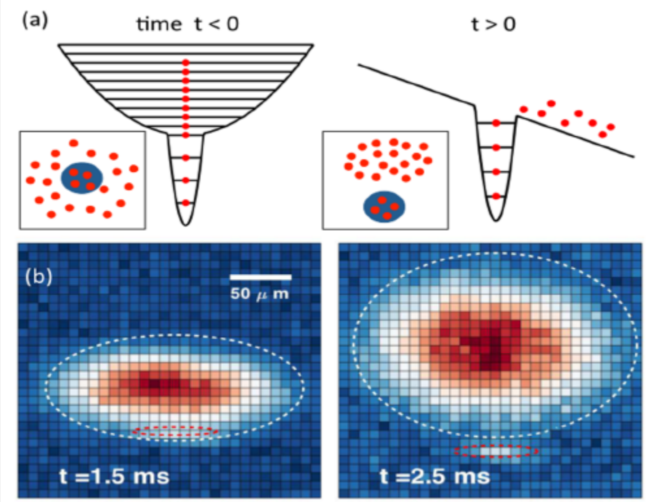
Singular nonlinearity

$f(|z|^2)z$ not locally Lipschitz



Quantum droplet

(Cabrera et al., **Science**, 2017)



Bose-Fermi mixture

(DeSalvo et al., **PRL**, 2017)

Problems to be Study Numerically

$$i\partial_t \psi = -\Delta \psi + V(\vec{x})\psi + f\left(|\psi|^2\right)\psi$$

1. **Optimal** error bounds on existing **popular** methods under
   - low regularity potential and nonlinearity:

$$V \in L^\infty \ \text{(bounded)}, \quad f(\rho) = \rho^\sigma \ (\sigma \in \mathbb{R}^+) \ \text{(local Lipschitz)}.$$

   - Singular potential: $V \in L^2$ (unbounded)
   - Singular nonlinearity: $f(\rho) = \ln \rho$ (not locally Lipschitz)

Well-posedness. well-posed in H^2 under all above: (Kato, '87; Cazenave, '03; Mauser, Wu, & Zhao, '24; Bao et al., '19)

$$\psi \in C([0,T]; H^2) \cap C^1([0,T]; L^2).$$

H^2 is sharp: Ill-posed in H^s $(s > 2)$ for $V \in L^2$; higher-than-H^2 open for LogSE.
Hence, focus on **time-splitting** and **EWI**.

2. **Design** novel **temporal** and **spatial** discretizations based on analysis: accuracy, efficiency, structure-preservation, etc

Review on Existing Results

$$i\partial_t \psi = -\Delta \psi + V(\vec{x})\psi + f\left(|\psi|^2\right)\psi$$

Low-regularity potential and nonlinearity

$$V \in L^\infty, \quad f(\rho) = \rho^\sigma \ (\sigma > 0).$$

The NLSE is well-posed in H^2: $\psi \in C([0,T]; H^2) \cap C^1([0,T]; L^2)$.

All methods can be directly applied but lack error estimates!

- **FDTD** (Henning & Peterseim, M3AS, '17)

$$V \in L^\infty, \ f \text{ smooth}, \ \psi \in C^2([0,T]; L^2) \implies \text{first-order in } L^2.$$

- **Time-splitting** with filter (Ignat, JDE, '11; Koh & Choi, DCDS, '21; Carles & Su, FoCM, '24)

$$V(\mathbf{x}) \equiv 0, \quad \sigma > 0, \quad H^2\text{-solution} \implies \text{half-order in } L^2(\Omega).$$

The filter **destroys ALL** structure-preserving properties of splitting methods! Valid only for **whole space**!

- **EWI** (Berland, Owren & Skaflestad, '06)

Observe advantages for low regularity potential but NO proof.

Difficulty: (i) Derive optimal order **LTE** estimate;

(ii) **Control the nonlinearity** at low regularity: $\psi^{n+1} = \Phi^\tau(\psi^n)$,

$$\|\Phi^\tau(v) - \Phi^\tau(w)\|_{L^2} \le (1 + C(\|v\|_{L^\infty}, \|w\|_{L^\infty})\tau)\|v - w\|_{L^2}.$$

Time-splitting Methods

The NLSE with non-integer power nonlinearity (C^1-nonlinearity if $\sigma > 0$)

$$\partial_t \psi = i\Delta\psi - i[V + \beta|\psi|^{2\sigma}]\psi =: A\psi + B(\psi)$$

Based on this decomposition, we obtain two sub-problems:

$$\begin{cases} \partial_t \psi = A\psi, \\ \psi(\mathbf{x}) = \psi_0, \end{cases} \qquad \begin{cases} \partial_t \psi = B(\psi), \\ \psi(0) = \psi_0, \end{cases}$$

$$\Longrightarrow \ \psi(t) = e^{it\Delta}\psi_0, \qquad \Longrightarrow \ \psi(t) = \Phi_B^t(\psi_0) := \psi_0 e^{-it(V+\beta|\psi_0|^{2\sigma})},$$

where $|\psi(t)| \equiv |\psi(0)|$ for $t \geq 0$ in B step.

Time-splitting Fourier spectral/pseudospectral (Trotter, '59; Strang, '68)

$$\psi^{[n+1]} = \Phi^\tau_{\text{Lie}}(\psi^{[n]}) := e^{i\tau\Delta}\Pi_N \Phi_B^\tau(\psi^{[n]}), \qquad \text{(Lie-Trotter)}$$

$$\psi^{[n+1]} = \Phi^\tau_{\text{Strang}}(\psi^{[n]}) := e^{i\frac{\tau}{2}\Delta}\Pi_N \Phi_B^\tau\left(e^{i\frac{\tau}{2}\Delta}\psi^{[n]}\right). \qquad \text{(Strang)}$$

- $\Pi_N = P_N$ for spectral (P_N: Fourier projection onto $X_N := \left\{e^{ilx} : l = -\frac{N}{2}, \cdots, \frac{N}{2} - 1\right\}$)
- $\Pi_N = I_N$ for pseudospectral (I_N: Fourier interpolation operator on X_N)

Estimates of Lie Splitting

Theorem (W. Bao & C. Wang, Math. Comp., 2024)

Assume $V \in H^2(\Omega)$, $\sigma > 0$ and H^2-solution,

$$\|\psi(\cdot, t_n) - \psi^{[n]}\|_{L^2} \lesssim \tau^{\frac{1}{2}+\sigma \wedge 1}.$$

LTE: with $B(\phi) = -i(V\phi + |\phi|^{2\sigma}\phi)$

$$\mathcal{L}^n \approx \tau^2 [B, i\Delta](\psi(t_n)) = -i\Delta B(\psi) + dB(\psi)[i\Delta\psi],$$

and $[B, i\Delta](\psi) \in L^2$ requires $V \in H^2$, $\psi \in H^2$, C^2-nonlinearity.

