Improved error estimates of the splitting methods for the long time dynamics for the weakly nonlinear Schrödinger equations

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1. Weakly nonlinear/perturbed Schrödinger equations
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Weakly nonlinear/perturbed Schrödinger equation

- Schrödinger equation (SE) with small potential on torus

$$i\partial_t\psi(\mathbf{x},t) = -\Delta\psi(\mathbf{x},t) + \varepsilon V(\mathbf{x})\psi(\mathbf{x},t)$$

- Weakly nonlinear Schrödinger equation (NLSE) on torus

$$i\partial_t\psi(\mathbf{x},t) = -\Delta\psi(\mathbf{x},t) \pm \varepsilon^2|\psi(\mathbf{x},t)|^2\psi(\mathbf{x},t)$$

- $0 < \varepsilon \ll 1$ a small parameter
- Initial value $\psi(\mathbf{x},0) = O(1)$

- Hamiltonian perturbation of linear PDEs on torus (J. Bourgain, Ann. Math., 98')

$$iu_t + Au + \varepsilon \partial_{\bar{u}} H(u, \bar{u}) = 0$$

-2D linear Schrödinger equation: quasi-periodic solutions

- 2D weakly nonlinear Schrödinger equation on torus (E. Faou, P. Germain, Z. Hani, JAMS, 16')

$$iu_t = -\Delta u \pm |u|^2 u$$

– global solution with small initial data
–small data $u(0) = O(\varepsilon)$, $u = \varepsilon\psi$, $\psi(0) = O(1)$

$$i\partial_t \psi = -\Delta\psi \pm \varepsilon^2 |\psi|^2 \psi$$

Property as $\varepsilon \to 0$

- SE with small potential: $i\partial_t\psi = -\Delta\psi + \varepsilon V\psi$

  trivial —$[0, T/\varepsilon^\alpha]$ ($\alpha \in [0,1)$)

  non-trivial behavior happens $\alpha = 1$

  $t \to t\varepsilon$: $i\partial_t\psi = -\frac{\Delta}{\varepsilon}\psi + V\psi$

- Weakly NLSE $i\partial_t\psi = -\Delta\psi \pm \varepsilon^2|\psi|^2\psi$

  trivial linear dynamics $[0, T/\varepsilon^\alpha]$ ($\alpha \in [0,2)$)

  non-trivial dynamics for $\alpha = 2$

  $t \to t\varepsilon^2$: $i\partial_t\psi = -\frac{\Delta}{\varepsilon^2}\psi \pm |\psi|^2\psi$

Limit as $\varepsilon \to 0$

- Nonlinear case: $i\partial_t\psi = -\frac{\Delta}{\varepsilon^2}\psi \pm |\psi|^2\psi$
- $\widetilde{\psi} = e^{-it\frac{\Delta}{\varepsilon^2}}\psi$:

$$i\partial_t\widetilde{\psi} = \pm F(t/\varepsilon^2, \widetilde{\psi}),\ F(s,\widetilde{\psi}) = e^{-is\Delta}\left(\left|e^{is\Delta}\widetilde{\psi}\right|^2 e^{is\Delta}\widetilde{\psi}\right)$$

RHS: $F(s,\widetilde{\psi})$ periodic in s

- in 1D torus
- 2D $[0, L_x] \times [0, L_y]$ with $(L_y/L_x)^2$ rational
- 3D $[0, L_x] \times [0, L_y] \times [0, L_z]$ with $(L_y/L_x)^2$, $(L_z/L_x)^2$ rational

- 1D $[0, L]$, $\widetilde{\psi} = \sum_{k\in\mathbb{Z}} a_k e^{2\pi ikx/L}$

$$F(s,\widetilde{\psi}) = \pm\sum_k\left(\sum_{\mathcal{I}_k} e^{-4\pi^2 si\delta/L^2} a_{k_1}\overline{a}_{k_2}a_{k_3}\right)e^{2\pi ikx/L}$$

$$\mathcal{I}_k = \left\{(k_1,k_2,k_3)\in\mathbb{Z}^3 : k_1 - k_2 + k_3 = k\right\},\ \delta = k^2 - k_1^2 + k_2^2 - k_3^2$$

