Numerical methods for nonlinear Schrödinger equations

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Discretisation of nonlinear Schrödinger equations

**Problem.** System of nonlinear Schrödinger equations

\[ i \partial_t \Psi(x, t) = \mathcal{H}(x, \Psi(x, t)) \Psi(x, t), \quad x \in \mathbb{R}^d, \quad 0 \leq t \leq T. \]

**Discretisation.** High accuracy approximations rely on

- pseudo-spectral methods in space and
- exponential operator splitting methods in time.

**Numerical analysis.** Theoretical analysis of integration methods (stability, convergence, long-term behaviour).

**Applications.**

- Gross–Pitaevskii systems (GPS)
- Multi-configuration time-dependent Hartree–Fock (MCTDHF) equations
Bose–Einstein condensation

In our laboratories temperatures are measured in micro- or nanokelvin ... In this ultracold world ... atoms move at a snail’s pace ... and behave like matter waves. Interesting and fascinating new states of quantum matter are formed and investigated in our experiments.

_Grimm et al._

**Practical realisation.** Observation of Bose–Einstein condensation in physical experiments.

**Theoretical model.** Mathematical description of multi-component Bose–Einstein condensates by Gross–Pitaevskii systems.

**Numerical simulation.** Favourable space and time discretisations rely on time-splitting pseudo-spectral methods. See recent work by _BAO ET AL._
Objectives

**Convergence analysis.**
- High-order time-splitting methods for nonlinear Schrödinger equations (GPS, MCTDHF).
- Minimisation method for ground state computation (1D/2D GPS).

**Implementation.**
- Numerical simulation of Gross–Pitaevskii systems in three space dimensions (ground state, time evolution).
Contents

- Gross–Pitaevskii systems
- Pseudo-spectral methods
  (Fourier, Sine, Hermite, Laguerre–Fourier–Hermite)
- Exponential operator splitting methods
  - Linear evolutionary Schrödinger equations
  - Nonlinear evolutionary Schrödinger equations
  - Stability and convergence analysis
- Illustrations
  - Pseudo-spectral methods
  - Ground state computation
  - Time evolution
Gross–Pitaevskii systems
Problem. System of coupled time-dependent Gross–Pitaevskii equations for $\Psi : \mathbb{R}^d \times [0, \infty) \to \mathbb{C}^J$

$$i \hbar \partial_t \Psi_j(x, t) = \left( -\frac{\hbar^2}{2m_j} \Delta + V_j(x) + \hbar^2 \sum_{k=1}^{J} g_{jk} |\Psi_k(x, t)|^2 \right) \Psi_j(x, t),$$

$$V_j(x) = \sum_{i=1}^{d} \left( \frac{m_j}{2} \omega_{ji}^2 (x_i - \zeta_{ji})^2 + \kappa_{ji} \left( \sin(q_{ji} x_i) \right)^2 \right),$$

$$\|\Psi_j(\cdot, 0)\|_{L^2}^2 = N_j, \quad x \in \mathbb{R}^d, \quad 0 \leq t \leq T, \quad 1 \leq j \leq J.$$

Normalisation. Linear transformation yields normalised problem for $\psi : \mathbb{R}^d \times [0, \infty) \to \mathbb{C}^J$

$$i \partial_t \psi_j(\xi, t) = \left( -c_j \Delta + U_j(\xi) + \sum_{k=1}^{J} \partial_{jk} |\psi_k(\xi, t)|^2 \right) \psi_j(\xi, t),$$

$$\|\psi_j(\cdot, 0)\|_{L^2}^2 = N_j, \quad \xi \in \mathbb{R}^d, \quad 0 \leq t \leq T, \quad 1 \leq j \leq J.$$
Special case \((J = 1)\). Gross–Pitaevskii equation subject to asymptotic boundary conditions and initial condition

\[
i \partial_t \psi(\xi, t) = \left( -\frac{1}{2} \Delta + U(\xi) + \vartheta |\psi(\xi, t)|^2 \right) \psi(\xi, t),
\]

\[
\Delta = \sum_{i=1}^{d} \partial_{\xi_i}^2, \quad U(\xi) = \frac{1}{2} U_H(\xi) = \frac{1}{2} \sum_{i=1}^{d} \gamma_i^4 \xi_i^2,
\]

\[
\|\psi(\cdot, 0)\|_{L^2}^2 = 1, \quad \xi \in \mathbb{R}^d, \quad 0 \leq t \leq T.
\]