Control the nonlinearity:

- $\underline{0 < \sigma \le 1/2}$: an unconditional L^2-stability

$$\|\Phi^\tau(v) - \Phi^\tau(w)\|_{L^2} \le (1 + C(M)\tau)\|v - w\|_{L^2},$$

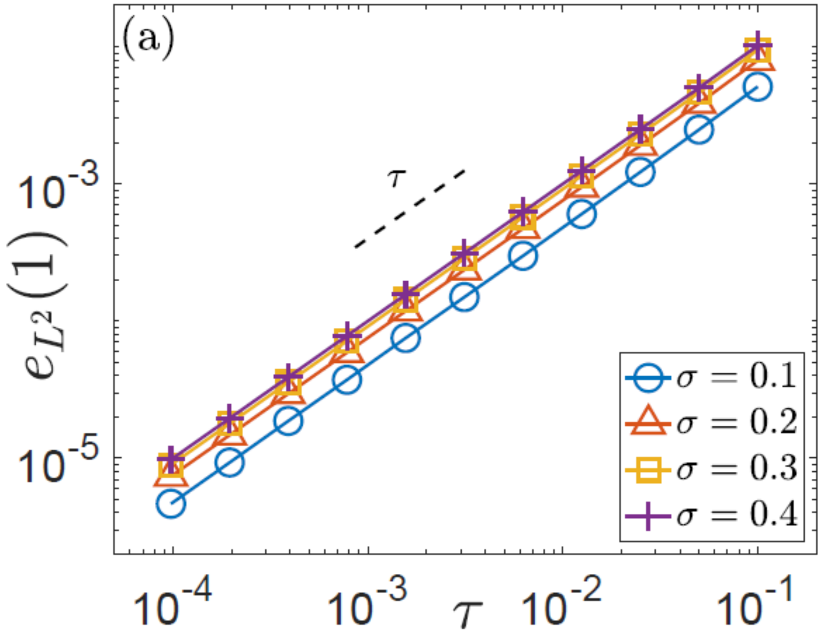
where $M := \min\{\|v\|_{L^\infty}, \|w\|_{L^\infty}\} < \infty$. (recall $\Phi^\tau(v) = e^{i\tau\Delta}(ve^{-i\tau f(|v|^2)})$).

- $\underline{\sigma \ge 1/2}$: fractional error bounds in H^1-norm with induction. (discrete Sobolev inequalities under $\tau \lesssim \frac{1}{|\ln h|}$ in 2D and $\tau \lesssim h$ in 3D)

[1] W. Bao & C. Wang, Error estimates of the time-splitting methods for the nonlinear Schrödinger equation with semi-smooth nonlinearity, Math. Comp., Vol 93 (2024), pp. 1599-1631.

Numerical Results: Low-regularity Nonlinearity

Take $V(x) \equiv 0$, $f(\rho) = -\rho^\sigma$ and $\psi_0(x) = xe^{-x^2/2}$, $x \in \Omega$.



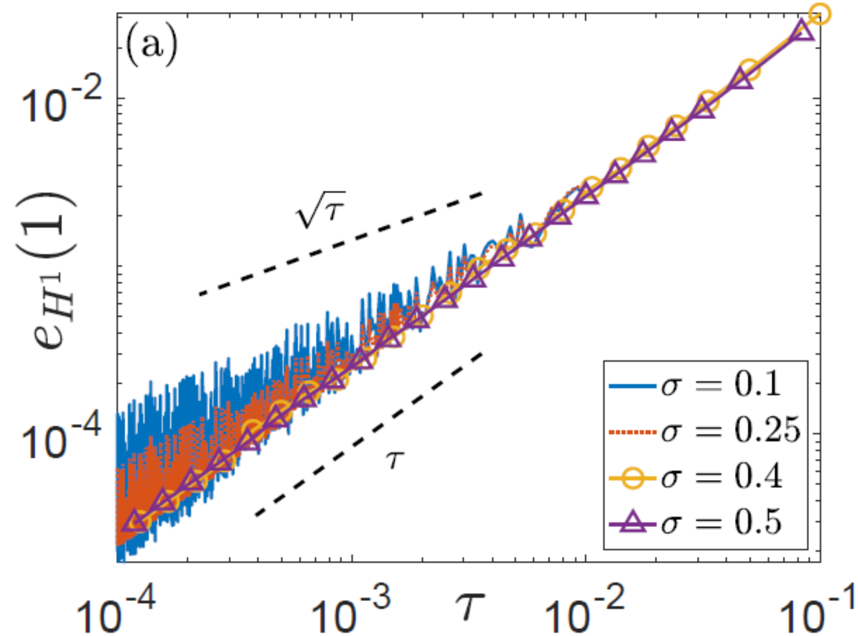


Figure 1: temporal errors in L^2-norm (left) and H^1-norm (right) for different σ.

First order in L^2 when $\sigma > 0$. First order in H^1 when $\sigma \geq 1/2$.

[1] W. Bao & C. Wang, Error estimates of the time-splitting methods for the nonlinear Schrödinger equation with semi-smooth nonlinearity, Math. Comp., Vol 93 (2024), pp. 1599-1631.