- Averaging as $\varepsilon \to 0$: formally, only $\delta = 0$ term in the limit $\varepsilon \to 0$
- averaging based methods (P. Chartier, A. Murua, J.M. Sanz-Serna, FOCM, 10',12')

- Linear $i\partial_t\psi = -\Delta\psi + \varepsilon V\psi$ over interval $[0, T/\varepsilon]$
- Nonlinear $i\partial_t\psi = -\Delta\psi \pm \varepsilon^2|\psi|^2\psi$ over interval $[0, T/\varepsilon^2]$
- Sufficiently regular initial data $\rightarrow$ uniform Sobolev norms
- Numerical methods (splitting methods) and performance?
    - splitting methods known for good performance over long time

Splitting methods for linear case

- 1D linear on periodic $[a, b]$: $i\partial_t\psi(x,t) = -\Delta\psi(x,t) + \varepsilon V(x)\psi(x,t)$
- split into two subporblems:
  - $i\partial_t\psi(x,t) = -\Delta\psi(x,t)$ solve exactly in phase space
    $\psi(\cdot,t) = e^{it\Delta}\psi_0(\cdot)$
  - $i\partial_t\psi(x,t) = \varepsilon V(x)\psi(x,t)$ integrate exactly in physical space
    $\psi(x,t) = e^{-i\varepsilon t V(x)}\psi_0(x)$
- Strang splitting $\psi^{[n+1]}(x) = \mathcal{S}_\tau(\psi^{[n]}) = e^{i\frac{\tau}{2}\Delta}e^{-i\varepsilon\tau V(x)}e^{i\frac{\tau}{2}\Delta}\psi^{[n]}(x)$
- Strang splitting with Fourier pseudo-spectral discretization:
  $\psi_j^n \approx \psi^{[n+1]}(x_j)$ $(x_j = a + jh,\ h = (b-a)/N)$
  $\psi_j^{(1)} = \sum_{l=-N/2}^{N/2-1} e^{-i\frac{\tau\mu_l^2}{2}}\ \widetilde{(\psi^n)}_l\ e^{i\mu_l(x_j-a)}$, $\psi_j^{(2)} = e^{-i\varepsilon\tau V(x_j)}\psi_j^{(1)}$
  $\psi_j^{n+1} = \sum_{l=-N/2}^{N/2-1} e^{-i\frac{\tau\mu_l^2}{2}}\ \widetilde{(\psi^{(2)})}_l\ e^{i\mu_l(x_j-a)}$
  $\widetilde{(\psi^n)}_l$ the discrete Fourier transform of ψ_j^n

Splitting methods for nonlinear case

- 1D nonlinear on periodic $[a, b]$: $i\partial_t\psi(x,t) = -\Delta\psi \pm \varepsilon^2|\psi|^2\psi$
- Strang splitting $\psi^{[n+1]}(x) = \mathcal{S}_\tau(\psi^{[n]}) = e^{i\frac{\tau}{2}\Delta} e^{\mp i\varepsilon^2\tau\left|e^{i\frac{\tau}{2}\Delta}\psi^{[n]}(x)\right|^2} e^{i\frac{\tau}{2}\Delta}\psi^{[n]}(x)$
- Strang splitting with Fourier pseudo-spectral discretization: $\psi_j^n \approx \psi^{[n+1]}(x_j)$ $(x_j = a + jh,\ h = (b-a)/N)$

$$\psi_j^{(1)} = \sum_{l=-N/2}^{N/2-1} e^{-i\frac{\tau\mu_l^2}{2}}\ \widetilde{(\psi^n)}_l\ e^{i\mu_l(x_j-a)}$$

$$\psi_j^{(2)} = e^{\mp i\varepsilon^2\tau\lambda|\psi_j^{(1)}|^2}\psi_j^{(1)}$$

$$\psi_j^{n+1} = \sum_{l=-N/2}^{N/2-1} e^{-i\frac{\tau\mu_l^2}{2}}\ \widetilde{(\psi^{(2)})}_l\ e^{i\mu_l(x_j-a)}$$

Some known properties of Splitting

- $\varepsilon = 1$

  Convergence in the linear case $O(\tau^2)$ (T. Jahnke, C. Lubich, BIT, 00'; S. Blanes, F. Casas, A. Murua, 14',$\cdots$)