**Geometric properties.** Preservation of particle number \(\|\psi(\cdot, t)\|_{L^2}^2\)

and energy functional

\[
E(\psi(\cdot, t)) = \left( \left( -\frac{1}{2} \Delta + U + \frac{1}{2} \vartheta |\psi(\cdot, t)|^2 \right) \psi(\cdot, t) \right) \left| \psi(\cdot, t) \right|_{L^2}.
\]
Pseudo-spectral methods
Spectral methods

- Fourier spectral method
- Sine spectral method
- Cosine spectral method
- Hermite spectral method
- Laguerre–Fourier–Hermite spectral method
Fourier pseudo-spectral method

**Spectral decomposition.** Let $\Omega = [-a, a]^d$ with $a > 0$. Fourier basis functions $(\mathcal{F}_m)_{m \in \mathbb{Z}^d}$ form orthonormal basis of $L^2(\Omega)$ and satisfy

$$-\frac{1}{2} \Delta \mathcal{F}_m = \lambda_m \mathcal{F}_m, \quad \lambda_m = \frac{\pi^2}{2a^2} \sum_{i=1}^d m_i^2.$$

Fourier decomposition for $\psi(\cdot, t) \in L^2(\Omega)$

$$\psi(\cdot, t) = \sum_m \psi_m(t) \mathcal{F}_m, \quad \psi_m(t) = \left(\psi(\cdot, t) \mid \mathcal{F}_m\right)_{L^2}.$$

**Numerical approximation.** Truncation of infinite sum and application of trapezoid quadrature formula

$$\psi_M(\cdot, t) = \sum_m \psi_m(t) \mathcal{F}_m,$$

$$\psi_m(t) = \int_{\Omega^d} \psi(\xi, t) \mathcal{F}_m(\xi) \, d\xi \approx \omega \sum_k \psi(\xi_k, t) \mathcal{F}_m(\xi_k).$$
Spectral decomposition. Hermite functions \((\mathcal{H}_m)_{m \geq 0}\) form orthonormal basis of \(L^2(\mathbb{R}^d)\) and satisfy
\[
\frac{1}{2} \left( - \Delta + U_H \right) \mathcal{H}_m = \lambda_m \mathcal{H}_m, \quad \lambda_m = \sum_{i=1}^{d} \gamma_i^2 \left( m_i + \frac{1}{2} \right).
\]

Hermite decomposition for \(\psi(\cdot, t) \in L^2(\mathbb{R}^d)\)
\[
\psi(\cdot, t) = \sum_m \psi_m(t) \mathcal{H}_m, \quad \psi_m(t) = (\psi(\cdot, t) | \mathcal{H}_m)_{L^2}.
\]

Numerical approximation. Truncation of infinite sum and application of Gauss–Hermite quadrature formula
\[
\psi_M(\cdot, t) = \sum_M \psi_m(t) \mathcal{H}_m, \\
\psi_m(t) = \int_{\mathbb{R}^d} \psi(\xi, t) \mathcal{H}_m(\xi) \, d\xi \approx \sum_k \omega_k e^{\xi_k^2} \psi(\xi_k, t) \mathcal{H}_m(\xi_k).
\]
Observations (GPE, 2D).