Improved Error Bounds for Lie-Splitting

Using Fourier spectral method in space and by refined analysis,

Theorem (W. Bao, Y. Ma & C. Wang, M3AS, 2024)

Assume $V \in L^\infty(\Omega)$, $\sigma > 0$, *and* H^2*-solution, when* $\tau \leq h^2/\pi$,

$$\|\psi(\cdot, t_n) - \psi^n\|_{L^2} \lesssim \tau + h^2.$$

- **Improvements**: by RCO, the **LTE** in time

$$\Delta(V\psi + f(|\psi|^2)\psi) \to \partial_t(V\psi + f(|\psi|^2)\psi).$$

By using Fourier spectral method, spatial error is optimal.

- **Stability compensation regularity:** $\tau \leq \frac{h^2}{\pi}$ compensates regularity loss

$$\psi^{n+1} = e^{i\tau\Delta}\left(\psi^n e^{-i\tau(V + f(|\psi^n|^2))}\right) \in L^\infty, \quad \text{if } V \in L^\infty, \psi^n \in H^2.$$

- Optimal **spatial** error is necessary for optimal **temporal** error

Selected in **M3AS 35th Anniversary Virtual Issue** as one of 18 highly cited papers published between 2019-2024 in M3AS

[1] W. Bao Y. Ma & C. Wang, Optimal error bounds on time-splitting methods for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, Math. Models Methods Appl. Sci., Vol 34 (2024), pp. 803-844.

A 1st Order Exponential Wave Integrator (EWI)

By Duhamel's formula, with $B(\phi) := V\phi + f(|\phi|^2)\phi$, $\partial_t\psi = i\Delta\psi - i[V + \beta|\psi|^{2\sigma}]\psi =: A\psi + B(\psi)$

$$\psi(t_{n+1}) = e^{i\tau\Delta}\psi(t_n) - i\int_0^\tau e^{i(\tau-s)\Delta}\underbrace{B(\psi(t_n+s))}_{\approx B(\psi(t_n))}\,\mathrm{d}s.$$

A first-order EWI (exponential Euler scheme)

$$\psi^{[n+1]} = e^{i\tau\Delta}\psi^{[n]} - i\tau\varphi_1(i\tau\Delta)B(\psi^{[n]}), \quad n \geq 0,$$

where $\varphi_1(z) = \frac{e^z - 1}{z}$ for $z \in \mathbb{C}$.

Remark

The filter function has smoothing effect: $\varphi_1(i\tau\Delta) \sim \tau^{-1}\Delta^{-1}$. If $B \in L^\infty$,

$$\psi^{[n+1]} = e^{i\tau\Delta}\psi^{[n]} - i\tau\varphi_1(i\tau\Delta)B(\psi^{[n]}) \in H^2, \qquad \text{(EWI)}$$

$$\psi^{[n+1]} = e^{i\tau\Delta}\left(\psi^{[n]}e^{-i\tau(V+f(|\psi^{[n]}|^2))}\right) \in L^\infty. \qquad \text{(Lie-Trotter)}$$

[1] W. Bao & C. Wang, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol. 62 (2024), pp. 93-118.

Error Bounds of EWI

Theorem (W. Bao & C.Wang, SINUM, 2024)

Assume $V \in L^\infty(\Omega)$, $\sigma > 0$, *and* H^2*-solution,*

$$\|\psi(\cdot, t_n) - \psi^{[n]}\|_{L^2} \lesssim \tau, \quad \|\psi^{[n]}\|_{H^2} \lesssim 1.$$

Remark: No time step size restriction is required; $\|\psi^{[n]}\|_{H^2} \lesssim 1$ recover the H^2 well-posedness.

Key ideas:

- From the construction of the EWI, optimal **LTE** in L^2-norm

$$\mathcal{L}^n = -i \int_0^\tau e^{i(\tau - s)\Delta}\left[B(\psi(t_n+s)) - B(\psi(t_n))\right]\mathrm{d}s \sim \tau^2 \partial_t B(\psi(t)) \implies \|\mathcal{L}^n\|_{L^2} \lesssim \tau^2.$$

- Smoothing effects **control nonlinearity** in high-order norm H^s $(s > \frac{d}{2})$.
  - Smoothing from equation for **LTE**: $\|\mathcal{L}^n\|_{H^2} \lesssim \tau \implies \|\mathcal{L}^n\|_{H^\alpha} \lesssim \tau^{2-\alpha/2}$
  - Smoothing from numerical scheme for **Stability**:

$$\|\varphi_1(i\tau\Delta)v\|_{H^\alpha} \lesssim \tau^{-\alpha/2}\|v\|_{L^2}, \quad 0 \le \alpha \le 2.$$

[1] W. Bao & C. Wang, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol. 62 (2024), pp. 93-118.

Numerical Results of EWI

With low regularity potential and nonlinearity:

$$V(x) = \begin{cases} -4, & x \in (-2,2) \\ 0, & \text{otherwise} \end{cases}, \quad \sigma = 0.1, \quad \psi_0 \in H^2.$$