  Convergence in the nonlinear case $O(\tau^2)$ (C. Lubich, MCOM, 08',$\cdots$)

  Convergence in the nonlinear fully discrete case (Z. Wang, J. Shen, FOCM, 13'; W. Bao, Y. Cai, 13',$\cdots$)

  Long time near conservation (L. Gauckler, C Lubich, FOCM, 10',$\cdots$)

  Convergence in low regularity/filtered case: (A. Ostermann, F. Rousset, K. Schratz, 22',$\cdots$)

- semi-classical case

  Best resolution in observables, etc. (W. Bao, S. Jin, P.A. Markowich, 02',$\cdots$)

  General splitting linear setup (P. Bader, A. Iserles, K. Kropielnicka, P. Singh, FOCM, 14',$\cdots$)

- what to be expected when $0 < \varepsilon \ll 1$?

Direct computation-linear case

- Local error: $\mathcal{S}_\tau(\psi^n) = e^{i\frac{\tau}{2}\Delta}e^{-i\varepsilon\tau V(x)}e^{i\frac{\tau}{2}\Delta}\psi^n$

$$\begin{aligned}
\mathcal{S}_\tau(\psi(t_n)) =& e^{i\tau\Delta}\psi(t_n) - i\varepsilon\tau\left(e^{i\frac{\tau}{2}\Delta}Ve^{i\frac{\tau}{2}\Delta}\psi(t_n)\right)\\
&-\frac{\varepsilon^2\tau^2}{2}e^{i\frac{\tau}{2}\Delta}V^2e^{i\frac{\tau}{2}\Delta}\psi(t_n) + O(\varepsilon^3\tau^3),\\
\psi(t_{n+1}) =& e^{i\tau\Delta}\psi(t_n) - i\varepsilon\int_0^\tau\left(e^{i(\tau-s)\Delta}V\psi(t_n+s)\right)ds\\
=& e^{i\tau\Delta}\psi(t_n) - i\varepsilon\int_0^\tau\left(e^{i(\tau-s)\Delta}Ve^{is\Delta}\psi(t_n)\right)ds\\
&-\varepsilon^2\int_0^\tau\int_0^s\left(e^{i(\tau-s)\Delta}Ve^{i(s-w)\Delta}Ve^{iw\Delta}\psi(t_n)\right)dwds + O(\varepsilon^3\tau^3)
\end{aligned}$$

- $\mathcal{S}_\tau(\psi(t_n)) - \psi(t_{n+1}) = O(\varepsilon\tau^3[\Delta,[\Delta,V]]) + O(\varepsilon^2\tau^3) + O(\varepsilon^3\tau^3)$
- stability $\|\mathcal{S}_\tau\psi\|_{H^1} \lesssim (1+\varepsilon\tau)\|\psi\|_{H^1}$, $\|\mathcal{S}_\tau\psi\|_{L^2} = \|\psi\|_{L^2}$
- over $[0, T/\varepsilon]$, global error $\frac{T}{\varepsilon\tau}O(\varepsilon\tau^3[\Delta,[\Delta,V]]) = O(\tau^2)$

Extension to weakly NLSE

- Local error

$$e^{i\frac{\tau}{2}\Delta}e^{\mp i\varepsilon^2\tau\left|e^{i\frac{\tau}{2}\Delta}\psi(t_n)\right|^2}e^{i\frac{\tau}{2}\Delta}\psi(t_n)-\psi(t_{n+1})=-i\varepsilon^2\tau f\left(\frac{\tau}{2}\right)+i\varepsilon^2\int_0^\tau f(s)ds+O(\varepsilon^4\tau^3)$$

- $f(s)=\pm e^{i(\tau-s)\Delta}|e^{is\Delta}\psi(t_n)|^2e^{is\Delta}\psi(t_n)$
- size: $O(\varepsilon^2\tau^3[\Delta,[\Delta,|\psi|^2]])+O(\varepsilon^4\tau^3)=O(\varepsilon^2\tau^3)$
- Direct extension would be $O(\tau^2)=O(\varepsilon^2\tau^2)\frac{T}{\tau\varepsilon^2}$ over $[0,T/\varepsilon^2]$