- Spectral methods show favourable behaviour regarding accuracy.
- For certain parameter ranges Hermite spectral error (bottom) is remarkably smaller than Fourier spectral error (top).
- Hermite transform error does not go below $\approx 10^{-14}$ (Matlab implementation).
Computation time

Mean computational cost of a single spectral transform in one (left picture) and two (right picture) space dimensions.
Preliminary tests

Preliminary tests in PYTHON/CYTHON by Johannes Traxl.

Computational cost of a single spectral transform in one to three space dimensions.
Ground state computation
**Problem.** Gross–Pitaevskii equation

\[ i \partial_t \psi(\xi, t) = \left( -\frac{1}{2} \Delta + U(\xi) + \vartheta |\psi(\xi, t)|^2 \right) \psi(\xi, t). \]

**Ground state.** Solution of special form \( \psi(\xi, t) = e^{-i\mu t} \varphi(\xi) \) that minimises energy functional. Used as reliable reference solution in time-integration.

**Imaginary time method (normalised gradient flow).** Artificial time integration by linearly-implicit Euler method, see BAO, CHERN, LIM (2006).

**Minimisation approach.** Direct minimisation of energy functional, see BAO, TANG (2003), CALIARI, OSTERMANN, RAINER, TH. (2008).
**Imaginary time method.** Artificial time integration of

\[ \partial_t \psi(\xi, t) = \left( \frac{1}{2} \Delta - U(\xi) - \vartheta |\psi(\xi, t)|^2 \right) \psi(\xi, t), \quad \| \psi(\cdot, 0) \|_{L^2}^2 = 1. \]

- Space discretisation by pseudo-spectral methods
- Time discretisation by linearly-implicit Euler method

**Illustration.** Computation of ground state \( \psi(\xi, t) = e^{-i\vartheta t} \varphi(\xi) \) for different values of \( \vartheta \).
*Illustration.* Computation of ground state $\psi(\xi, t) = e^{-i\mu t} \varphi(\xi)$ for $\vartheta = 0$. Random initial value. Exact solution $\varphi = \mathcal{H}_0$. 
Illustration (1D). Computation of ground state $\psi(\xi, t) = e^{-i\mu t} \varphi(\xi)$ for $\vartheta = 0$ by imaginary time method (time stepsize $\Delta t$, number of steps $N$, tolerance $\text{tol} \parallel \Delta \varphi \parallel_{L^2} = 10^{-13}$, random initial value). Exact solution $\varphi = \mathcal{H}_0$. Determine $\Delta \varphi = \parallel \varphi - \mathcal{H}_0 \parallel_{L^2}$, $\Delta E = |E(\varphi) - E(\mathcal{H}_0)|$.

<table>
<thead>
<tr>
<th>Method     (dof)</th>
<th>$\Delta t$</th>
<th>$N$</th>
<th>$\Delta \varphi$</th>
<th>$\Delta E$</th>
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<tbody>
<tr>
<td>Hermite 1D (256)</td>
<td>$1 \cdot 10^{-1}$</td>
<td>285</td>
<td>$9.9 \cdot 10^{-13}$</td>
<td>0</td>
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<tr>
<td>Fourier 1D (256)</td>
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<td>6062</td>
<td>$3.0 \cdot 10^{-11}$</td>
<td>$2.8 \cdot 10^{-16}$</td>
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<td>Sine 1D (256)</td>
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<td>6569</td>
<td>$3.0 \cdot 10^{-11}$</td>
<td>$1.1 \cdot 10^{-16}$</td>
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<td>6005</td>
<td>$3.0 \cdot 10^{-11}$</td>
<td>0</td>
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</table>
Illustration (2D). Computation of ground state $\psi(\xi, t) = e^{-i\mu t} \varphi(\xi)$ for $\vartheta = 0$ by imaginary time method (time stepsize $\Delta t$, number of steps $N$, $N_{\text{max}} = 1000$, tolerance $\text{tol} \|\Delta \varphi\|_{L^2} = 10^{-13}$, random initial value). Exact solution $\varphi = H_0$. Determine $\Delta \varphi = \|\varphi - H_0\|_{L^2}$, $\Delta E = |E(\varphi) - E(H_0)|$.