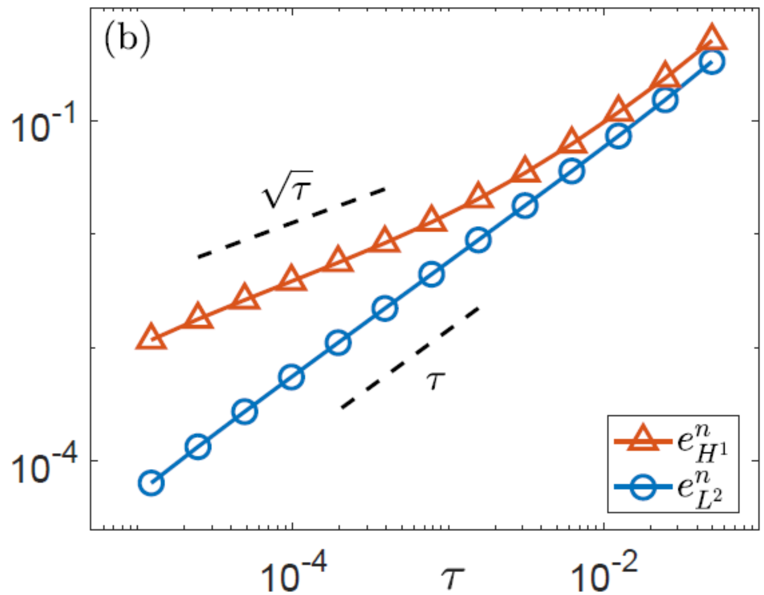
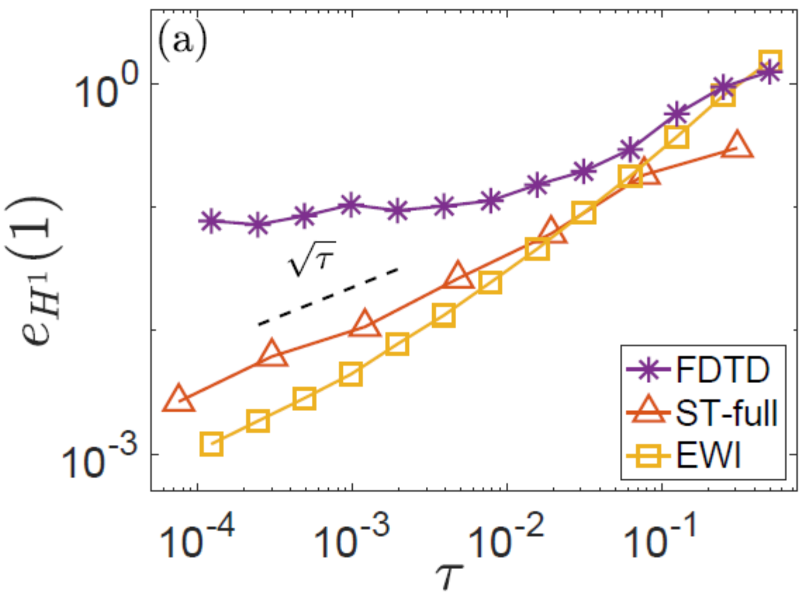


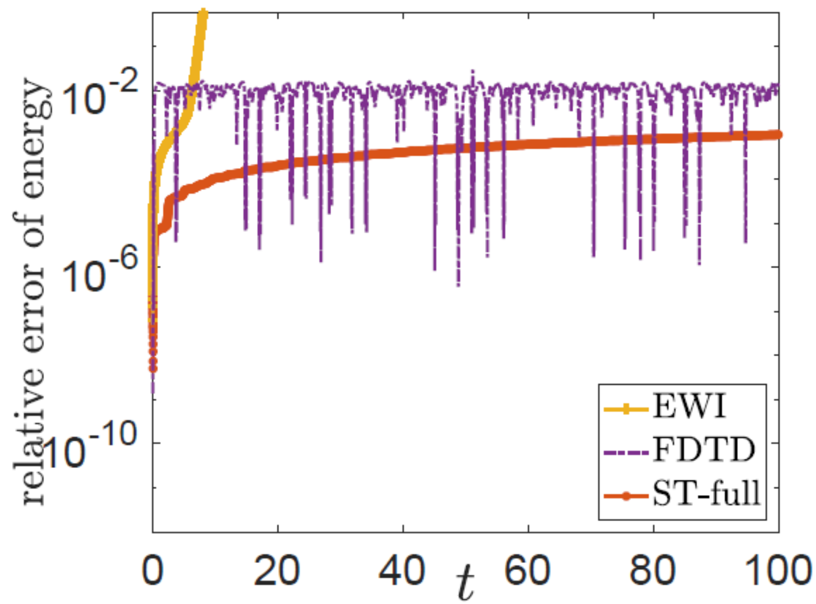
Figure 2: EWI with low regularity potential and nonlinearity (semi-discretization)

[1] W. Bao & C. Wang, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol. 62 (2024), pp. 93-118.

Comparison of Different Numerical Methods

Solve the NLSE with low regularity potential and nonlinearity:





(a) Errors in H^1 up to short time $T = 1$ (b) Energy errors up to long time $T = 100$

Explicit, **structure-preserving** and **high-order** **EWI** is needed!

[1] W. Bao & C. Wang, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol. 62 (2024), pp. 93-118.

A Novel Explicit & Symmetric EWI

Recalling the Duhamel's formula, $\partial_t \psi = i\Delta\psi - i[V + \beta|\psi|^{2\sigma}]\psi =: A\psi + B(\psi)$

$$e^{-i\zeta\Delta}\psi(t_n + \zeta) = \psi(t_n) - i\int_0^\zeta e^{-is\Delta}B(\psi(t_n + s))\mathrm{d}s. \qquad (*)$$

Taking $\zeta = \pm\tau$ in $(*)$, subtracting, multiplying $e^{i\tau\Delta}$,

$$\psi(t_{n+1}) = e^{2i\tau\Delta}\psi(t_{n-1}) - ie^{i\tau\Delta}\int_{-\tau}^{\tau} e^{-is\Delta}B(\psi(t_n + s))\mathrm{d}s.$$

Applying an explicit exponential mid-point rule, we get

$$\int_{-\tau}^{\tau} e^{-is\Delta}B(\psi(t_n+s))\mathrm{d}s \approx \int_{-\tau}^{\tau} e^{-is\Delta}B(\psi(t_n))\mathrm{d}s = 2\tau\mathrm{sinc}(\tau\Delta)B(\psi(t_n)),$$

which yields

$$\psi(t_{n+1}) \approx e^{2i\tau\Delta}\psi(t_{n-1}) - 2i\tau e^{i\tau\Delta}\,\mathrm{sinc}(\tau\Delta)B(\psi(t_n)).$$

[1] W. Bao & C. Wang, An explicit and symmetric exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol 62 (2024), pp. 1901-1928.

sEWI & its Error Bounds

Recall $B(v) = Vv + f(|v|^2)v$. Let $\psi^{[n]}$ approximates $\psi(t_n)$.