Known results in the nonlinear case

- Improved error in weakly NLSE $0 < \varepsilon \ll 1$ (P. Chartier, F. Méhats, M. Thalhammer, Y. Zhang, MCOM, 16')
- $e^{it\Delta}$ periodic with period ΔT ($L^2/4\pi^2$, 1D), $\tau = \frac{\Delta T}{N}$
- Strang splitting error improved!

$$\|\psi^{[n]} - \psi(t_n)\| \lesssim \varepsilon^2 \tau^2 + N^{-m}$$

  m-regularity dependent parameter
- A factor of ε^2 improved!
- Drawback: periodicity highly involved

Main results

For weakly NLSE, Strang splitting with Fourier pseudo-spectral

Theorem

Let ψ^n be the numerical approximation obtained from the TSFP. For sufficiently regular data, for any $0 < \varepsilon \le 1$, when $0 < \tau \le \alpha \frac{\tau_0^2 (b-a)^2}{4\pi(1+\tau_0)^2} < 1$ with a constant $\alpha \in (0,1)$, there holds

$$\|\psi(x,t_n) - I_N\psi^n\|_{H^1} \lesssim h^{m-1} + \varepsilon^2\tau^2 + \tau_0^{m-1},$$

$$\|I_N\psi^n\|_{H^1} \le 1 + M,\ 0 \le n \le \frac{T/\varepsilon^2}{\tau},$$

$M := \|\psi\|_{L^\infty([0,T_\varepsilon];H^1)}$. If the exact solution is smooth, i.e. $\psi(x,t) \in H^\infty_{\mathrm{per}}$, the τ_0^{m-1} can be ignored in practical computation when τ_0 is small but fixed, the estimates become

$$\|\psi(x,t_n) - I_N\psi^n\|_{H^1} \lesssim h^{m-1} + \varepsilon^2\tau^2.$$

Results for linear case

TSFP for SE with small potential

Theorem

For $\varepsilon \in (0,1]$ and a fixed $\tau_0 \in (0,1)$, for $\tau \in \left(0, \alpha \frac{(b-a)^2}{2\pi(1+\tau_0)^2}\tau_0^2\right)$ ($\alpha \in (0,1)$) and sufficiently regular data, the error reads

$$\|\psi(x,t_n) - I_N\psi^n\|_{H^1} \lesssim h^{m-1} + \varepsilon\tau^2 + \tau_0^{m-1}, \quad 0 \le n \le \frac{T/\varepsilon}{\tau}.$$

Again for smooth solution, i.e. $\psi(x,t) \in H^\infty_{\mathrm{per}}$, the τ_0^{m-1} part can be ignored in practical computation, the improved error bounds read

$$\|\psi(x,t_n) - I_N\psi^n\|_{H^1} \lesssim h^{m-1} + \varepsilon\tau^2, \quad 0 \le n \le \frac{T/\varepsilon}{\tau}.$$

Estimates revisited-linear case

- Local error-full discretization: $\mathcal{S}_\tau : \psi \to e^{i\frac{\tau}{2}\Delta} e^{-i\varepsilon\tau V(x)}\psi$ (propagator of semi discretization)

$$\mathcal{E}^n(x) := P_N \mathcal{S}_\tau(P_N\psi(t_n)) - P_N\psi(t_{n+1}) = P_N\mathcal{F}(P_N\psi(t_n)) + R_n$$

  P_N projection onto Fourier modes $k = -N/2, \ldots, N/2-1$

- $$\mathcal{F}(P_N\psi(t_n)) = -i\varepsilon\tau f^n\left(\frac{\tau}{2}\right) + i\varepsilon\int_0^\tau f^n(s)\, ds$$

  with $f^n(s) = e^{i(\tau-s)\Delta} V e^{is\Delta} P_N\psi(t_n)$
- $\|R_n\|_{H^1} \lesssim \varepsilon^2\tau^3 + \varepsilon\tau h^{m-1}$, $\|\mathcal{F}(P_N\psi(t_n))\|_{H^1} \lesssim \varepsilon\tau^3$
- Naive estimates over $0 \le n \le \frac{T}{\tau\varepsilon}$ interval gives $h^{m-1} + \varepsilon\tau^2 + \tau^2$
- Improved error?