<table>
<thead>
<tr>
<th>Method (dof)</th>
<th>$\Delta t$</th>
<th>$N$</th>
<th>$\Delta \varphi$</th>
<th>$\Delta E$</th>
</tr>
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<tbody>
<tr>
<td>Hermite 2D (128 $\times$ 128)</td>
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<td>279</td>
<td>$1.1 \cdot 10^{-12}$</td>
<td>$2.7 \cdot 10^{-15}$</td>
</tr>
<tr>
<td>Fourier 2D (128 $\times$ 128)</td>
<td>$1 \cdot 10^{-3}$</td>
<td>$N_{\text{max}}$</td>
<td>$1.3 \cdot 10^{-1}$</td>
<td>$3.5 \cdot 10^{-2}$</td>
</tr>
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<td>Sine 2D (128 $\times$ 128)</td>
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<td>$N_{\text{max}}$</td>
<td>$1.5 \cdot 10^{-1}$</td>
<td>$4.3 \cdot 10^{-2}$</td>
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<td>$N_{\text{max}}$</td>
<td>$1.4 \cdot 10^{-1}$</td>
<td>$3.7 \cdot 10^{-2}$</td>
</tr>
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<td>274</td>
<td>$1.1 \cdot 10^{-12}$</td>
<td>$4.4 \cdot 10^{-16}$</td>
</tr>
<tr>
<td>Laguerre 2D (40 $\times$ 40)</td>
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<td>281</td>
<td>$1.1 \cdot 10^{-12}$</td>
<td>$1.8 \cdot 10^{-15}$</td>
</tr>
</tbody>
</table>
Illustration (1D). Computation of ground state $\psi(\xi, t) = e^{-i\mu t} \varphi(\xi)$ for $\vartheta = 1, 10, 100$ by imaginary time method (time stepsize $\Delta t$, number of steps $N$, $N_{\text{max}} = 10000$, $\text{tol} \|\Delta \varphi\|_{L^2} = 10^{-13}$, initial value $H_0$). Determine energy $E$ and chemical potential $\mu$.

<table>
<thead>
<tr>
<th>$\vartheta$</th>
<th>Method (dof)</th>
<th>$\Delta t$</th>
<th>$N$</th>
<th>$E$</th>
<th>$\mu$</th>
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<td>$N_{\text{max}}$</td>
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<td>5768</td>
<td>8.508526756216648</td>
<td>14.13428708652637</td>
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</tbody>
</table>
Illustration (1D). Harmonic and optical lattice potential.
Parameters $\vartheta = 400, \kappa = 0$ (first row), $\vartheta = 250, \kappa = 25$ (second row).
**Ground and excited states**

**Illustration (1D).** Harmonic and optical lattice potential \((\vartheta = 400, \kappa = 0)\). Ground state (first table), first excited state (second table).

<table>
<thead>
<tr>
<th>Method (dof)</th>
<th>N</th>
<th>(E)</th>
<th>(\mu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fourier 1D (128)</td>
<td>1652</td>
<td>21.36006969604896</td>
<td>35.57746088822537</td>
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<table>
<thead>
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<th>Method (dof)</th>
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<th>(E)</th>
<th>(\mu)</th>
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</table>
Illustration (2D). Harmonic and optical lattice potential. Parameters $\vartheta = 500, \kappa = 50$. 
**Problem.** Description of two-component Bose–Einstein condensate with external driving field by Gross–Pitaevskii system

\[
i \partial_t \psi_1(\xi, t) = \left( -c_1 \Delta + U_1(\xi) + \delta_1 + \vartheta_{11} |\psi_1(\xi, t)|^2 \\
+ \vartheta_{12} |\psi_2(\xi, t)|^2 \right) \psi_1(\xi, t) + \lambda_1 \psi_2(\xi, t),
\]