sEWI (W. Bao & C. Wang, SINUM, 2024)

$$\psi^{[n+1]} = e^{2i\tau\Delta}\psi^{[n-1]} - 2i\tau e^{i\tau\Delta}\,\mathrm{sinc}(\tau\Delta)B(\psi^{[n]}), \quad n \geq 1,$$
$$\psi^{[1]} = \mathcal{G}^\tau(\psi_0), \quad \psi^{[0]} = \psi_0.$$

Properties: explicit, symmetric, unconditionally (linearly) stable, A-stable

Theorm [1] Optimal error bounds of sEWI

– Under $V \in H^2, \sigma \geq 1, \psi \in H^4$, we have

$$\left\|\psi(\bullet,t_n)-\psi_h^n\right\|_{L^2} \leq C\left(\tau^2+h^4\right), \quad \left\|\psi(\bullet,t_n)-\psi_h^n\right\|_{H^1} \leq C\left(\tau^{3/2}+h^3\right), \quad 0\leq n\leq T/\tau$$

– Under $V \in L^\infty, \sigma > 0, \psi \in H^2$, we have

$$\left\|\psi(\bullet,t_n)-\psi_h^n\right\|_{L^2} \leq C\left(\tau+h^2\right), \quad \left\|\psi(\bullet,t_n)-\psi_h^n\right\|_{H^1} \leq C\left(\tau^{1/2}+h\right), \quad 0\leq n\leq T/\tau$$

[1] W. Bao & C. Wang, An explicit and symmetric exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol 62 (2024), pp. 1901-1928.

Comparison of Different Methods

$$V(x) = \frac{x^2}{2} + V_{\mathrm{well}}(x), \quad \sigma = 0.1, \quad \psi_0(x) = e^{-x^2/2+2ix}.$$

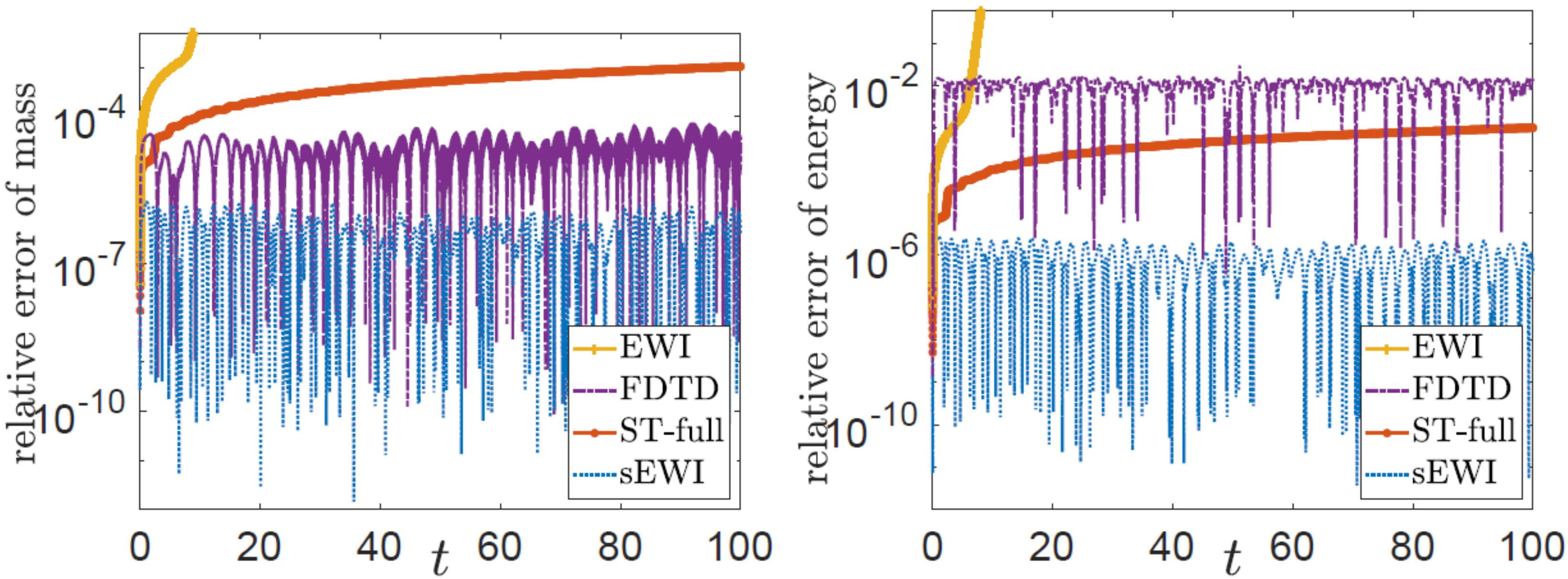


Figure 3: Relative errors of (a) mass and (b) energy up to $T = 100$

The sEWI performs significantly better than other time integrators under low regularity potential and nonlinearity!

[1] W. Bao & C. Wang, An explicit and symmetric exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol 62 (2024), pp. 1901-1928.

Summary on Different Methods for NLSE

Under (A) L^∞-potential, C^1-nonlinearity, and (B) H^2-solution

	in L^2	in H^1
Splitting ($V = 0$, $\sigma > 0$)	$\tau^{1/2+\sigma} + h^{1+2\sigma}$	–
Splitting ($\tau \lesssim h^2$)	$\tau + h^2$	$\tau^{\frac{1}{2}} + h$
EWI/sEWI	$\tau + h^2$	$\tau^{\frac{1}{2}} + h$

To obtain given convergence order, we need

	First-order in L^2-norm		**Second-order** in L^2-norm	
	potential	nonlinearity	potential	nonlinearity
Splitting	H^2	C^2	H^4	C^4
Splitting ($\tau \lesssim h^2$)	L^∞	C^1	H^2	C^3
EWI/sEWI	L^∞	C^1	H^2	C^3
sEWI ($\tau \lesssim h^2$)	L^∞	C^1	H^2	C^2

[1] W. Bao & C. Wang, An explicit and symmetric exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol 62 (2024), pp. 1901-1928.