Estimates of global error

Global error

- pseudo-spectral v.s. spectral (local error)

$$I_N\psi^{n+1} = e^{i\frac{\tau}{2}\Delta}(I_N\psi^{(2)}),\ I_N(\psi^{(2)}) = I_N(e^{-i\varepsilon\tau V(x)}\psi^{(1)}),\ I_N\psi^{(1)} = e^{i\frac{\tau}{2}\Delta}I_N\psi^n$$
$$P_N(\mathcal{S}_\tau(\psi(t_n))) = e^{i\frac{\tau}{2}\Delta}(P_N\psi^{\langle 2\rangle}),\ \psi^{\langle 2\rangle} = e^{-i\varepsilon\tau V(x)}\psi^{\langle 1\rangle},\ \psi^{\langle 1\rangle} = e^{i\frac{\tau}{2}\Delta}P_N\psi(t_n)$$

- error: $e^n := e^n(x) = I_N\psi^n - P_N\psi(t_n)$:

$$e^{n+1} = \ e^{i\tau\Delta}e^n + Q^n(x) + \mathcal{E}^n$$

$\mathcal{E}^n$-local error

$$Q^n(x) = -i\varepsilon\tau e^{i\frac{\tau}{2}\Delta}\left(I_N(V(x)\int_0^1 e^{-i\varepsilon\theta\tau V(x)}\,d\theta\psi^{(1)})\right) + i\varepsilon\tau e^{i\frac{\tau}{2}\Delta}\left(P_N(V(x)\int_0^1 e^{-i\varepsilon\theta\tau V(x)}\,d\theta\psi^{\langle 1\rangle})\right)$$

- $\|Q^n(x)\|_{H^1} \lesssim \varepsilon\tau\left(h^{m-1} + \|e^n\|_{H^1}\right)$

$$e^{n+1} = e^{i(n+1)\tau\Delta}e^0 + \sum_{k=0}^{n} e^{i(n-k)\tau\Delta}\left(Q^k(x) + \mathcal{E}^k\right)$$

- Global error

$$\|e^{n+1}\|_{H^1} \lesssim h^{m-1} + \varepsilon\tau^2 + \varepsilon\tau\sum_{k=0}^{n}\|e^k\|_{H^1} + \left\|\sum_{k=0}^{n} e^{i(n-k)\tau\Delta}P_N\mathcal{F}(P_N\psi(t_k))\right\|_{H^1}$$

Refined error analysis

- Refined estimates on $\sum_{k=0}^{n} e^{i(n-k)\tau\Delta} P_N \mathcal{F}(P_N\psi(t_k))$

  $\mathcal{F}(P_N\psi(t_n)) = -i\varepsilon\tau f^n\left(\frac{\tau}{2}\right) + i\varepsilon\int_0^\tau f^n(s)\,ds$, $f^n(s) = e^{i(\tau-s)\Delta} V e^{is\Delta} P_N\psi(t_n)$

- Periodicity approach: $\tau = L^2/4\pi^2/N^*$ $(N^* \in \mathbb{Z}^+)$

  sum $k = 0, \ldots, N^*-1$ is equivalent to a midpoint rule for a periodic function—spectral in time $(N^*)^{-m}$!
  $O(\varepsilon\tau^3)$ only accumulate at most in one period to $O(\varepsilon\tau^2)$–desired!

- Our approach: (regularity compensate oscillation)
  - Separate high frequency and low frequency: $> 1/\tau_0$ and $\leq 1/\tau_0$ (τ_0 parameter)
  - High modes controlled by regularity (projection): $N_0 = 2\lceil 1/\tau_0\rceil \in \mathbb{Z}^+$

    $$\left\| P_{N_0}\mathcal{F}(P_{N_0}\psi(t_n)) - P_N\mathcal{F}(P_N\psi(t_n))\right\|_{H^1} \lesssim \varepsilon\tau(h^{m-1} + \tau_0^{m-1})$$

  - Calculate phase cancellation for low modes $\leq 1/\tau_0$ (summation by parts), i.e. the phase in $f^n(s)$

RCO for phase cancellation

- gain order in ε: $\partial_t\psi(x,t) - i\Delta\psi(x,t) = O(\varepsilon)$, 'twisted variable' as

$$\phi(x,t) = e^{-it\Delta}\psi(x,t), \quad \partial_t\phi(x,t) = O(\varepsilon)$$

