High-order time-splitting spectral methods for nonlinear Schrödinger equations

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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 by systems of nonlinear Schrödinger equations.

Numerical simulation. Favourable discretisations rely on time-splitting pseudospectral methods. See recent work by Bao, Cancès, Dion, Du, Jaksch, Markowich, Pérez-García, Shen, Tang, Tiwari, Shukla, Vazquez, Zhang etc.
**Theoretical model.** Mathematical description of Bose–Einstein condensate by Gross–Pitaevskii equation

\[
  i \hbar \frac{\partial}{\partial t} \psi(x, t) = \left( -\frac{\hbar^2}{2m} \Delta + U(x) + \frac{4\pi \hbar^2 a N}{m} |\psi(x, t)|^2 \right) \psi(x, t).
\]

**Numerical discretisation.** High accuracy approximations rely on
- Hermite and Fourier spectral methods in space and
- exponential operator splitting methods in time.
Objectives

Convergence analysis.
- High-order splitting methods for nonlinear Schrödinger equations.
- Minimisation method for ground state computation.

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

- Gross–Pitaevskii equation
- Pseudospectral methods
- Exponential operator splitting methods
  - Linear evolutionary Schrödinger equations
  - Nonlinear evolutionary Schrödinger equations
  - Stability and convergence analysis
Gross–Pitaevskii equation
Nonlinear Schrödinger equation. Normalised Gross–Pitaevskii equation for $\psi : \mathbb{R}^d \times [0, \infty) \rightarrow \mathbb{C}$

$$i \partial_t \psi(x, t) = \left( -\frac{1}{2} \Delta + V(x) + \partial |\psi(x, t)|^2 \right) \psi(x, t),$$

$$\Delta = \sum_{j=1}^{d} \partial_{x_j}^2,$$

$$V(x) = \frac{1}{2} V_H(x) = \frac{1}{2} \sum_{j=1}^{d} \gamma_j^4 x_j^2,$$

subject to asymptotic boundary conditions and initial condition

$$\|\psi(\cdot, 0)\|_{L^2}^2 = 1.$$

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

$$E(\psi(\cdot, t)) = \left( \left( -\frac{1}{2} \Delta + V + \frac{1}{2} \partial |\psi(\cdot, t)|^2 \right) \psi(\cdot, t) \right|_{L^2}.$$
**Nonlinear Schrödinger equation.** Gross–Pitaevskii equation

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

**Ground state.** Solution of form

\[ \psi(x, t) = e^{-i\mu t} \phi(x) \]

that minimises energy functional.

**Minimisation approach.** Compute ground state by direct minimisation of energy functional, see Bao and Tang (2003) and Caliari et al. (2008). Use ground state solution as reliable reference solution in time-integration.
Spatial discretisation
Hermite pseudospectral method

**Spectral decomposition.** Hermite functions \((\mathcal{H}_m)_{m \geq 0}\) form orthonormal basis of \(L^2(\mathbb{R}^d)\) and satisfy

\[
\frac{1}{2} \left( - \Delta + V_H \right) \mathcal{H}_m = \lambda_m \mathcal{H}_m, \quad \lambda_m = \sum_{j=1}^{d} \gamma_j^2 (m_j + \frac{1}{2}).
\]

Hermite decomposition for \(\psi(\cdot, t) \in L^2(\mathbb{R}^d)\)

\[
\psi(\cdot, t) = \sum_m \psi_m(t) \mathcal{H}_m, \quad \psi_m(t) = \left( \psi(\cdot, t) | \mathcal{H}_m \right)_{L^2}.
\]

**Numerical approximation.** Truncation of infinite sum and application of Gauss–Hermite quadrature formula

\[
\psi_M(\cdot, t) = \sum_m \psi_M(t) \mathcal{H}_m, \quad \psi_M(t) = \int_{\mathbb{R}^d} \psi(x, t) \mathcal{H}_m(x) \, dx \approx \sum_k \omega_k e^{\xi_k^2} \psi(\xi_k, t) \mathcal{H}_m(\xi_k).
\]
Spectral decomposition. Let $\Omega = [-a, a]$ with $a > 0$. Fourier basis functions $(F_m)_{m \in \mathbb{Z}^d}$ form orthonormal basis of $L^2(\Omega^d)$ and satisfy

$$-\frac{1}{2} \Delta F_m = \lambda_m F_m, \quad \lambda_m = \frac{\pi^2}{2a^2} \sum_{j=1}^{d} m_j^2.$$ 

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

$$\psi(\cdot, t) = \sum_{m} \psi_m(t) F_m, \quad \psi_m(t) = (\psi(\cdot, t) | F_m)_{L^2}.$$ 

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

$$\psi_M(\cdot, t) = \sum_{m} \psi_m(t) F_m,$$

$$\psi_m(t) = \int_{\Omega^d} \psi(x, t) F_m(x) \, dx \approx \omega \sum_{k=M}^{\infty} \psi(\xi_k, t) F_m(\xi_k).$$
Time integration
Evolutionary Schrödinger equations. Formulate nonlinear Schrödinger equations such as Gross–Pitaevskii equation

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

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

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

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

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

**Aim.** For linear evolutionary Schrödinger equation

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

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

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

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 \((B_m)\) and pointwise multiplication yields

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

\[ (w(t))(x) = (e^{tB} w(0))(x) = e^{tB(x)} (w(0))(x). \]
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

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

**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.
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

$$\| u_n - u(t_n) \|_X \leq C \| u(0) - u_0 \|_X + C h^p, \quad 0 \leq nh \leq T.$$
Abstract formulation. Rewrite nonlinear Schrödinger equation

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

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

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

\[ i A = -\frac{1}{2} \Delta, \quad i B(u) = V + \vartheta |u|^2. \quad \text{(Fourier)} \]
Temporal convergence orders of various time-splitting Hermite (first row) and Fourier (second row) pseudospectral methods (GPE in 2d, \( \vartheta = 1, M = 128 \)).

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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:

$$\| u_n - u(t_n) \|_X \leq C \| u(0) - u_0 \|_X + C h^p, \quad 0 \leq nh \leq T.$$
Conclusions and future work

**Contents.** High accuracy discretisations of nonlinear Schrödinger equations by time-splitting spectral methods.

- Convergence analysis for linear evolutionary Schrödinger equations.
- Numerical illustrations.

**Future work.**

- Extend error analysis to nonlinear problems (see GAUCKLER, 2009).
- Extend implementation to systems of coupled Gross–Pitaevskii equations in three space dimensions.