An EWI for NLSE with Singular Potential

- Consider the NLSE in the whole space

$$i\partial_t\psi = -\Delta\psi + V(\vec{x})\psi + \beta|\psi|^2\psi, \quad t>0$$

  - where $$\psi(\vec{x},0)=\psi_0(\vec{x}), \quad \vec{x}\in\mathbb{R}^d \ (d=1,2,3)$$

$$V\in L^p(\mathbb{R}^d)+L^\infty(\mathbb{R}^d), \quad p\geq 1\,\&\, p>d/2, \quad d=1,2,3$$

- Exponential wave integrator (EWI):

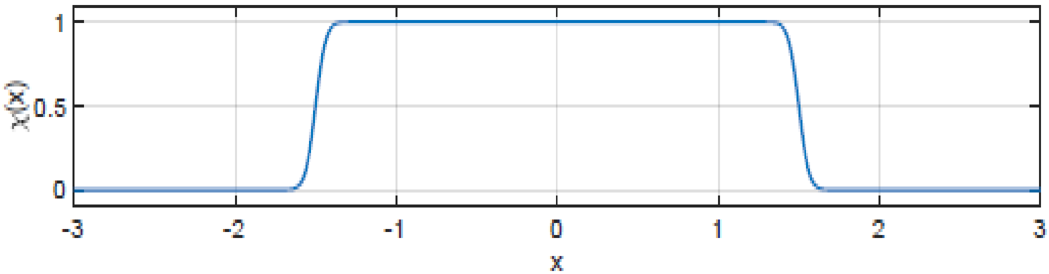
$$\psi^{n+1}=e^{i\tau\Delta}\psi^n - i\tau\phi_1(i\tau\Delta)\Pi_\tau(V\psi^n+\beta\left|\psi^n\right|^2\psi^n), \quad n\geq 0$$

$$\psi^0=\Pi_\tau\psi_0$$

  - where

$$\phi_1(z)=(e^z-1)/z$$

$$\Pi_\tau\phi = F^{-1}(\chi(\tau^{1/2}\xi)F(\phi)(\xi))$$



[1] W. Bao & C. Wang, Error estimates of an exponential wave integrator for the nonlinear Schrödinger equation with singular potential, SIAM J. Numer. Anal., to appear (arXiv: 2504.03346).

Optimal Error Bounds

- Theorem 1 [1,2] Assume

$$V \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d) \text{ with } p \ge 2 \;\&\; \psi_0 \in H^2(\mathbb{R}^d) \text{ for } d = 1,2,3$$

$\exists\, \tau_0 > 0$ sufficiently small such that when $0 < \tau \le \tau_0$, we have

$$\left\|\psi(\bullet,t_n)-\psi^n(\bullet)\right\|_{L^2} \le C\tau, \quad 0 \le n \le \frac{T}{\tau} \Rightarrow \left\|\psi(\bullet,t_n)-\psi^n(\bullet)\right\|_{H^1} \le C\tau^{1/2}, \quad 0 \le n \le \frac{T}{\tau}$$

- Optimality of the first-order L^2-norm is two-fold:
  - The convergence order is optimal for the EWI under L^2_{loc}-potentials
  - The L^2_{loc}-potentials is the weakest regularity for the EWI to achieve the 1st convergence
- Main difficulty: loss of integrability due to $V \in L^2$
- Key techniques [1,2]:
  - Discrete space-time Lebesgue spaces + discrete Stricharitz estimates to establish the stability
  - Normal form transformation + frequency decompositions to obtain optimal error bounds

[1] W. Bao & C. Wang, Error estimates of an exponential wave integrator for the nonlinear Schrödinger equation with singular potential, SIAM J. Numer. Anal., to appear (arXiv: 2504.03346).

[2] W. Bao, C. Wang & Y. Wu, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with highly singular potential, arXiv: 2605.03355.

Optimal Error Bounds for NLSE with Coulomb Potential

- Corollary 1 [1,2] For Coulomb potential in 2D & 3D as

$$V(\vec{x}) = \sum_{j=1}^{J} \frac{Z_j}{|\vec{x}-\vec{x}_j|}, \quad \vec{x} \in \mathbb{R}^d, \quad J \in \mathbb{Z}^+, \quad \vec{x}_j \in \mathbb{R}^d, \quad Z_j \in \mathbb{R}, \quad d = 2,3$$

$\exists \tau_0 > 0$ sufficiently small such that when $0 < \tau \le \tau_0$, we have

$$\|\psi(\bullet, t_n) - \psi^n(\bullet)\|_{L^2} \le C\tau, \quad 0 \le n \le \frac{T}{\tau}$$

$$\Rightarrow \|\psi(\bullet, t_n) - \psi^n(\bullet)\|_{H^1} \le C\tau^{1/2}, \quad 0 \le n \le \frac{T}{\tau}$$

- Corollary 2 [1,2] Similar optimal error bounds for sEWI

[1] W. Bao & C. Wang, Error estimates of an exponential wave integrator for the nonlinear Schrödinger equation with singular potential, SIAM J. Numer. Anal., to appear (arXiv: 2504.03346).
[2] W. Bao, C. Wang & Y. Wu, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with highly singular potential, arXiv: 2605.03355.

Error Bounds

- Theorem 2 [1,2] Assume

$$V \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d) \text{ with } d/2 < p < 2 \,\&\, p \geq 1, \quad \psi_0 \in H^{2-\alpha}(\mathbb{R}^d) \text{ for } d = 1,2,3$$

$\exists \tau_0 > 0$ sufficiently small such that when $0 < \tau \leq \tau_0$, we have

$$\left\|\psi(\bullet, t_n) - \psi^n(\bullet)\right\|_{L^2} \leq C \begin{cases} \tau^{1-\alpha} & d = 1, 1 \leq p < 2, \\ \tau^{1-\alpha} & d = 2, 1 < p < 2, \\ \tau^{1-3\alpha/2} & d = 3, 3/2 < p < 2, \end{cases} \qquad 0 \leq n \leq \frac{T}{\tau}$$