- low modes left: $\left\|e^{n+1}\right\|_{H^1} \lesssim h^{m-1} + \tau_0^{m-1} + \varepsilon\tau^2 + \varepsilon\tau\sum_{k=0}^{n}\left\|e^k\right\|_{H^1} + \|\mathcal{R}^n\|_{H^1}$

  $\mathcal{R}^n(x) = \sum\limits_{k=0}^{n} e^{-i(k+1)\tau\Delta} P_{N_0}\mathcal{F}(e^{it_k\Delta}(P_{N_0}\phi(t_k)))$

- $\mathcal{T}_{N_0} = \{-N_0/2, -N_0/2+1, \ldots, N_0/2-1\}$, $\mathcal{I}_l^{N_0} = \left\{(l_1,l_2) \mid l_1 + l_2 = l,\ l_1 \in \mathbb{Z},\ l_2 \in \mathcal{T}_{N_0}\right\}$
- $\phi(t) = \sum_{l\in\mathbb{Z}} \widehat{\phi}_l(t) e^{i\mu_l(x-a)}$ $(t \geq 0)$, $P_{N_0}\phi(t) = \sum_{l\in\mathcal{T}_{N_0}} \widehat{\phi}_l(t) e^{i\mu_l(x-a)}$
- $\mathcal{R}^n(x) = i\varepsilon \sum\limits_{k=0}^{n} \sum\limits_{l\in\mathcal{T}_{N_0}} \sum\limits_{(l_1,l_2)\in\mathcal{I}_l^{N_0}} \lambda_{k,l,l_1,l_2} e^{i\mu_l(x-a)}$
- $\lambda_{k,l,l_1,l_2} = -\tau\mathcal{G}_{k,l,l_1,l_2}(\tau/2) + \int_0^\tau \mathcal{G}_{k,l,l_1,l_2}(s)\,ds = r_{l,l_2} e^{it_k\delta_{l,l_2}} c_{k,l,l_1,l_2}$
- $\mathcal{G}_{k,l,l_1,l_2}(s) = e^{i(t_k+s)\delta_{l,l_2}} \widehat{V}_{l_1}\widehat{\phi}_{l_2}(t_k), \quad \delta_{l,l_2} = \delta_l - \delta_{l_2}, \quad \delta_l = \mu_l^2$

  $r_{l,l_2} = \ -\tau e^{i\frac{\tau\delta_{l,l_2}}{2}} + \int_0^\tau e^{is\delta_{l,l_2}}\,ds = O(\tau^3(\delta_{l,l_2})^2)$