\[
i \partial_t \psi_2(\xi, t) = \left( -c_2 \Delta + U_2(\xi) + \delta_2 + \vartheta_{12} |\psi_1(\xi, t)|^2 \\
+ \vartheta_{22} |\psi_2(\xi, t)|^2 \right) \psi_2(\xi, t) + \lambda_1 \psi_1(\xi, t),
\]

\[
\| \psi_1(\cdot, 0) \|^2_{L^2} = N_1, \quad \| \psi_2(\cdot, 0) \|^2_{L^2} = N_2, \quad \xi \in \mathbb{R}^d, \quad 0 \leq t \leq T.
\]

**Ground state.** Numerical computation of ground state solutions

\[
\psi_1(\xi, t) = e^{-i\mu t} \varphi_1(\xi), \quad \psi_2(\xi, t) = e^{-i\mu t} \varphi_2(\xi),
\]

by imaginary time method, see also BAO, CAI (2009).
**Illustration.** Harmonic potential. Raman transition constant, effective Rabi frequency, interaction constants

\[\delta = (0, 0), \quad \lambda = (-1, -1), \quad \vartheta_{12} = 0.94 \vartheta_{11}, \quad \vartheta_{22} = 0.97 \vartheta_{11}.\]

Particle numbers \(N_1 = \frac{1}{2} = N_2\). Ground state computation for different \(\vartheta_{11}\).

<table>
<thead>
<tr>
<th>Method</th>
<th>(dof)</th>
<th>(\vartheta_{11})</th>
<th>(N)</th>
<th>(E)</th>
<th>(\mu)</th>
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<td>2767</td>
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<td>39.20595346564230</td>
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Ground state (External driving field)

Ground state solutions for $\theta_{11} = 0, 10, 50, 100, 250, 500$ (left).
Particle numbers, total energy and chemical potential versus $\theta_{11}$ (right).
Exponential operator splitting methods
Evolutionary Schrödinger equations. Formulate nonlinear Schrödinger equations such as Gross–Pitaevskii equation

\[ i \partial_t \psi(\xi, t) = \left( -\frac{1}{2} \Delta + U(\xi) + \vartheta |\psi(\xi, t)|^2 \right) \psi(\xi, t) \]

as abstract differential equation for \( u(t) = \psi(\cdot, t) \)

\[ u'(t) = A u(t) + B(u(t)) u(t) . \]

Choose differential operator \( A \) and multiplication operator \( B(u) \) according to spectral space discretisation

\[
\begin{align*}
    i A &= -\frac{1}{2} (\Delta - U_H), \\
    i B(u) &= U - \frac{1}{2} U_H + \vartheta |u|^2, \quad \text{(Hermite)} \\
    i A &= -\frac{1}{2} \Delta, \\
    i B(u) &= U + \vartheta |u|^2. \quad \text{(Fourier)}
\end{align*}
\]

Abstract formulation convenient for construction and theoretical analysis of time integration methods.
Splitting methods for linear equations

**Aim.** For linear evolutionary Schrödinger equation

\[ u'(t) = A u(t) + B u(t), \quad t \geq 0, \quad u(0) \text{ given,} \]

\[ i A = - \frac{1}{2} (\Delta - U_H), \quad i B = U - \frac{1}{2} U_H, \quad \text{(Hermite)} \]

\[ i A = - \frac{1}{2} \Delta, \quad i B = U, \quad \text{(Fourier)} \]

determine numerical approximation \( u_n \approx u(t_n) \) at \( t_n = nh \).