– With

$$\alpha := \begin{cases} 1/2 & p = 1, d = 1 \\ 1/p - 1/2 & 1 < p < 2, d = 1 \\ d\left(1/p - 1/2\right) & d/2 < p < 2, d = 2,3 \end{cases} \quad \Rightarrow \quad \alpha \in \begin{cases} [0, 1/2] & d = 1 \\ [0, 1) & d = 2 \\ [0, 1/2) & d = 3 \end{cases}$$

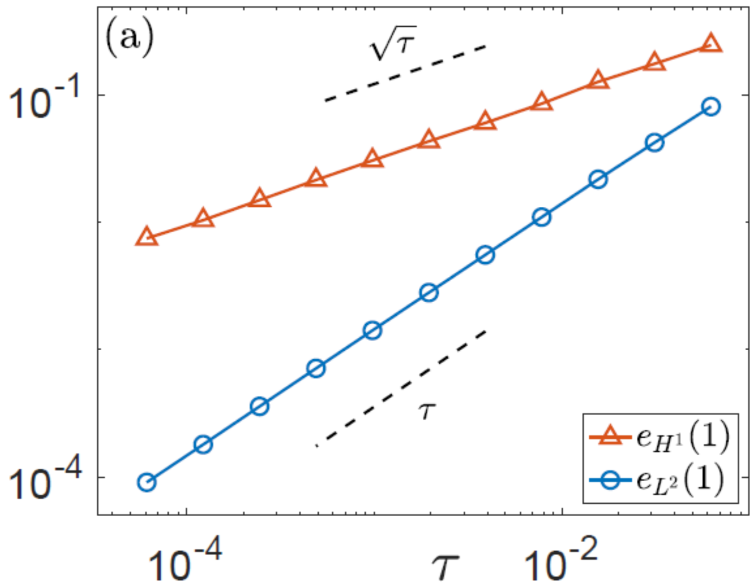
– If $\left\|\psi(\bullet, t_n) - \psi^n(\bullet)\right\|_{L^2} \approx \tau^\gamma$ with $\gamma > \dfrac{1}{2} \Rightarrow \left\|\psi(\bullet, t_n) - \psi^n(\bullet)\right\|_{H^1} \approx \tau^{\gamma - 1/2}$

[1] W. Bao & C. Wang, Error estimates of an exponential wave integrator for the nonlinear Schrödinger equation with singular potential, SIAM J. Numer. Anal., to appear (arXiv: 2504.03346).

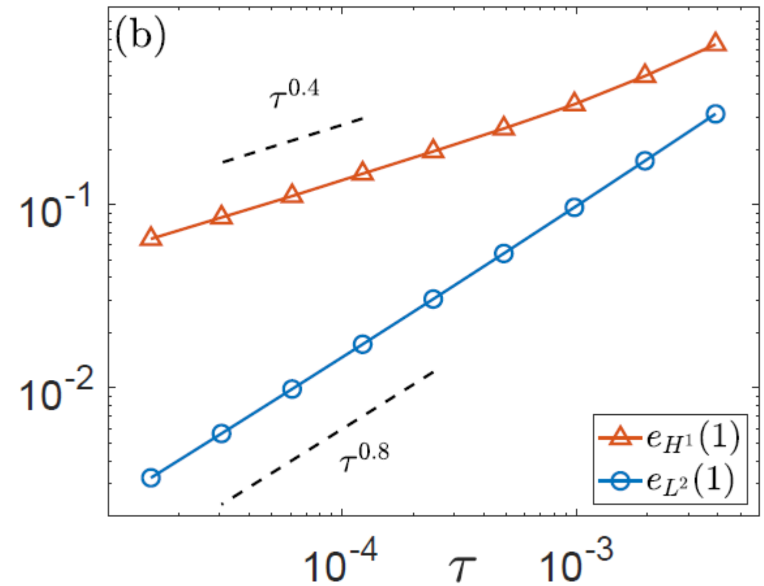
[2] W. Bao, C. Wang & Y. Wu, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with highly singular potential, arXiv: 2605.03355.

Convergence Tests in 1D

$$\psi_0(\mathbf{x}) = e^{-\frac{|\mathbf{x}|^2}{2}}, \quad \mathbf{x} \in \mathbb{R}^d, \quad \beta = 1, \quad \sigma = 1.$$



(a) $V(x) = \frac{1}{\sqrt{|x|}}$ (L^{2^-});



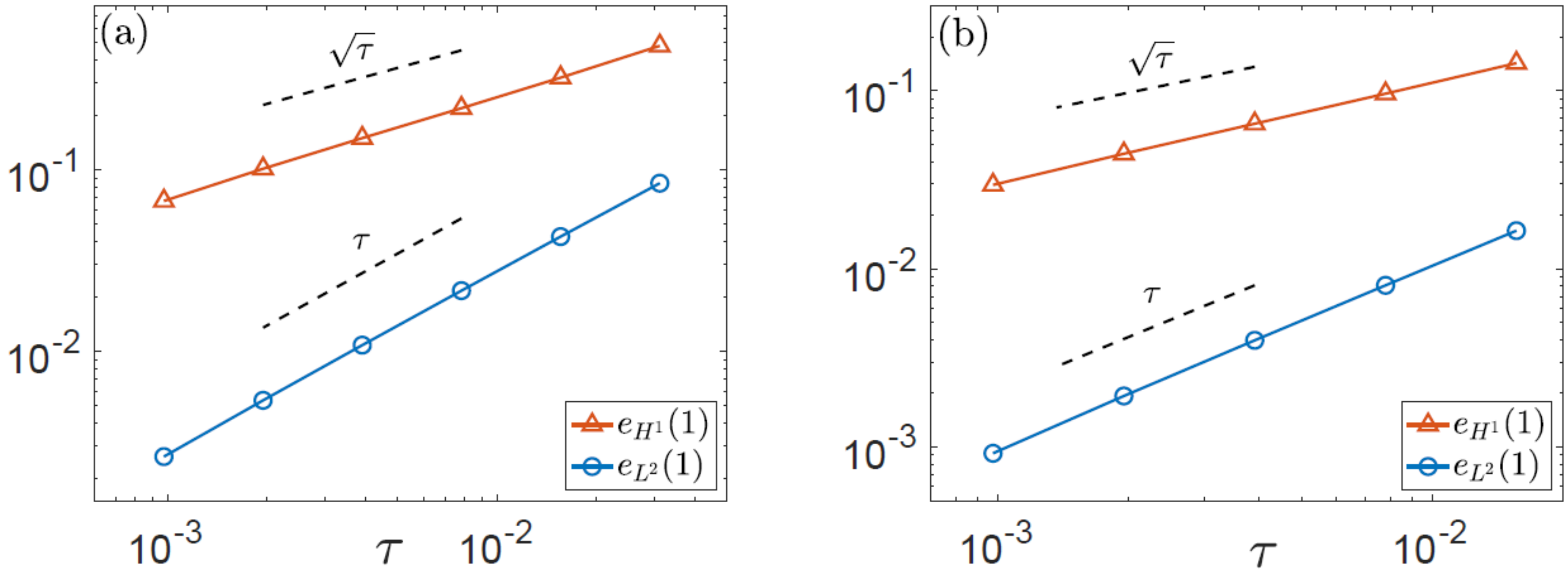
(b) $V(x) = \frac{1}{|x|^{\frac{3}{4}}}$ $(L^{\frac{4}{3}^-})$.