RCO

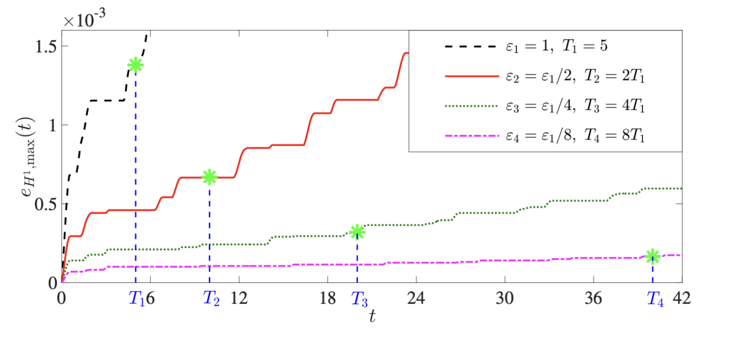
- summation by parts in time: exponential sums $S_{n,l,l_2} = \sum_{k=0}^{n} e^{it_k \delta_{l,l_2}}$
- For $0 < \tau \leq \alpha \frac{2\pi}{\mu_1^2(1+\tau_0)^2}\tau_0^2$, $|S_{n,l,l_2}| \leq C/\tau|\delta_{l,l_2}|$
- $\sum_{k=0}^{n} \lambda_{k,l,l_1,l_2} = r_{l,l_2} \sum_{k=0}^{n-1} S_{k,l,l_2}(c_{k,l,l_1,l_2} - c_{k+1,l,l_1,l_2}) + S_{n,l,l_2}\ r_{l,l_2}\ c_{n,l,l_1,l_2}$
- $r_{l,l_2} = O(\tau^3(\delta_{l,l_2})^2)$, $c_{k,l,l_1,l_2} - c_{k+1,l,l_1,l_2} = \widehat{V}_{l_1}\left(\widehat{\phi}_{l_2}(t_k) - \widehat{\phi}_{l_2}(t_{k+1})\right) = O(\varepsilon\tau)$
- $\left|\sum_{k=0}^{n} \lambda_{k,l,l_1,l_2}\right| \lesssim \tau^2|\delta_{l,l_2}|\left|\widehat{V}_{l_1}\right|\left[\sum_{k=0}^{n-1}\left|\widehat{\phi}_{l_2}(t_k) - \widehat{\phi}_{l_2}(t_{k+1})\right| + \left|\widehat{\phi}_{l_2}(t_n)\right|\right]$
- $\|\mathcal{R}^n(x)\|_{H^1} \lesssim \varepsilon\tau^2$ for $n\tau \leq T/\varepsilon$ (Improved estimates by Gronwall inequality)
- $\|\mathcal{R}^n(x)\|_{H^1}^2 = \varepsilon^2 \sum_{l\in\mathcal{T}_{N_0}} (1+\mu_l^2)\left|\sum_{(l_1,l_2)\in\mathcal{I}_l^{N_0}} \sum_{k=0}^{n} \lambda_{k,l,l_1,l_2}\right|^2$
- Estimates sums instead by considering $U(x) = \sum_{l\in\mathbb{Z}}(1+\mu_l^2)^{3/2}\left|\widehat{V}_l\right| e^{i\mu_l(x-a)}$ and $\xi(x) = \sum_{l\in\mathbb{Z}}(1+\mu_l^2)^{3/2}\left|\widehat{\phi}_l(t_n)\right| e^{i\mu_l(x-a)}$

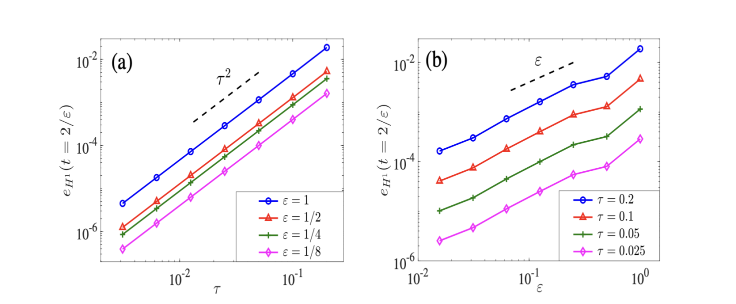
- τ_0-artificial parameter (truncation of Fourier modes)-depend on the exact solution
- structure of Fourier functions $e^{i\mu_l(x-a)}e^{i\mu_k(x-a)} = e^{i\mu_{l+k}(x-a)}$
- valid for non-periodic evolutionary Schrödinger operator
- more choices of time step size τ
  - need $|S_{n,l,l_2}| = |\sum_{k=0}^{n} e^{it_k\delta_{l,l_2}}| \lesssim \frac{1}{\tau|\delta_{l,l_2}|^{\beta}}$ $(\beta \leq 2)$

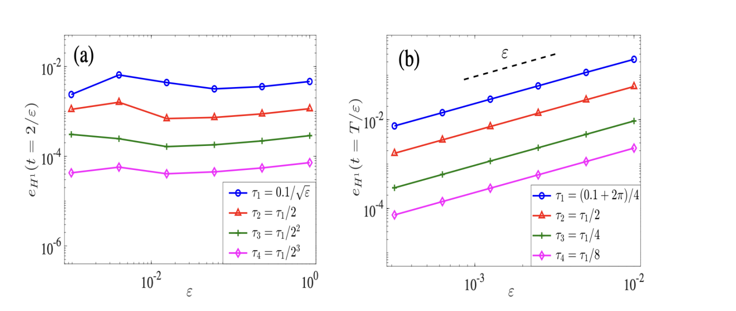
    Diophantine condition (Z. Shang, 00')

$$\left|\frac{1-e^{i\tau\mu_1^2 K}}{\tau}\right| \geq \frac{\gamma}{|K|^{\nu}}, \quad \forall K \in \mathbb{Z},\ K \neq 0,$$

independent of τ_0, h, let $\tau_0, h \to 0^+$, recover $\varepsilon\tau^2$ for the semi-discrete-in-time splitting error