**Approach.** Splitting methods rely on suitable composition of

\[ v'(t) = A v(t), \quad w'(t) = B w(t). \]

Spectral decomposition with respect to basis functions \( \mathcal{B}_m \) and pointwise multiplication yields

\[ v(t) = e^{tA} v(0) = \sum_m v_m e^{-i t \lambda_m} \mathcal{B}_m, \quad v(0) = \sum_m v_m \mathcal{B}_m, \]

\[ \left( w(t) \right)(x) = \left( e^{tB} w(0) \right)(x) = e^{tB(x)} \left( w(0) \right)(x). \]
Splitting methods for linear equations (Examples)

- **Lie–Trotter splitting method** yields first-order approximation
  \[ u_{n+1} = e^{hB} e^{hA} u_n \approx u(t_{n+1}) = e^{h(A+B)} u(t_n). \]

- **Second-order Strang splitting method** given through
  \[ u_{n+1} = e^{\frac{1}{2}hB} e^{hA} e^{\frac{1}{2}hB} u_n, \quad u_{n+1} = e^{\frac{1}{2}hA} e^{hB} e^{\frac{1}{2}hA} u_n. \]

- **Higher-order splitting methods** by Blanes and Moan, Kahan and Li, McLachlan, Suzuki, and Yoshida are cast into form
  \[ u_{n+1} = \prod_{j=1}^{s} e^{b_j hB} e^{a_j hA} u_n = e^{b_s hB} e^{a_s hA} \cdots e^{b_1 hB} e^{a_1 hA} u_n \]
  with real (possible negative) method coefficients \((a_j, b_j)_{j=1}^{s}\).
**Situation.** Exponential operator splitting methods for linear evolutionary Schrödinger equations

\[
\begin{align*}
    u'(t) &= A u(t) + B u(t), \quad t \geq 0, \\
    u(t_{n+1}) &= e^{h(A+B)} u(t_n), \quad n \geq 0, \quad u(0) \text{ given}, \\
    u_{n+1} &= \prod_{j=1}^{s} e^{b_j h B} e^{a_j h A} u_n, \quad n \geq 0, \quad u_0 \text{ given}.
\end{align*}
\]

**Objective.** Derive stiff order conditions and error estimate for general exponential operator splitting method.

**Approach.** Extend error analysis by Jahnke and Lubich (2000) for second-order scheme to splitting methods of arbitrary order.
Convergence result

**Theorem (Th. 2007, Neuhauser and Th. 2008)**

Suppose that the coefficients of the splitting method fulfill the classical order conditions for $p \geq 1$. Then, provided that the exact solution is sufficiently regular, the following error estimate holds

$$\| u_n - u(t_n) \|_X \leq C \| u(0) - u_0 \|_X + C h^p, \quad 0 \leq nh \leq T.$$
Sketch of the proof

**Approach.** Relate global and local error (*Lady Windermere’s Fan*)

\[ u_n - u(t_n) = S^n (u_0 - u(0)) - \sum_{j=0}^{n-1} S^{n-j-1} d_{j+1}, \]

\[ S = \prod_{j=1}^{s} e^{b_j hB} e^{a_j hA}, \quad d_{j+1} = u(t_{j+1}) - Su(t_j). \]

Deduce **stability bound** for powers of splitting operator and suitable estimate for local error.

- Variation-of-constants formula
- Stepwise expansion of $e^{tB}$
- Quadrature formulas for multiple integrals
- Bounds for iterated commutators
- Characterise domains of unbounded operators
Splitting methods for nonlinear equations

**Abstract formulation.** Rewrite nonlinear Schrödinger equation

\[ i \partial_t \psi(\xi, t) = \left( -\frac{1}{2} \Delta + U(\xi) + \vartheta |\psi(\xi, t)|^2 \right) \psi(\xi, t) \]

as abstract differential equation for \( u(t) = \psi(\cdot, t) \)

\[ u'(t) = A u(t) + B(u(t)) u(t). \]