The assumption of L^2-potential for optimal convergence is optimally weak!

[1] W. Bao & C. Wang, Error estimates of an exponential wave integrator for the nonlinear Schrödinger equation with singular potential, SIAM J. Numer. Anal., to appear (arXiv: 2504.03346).
[2] W. Bao, C. Wang & Y. Wu, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with highly singular potential, arXiv: 2605.03355.

Convergence Tests in 2D & 3D

$$\psi_0(\mathbf{x}) = e^{-\frac{|\mathbf{x}|^2}{2}}, \quad \mathbf{x} \in \mathbb{R}^d, \quad \beta = 1, \quad \sigma = 1.$$



(a) 2D Coulomb: $V(\mathbf{x}) = \frac{1}{|\mathbf{x}|}$; (b) L^2-potential in 3D.

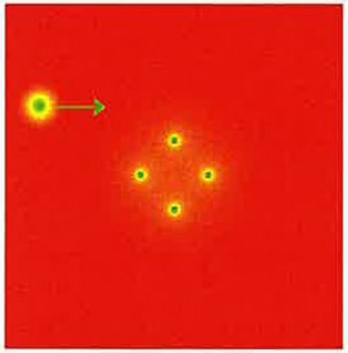
Remark. Convergence order reduction in 3D is not observed.

[1] W. Bao & C. Wang, Error estimates of an exponential wave integrator for the nonlinear Schrödinger equation with singular potential, SIAM J. Numer. Anal., to appear (arXiv: 2504.03346).

[2] W. Bao, C. Wang & Y. Wu, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with highly singular potential, arXiv: 2605.03355.

Dynamics in 2D under Coulomb Potential

$$V(\mathbf{x}) = -\sum_{j=1}^{4} \frac{1}{|\mathbf{x} - \mathbf{x}_j|}, \quad \mathbf{x} \in \mathbb{R}^2, \quad \mathbf{x}_j \in \left\{(\pm 1, 0)^T, (0, \pm 1)^T\right\}.$$



Conclusions & Future Challenges

- Conclusions --Under low-regularity or singular potential and nonlinearity
  - EWIs are advantageous over time-splitting & both are better than FDTD
  - sEWI is excellent at long time simulation
  - Fourier spectral method can obtain optimal spatial convergence with respect to the regularity of the solution & it is better than FD & FEM!!

- Future Challenges
  - Time dependent low-regularity/singular potential
  - Spatial Dirac delta potential & temporal Dirac delta potential – quantum kicks
  - Singular nonlinearity $f(\rho)=\rho^{\alpha}$ with $-1<\alpha<0$
  - Other dispersive PDEs, e.g. Klein-Gordon equation, Dirac equation, ….
  - Dissipative PDEs with low-regularity/singular potential & nonlinearity
  - Coupled PDEs with low-regularity/singular potential & nonlinearity
  - Error estimates of FDTD or FD+FEM, or under low-regularity/singular terms

Related Recent Publications

[1] W. Bao, C. Wang & Y. Wu, Optimal error bounds of the exponential wave integrator for the nonlinear Schrödinger equations with highly singular potential, arXiv: 2605.03355.

[2] W. Bao & C. Wang, Error estimates of an exponential wave integrator for the nonlinear Schrödinger equation with singular potential, SIAM J. Numer. Anal., to appear (arXiv: 2504.03346).

[3] W. Bao, Y. Ma & C. Wang, Optimal error bounds on an exponential wave integrator Fourier spectral method for the Logarithmic Schrödinger equation, IMA J. Numer. Anal., to appear (arXiv: 2412.16902).

[4] W. Bao & C. Wang, An explicit and symmetric exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol 62 (2024), pp. 1901-1928.

[5] W. Bao, B. Lin, Y. Ma & C. Wang, An extended Fourier pseudospectral method for the Gross-Pitaevskii equation with low regularity potential, East Asian J. Appl. Math., Vol 14 (2024), pp. 530-550.

[6] W. Bao, Y. Ma & C. Wang, Optimal error bounds on time-splitting methods for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, Math. Models Methods Appl. Sci., Vol 34 (2024), pp. 803-844.

[7] W. Bao & C. Wang, Error estimates of the time-splitting methods for the nonlinear Schrödinger equation with semi-smooth nonlinearity, Math. Comp., Vol 93 (2024), pp. 1599-1631.

[8] W. Bao & C. Wang, Optimal error bounds on the exponential wave integrator for the nonlinear Schrödinger equation with low regularity potential and nonlinearity, SIAM J. Numer. Anal., Vol. 62 (2024), pp. 93-118.

[9] W. Bao, Y. Feng & Y. Ma, Regularized numerical methods for the nonlinear Schrödinger equation with singular nonlinearity, East Asian J. Appl. Math., Vol. 13 (2023), pp. 646–670.