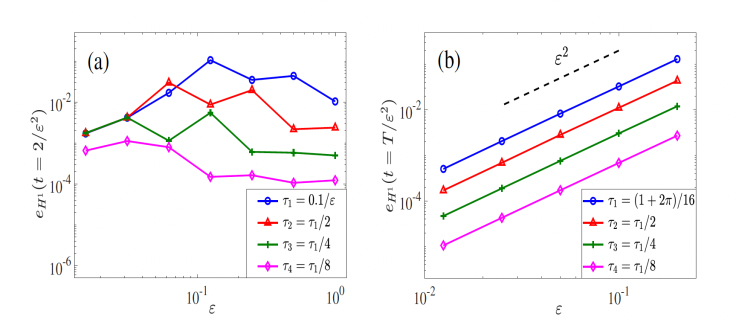

×10^-3
1.5
1
0.5
0
$e_{H^1,\max}(t)$
0
T_1
6
T_2
12
18
T_3
24
30
36
T_4
42
t
$\varepsilon_1 = 1,\ T_1 = 5$
$\varepsilon_2 = \varepsilon_1/2,\ T_2 = 2T_1$
$\varepsilon_3 = \varepsilon_1/4,\ T_3 = 4T_1$
$\varepsilon_4 = \varepsilon_1/8,\ T_4 = 8T_1$


(a)
τ^2
10^{-2}
10^{-4}
10^{-6}
$e_{H^1}(t=2/\varepsilon)$
10^{-2}
10^{-1}
τ
$\varepsilon=1$
$\varepsilon=1/2$
$\varepsilon=1/4$
$\varepsilon=1/8$
(b)
ε
10^{-2}
10^{-4}
10^{-6}
$e_{H^1}(t=2/\varepsilon)$
10^{-2}
10^{-1}
10^{0}
ε
$\tau=0.2$
$\tau=0.1$
$\tau=0.05$
$\tau=0.025$


(a)
10^{-2}
10^{-4}
10^{-6}
$e_{H^1}(t = 2/\varepsilon)$
10^{-2}
10^{0}
ε
$\tau_1 = 0.1/\sqrt{\varepsilon}$
$\tau_2 = \tau_1/2$
$\tau_3 = \tau_1/2^2$
$\tau_4 = \tau_1/2^3$
(b)
ε
10^{-2}
10^{-4}
$e_{H^1}(t = T/\varepsilon)$
10^{-3}
10^{-2}
ε
$\tau_1 = (0.1 + 2\pi)/4$
$\tau_2 = \tau_1/2$
$\tau_3 = \tau_1/4$
$\tau_4 = \tau_1/8$

Extension to nonlinear case

- Diophantine type non-resonant time step size τ
- Higher dimensions with tensor grids–straightforward!
- Arbitrary aspect ratios in higher dimensions–no periodicity needed!
- Polynomial type nonlinearities—ok!
- extra larger step size ok– $\tau = O(1/\varepsilon)$-non-resonant for the nonlinear case $\tau = O(1/\sqrt{\varepsilon})$-non-resonant for the linear case
- Higher order splitting—ok but need work out


(a)
10^{-2}
10^{-4}
10^{-6}
$e_{H^1}(t = 2/\varepsilon^2)$
10^{-1}
10^{0}
ε
$\tau_1 = 0.1/\varepsilon$
$\tau_2 = \tau_1/2$
$\tau_3 = \tau_1/4$
$\tau_4 = \tau_1/8$
(b)
ε^2
10^{-2}
10^{-4}
$e_{H^1}(t = T/\varepsilon^2)$
10^{-2}
10^{-1}
ε
$\tau_1 = (1+2\pi)/16$
$\tau_2 = \tau_1/2$
$\tau_3 = \tau_1/4$
$\tau_4 = \tau_1/8$

Summary

- Improved error bounds of splitting methods for SE with small potential and weakly NLSE
- Resonance is important
- RCO approach efficient tool for analyzing Schrödinger type equations
- Larger time step size could be accurate

THANK YOU!