**Approach.** Splitting methods rely on suitable composition of

\[ v'(t) = A v(t), \quad w'(t) = B(w(t)) w(t), \]

with \( A, B \) chosen according to spectral space discretisation

\[ i A = -\frac{1}{2} \left( \Delta - U_H \right), \quad i B(u) = U - \frac{1}{2} U_H + \vartheta |u|^2, \quad \text{(Hermite)} \]

\[ i A = -\frac{1}{2} \Delta, \quad i B(u) = U + \vartheta |u|^2. \quad \text{(Fourier)} \]
**Approach.** Splitting methods rely on suitable composition of

\[
v'(t) = A v(t), \quad w'(t) = B(w(t)) w(t),
\]

\[
i A = -\frac{1}{2} \left( \Delta - U_H \right), \quad i B(u) = U - \frac{1}{2} U_H + \vartheta |u|^2, \quad \text{(Hermite)}
\]

\[
i A = -\frac{1}{2} \Delta, \quad i B(u) = U + \vartheta |u|^2. \quad \text{(Fourier)}
\]

**Spectral decomposition** with respect to basis functions \((B_m)\) and invariance property \(B(w(t)) = B(w(0))\) yields

\[
v(t) = e^{tA} v(0) = \sum_m v_m e^{-it\lambda_m B_m}, \quad v(0) = \sum_m v_m B_m,
\]

\[
\left( w(t) \right)(x) = \left( e^{tB(w(0))} w(0) \right)(x) = e^{tB(w(0))(x)} \left( w(0) \right)(x).
\]
Splitting methods for nonlinear equations

**Splitting methods.** Consider initial value problem

\[ u'(t) = A u(t) + B(u(t)) u(t), \quad u(t_n) \text{ given}, \]

and solutions of associated initial value problems

\[ v(t) = e^{(t-t_n)A} v(t_n), \quad w(t) = e^{(t-t_n)B(w(t_n))} w(t_n). \]

**Strang splitting.** Second-order scheme given by

\[ u_{n+1} = e^{\frac{1}{2}hB(U_n)} e^{hA} e^{\frac{1}{2}hB(u_n)} u_n. \]

**High-order splitting.** General scheme can be cast into form

\[ u_{n+1} = e^{b_s hB(U_{ns})} U_{ns}, \]

\[ U_{n1} = e^{a_1 hA} u_n, \quad U_{nj} = e^{a_j hA} e^{b_{j-1} hB(U_{n,j-1})} U_{n,j-1}. \]
Temporal convergence orders of various time-splitting Fourier (first row) and Hermite (second row) pseudospectral methods (GPE in 2d, $\theta = 1$, $M = 128$).
Convergence analysis

Conjecture

Suppose that the coefficients of the splitting method fulfill the classical order conditions for $p \geq 1$. Then, provided that the exact solution is sufficiently regular, the following error estimate holds

$$\| u_n - u(t_n) \|_X \leq C \| u(0) - u_0 \|_X + C h^p, \quad 0 \leq nh \leq T.$$
Convergence analysis


**Main tools.**

- Formal calculus of Lie derivatives
- Nonlinear variation-of-constants formula
- Stepwise expansion of exponential involving nonlinear part
- Quadrature formulas for multiple integrals
- Bounds for iterated Lie commutators (Sobolev embedding)

**Remark.** Convergence analysis for high-order splitting methods applied to MCTDHF equations, see Koch, Neuhauser, Th. (2009).
Illustration. Perform long-term integration of the GPE (breathing) with $\vartheta = 1$ up to $T = 400$. For a prescribed tolerance display optimal performances (smallest values of required number of basis functions and spectral transforms).

Numerical solution $\psi(x_1, 0, t)$ of the GPE (breathing) for $\vartheta = 1$ up to a final time $T = 13$. Slice along $x_2 = 0$.
### Long-term integration (Breathing)

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Conclusions

**Theoretical aspects.**
- Numerical methods
- Ordinary differential equations
  (Lie derivatives, BCH, etc.)
- Functional analysis

**Practical aspects.**
- Practical implementation in 3D