High-order time-splitting spectral methods for Gross–Pitaevskii systems

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Mathematical Models of Quantum Fluids
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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 work by BAO, CANCÈS, DION, DU, JAKSCH, MARKOWICH, PÉREZ-GARCÍA, SHEN, TANG, TSUBOTA, TIWARI, SHUKLA, VAZQUEZ, ZHANG etc.
Discretisation of nonlinear Schrödinger equations

**Theoretical model.** Mathematical description of Bose–Einstein condensate by Gross–Pitaevskii equation

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

**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 Gross–Pitaevskii systems 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 $\psi : \mathbb{R}^d \times [0, \infty) \rightarrow \mathbb{C}$

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

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

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

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

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

Ground state. Solution of form

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

that minimises energy functional.

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

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

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

\[
\psi_M(\cdot, t) = \sum_{m} \psi_M(t) \mathcal{H}_m, \quad \psi_M(t) = \int_{\mathbb{R}^d} \psi(x, t) \mathcal{H}_m(x) \, dx \approx \sum_{k} \omega_k \, e^{\xi_k^2} \psi(\xi_k, t) \mathcal{H}_m(\xi_k) .
\]
Fourier pseudospectral method

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

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

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

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

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

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

$$\psi_m(t) = \int_{\Omega^d} \psi(x, t) \mathcal{F}_m(x) \, dx \approx \omega \sum_{k} \psi(\xi_k, t) \mathcal{F}_m(\xi_k).$$
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.
**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 \( (\mathcal{B}_m) \) and pointwise multiplication yields

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

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

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

\[ u(t_{n+1}) = e^{h(A+B)} u(t_n), \quad n \geq 0, \quad u(0) \text{ given}, \]

\[ u_{n+1} = \prod_{j=1}^{s} e^{b_j hB} e^{a_j hA} u_n, \quad n \geq 0, \quad u_0 \text{ given}. \]

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

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

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

Temporal convergence orders of various time-splitting methods for a two-dimensional linear Schrödinger equation. Error versus stepsize.
Sketch of the proof

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

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

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

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

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

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

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

**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

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

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

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

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

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

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

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

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

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

**Theoretical analysis.** Employ formal calculus of Lie-derivatives.
Temporal convergence orders of various time-splitting Hermite (first row) and Fourier (second row) pseudospectral methods (GPE in 2d, $\vartheta = 1$, $M = 128$).
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

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

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

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

**Current research.**

- Extend error analysis to **nonlinear problems** (GPS, MCTDHF equations).
- Employ different approach to study time-splitting methods for linear and nonlinear Schrödinger equations in semi-classical regime.