ENERGY PRESERVING METHOD FOR NONLINEAR Schrodinger EQUATIONS

by

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Outline of the Talk

1. Motivations
2. Not energy conservative schemes
3. Numerical schemes with preservation properties
4. Numerical experiments
Mean-field modeling of BEC: GP equation

**Gross-Pitaevskii equation**

\[
i\partial_t \varphi(t, x) = \left( -\frac{1}{2} \Delta + V(x) + \beta |\varphi|^{2\sigma}(t, x) + \lambda (U * |\varphi(t, \cdot)|^2)(x) - \Omega L \right) \varphi(t, x),
\]

with \( \varphi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C} \) or \( \mathbb{R} \times \mathbb{T}_\delta^d \to \mathbb{C} \), and \( \beta \in \mathbb{R} \) and \( \lambda \in \mathbb{R} \): local and nonlocal nonlinearity strengths.

\( \sigma = 1 \): standard GPE; \( \sigma = 2 \): extended GPE (see B. Blakie yesterday talk)

GPE is **hamiltonian** for the energy functional: 

\[
i\partial_t \varphi = \frac{\delta E(\varphi)}{\delta \varphi}
\]

\[
E(\varphi) = \frac{1}{2} \int \left( \frac{1}{2} |\nabla \varphi|^2 + V|\varphi|^2 + \frac{\beta}{\sigma + 1} |\varphi|^{2\sigma + 2} + \frac{\lambda}{2} (U * |\varphi|^2)|\varphi|^2 - \Omega \varphi L \varphi \right) dx
\]

provided \( U \) is a real-valued convolution kernel, symmetric with respect to the origin.

The total mass is preserved:

\[
\int |\varphi(t, x)|^2 dx = \int |\varphi(0, x)|^2 dx.
\]
Mean-field modeling of BEC: GP equation

\[ i\partial_t \varphi(t, x) = \left( -\frac{1}{2} \Delta + V(x) + \beta |\varphi|^2 \varphi(t, x) + \lambda \left( U \ast |\varphi(t, \cdot)|^2 \right)(x) - \Omega \cdot L \right) \varphi(t, x), \]

- **V** confining potential, usually \( V(x) = (\gamma_{x_1}^2 x_1^2 + \gamma_{x_2}^2 x_2^2 + \gamma_{x_3}^2 x_3^2)/2 \).
- **Rotation**: vortex nucleation by increasing rotation speed by Dalibard’s group (2001)

\( \Omega \in \mathbb{R}^d \): direction and the speed of the rotation, \( L = x \wedge (-i \nabla) \): rotation operator.

- **Dipolar interactions**, important for Chromium \( ^{52} \text{Cr} \) for example: convolution kernel \( U \)
What do we ask to numerical schemes?

- Time reversible
- Mass Conservation
- Energy Conservation
- Unconditional Stability
- Time and Spatial Accuracy
- Efficiency
- Very fine structures: high order numerical schemes in space (spectral, FEM) and if possible in time.

Excluded here

- Time Transverse Invariant (for linear equation with potential)
- Dispersion Relation (linear equation)
- Behavior with respect to small parameters (Asymptotic Preserving and Uniformly Accurate schemes)

Carles 2013, CB-Carles-Mehats 2013, Mehats et al. 2015-16, Bao et al. 2016-17, Jin et al., Cai et al. 2018, ...

- Order reduction:  A. Ostermann & K. Schratz, 2018
1 Motivations

2 Not energy conservative schemes

3 Numerical schemes with preservation properties

4 Numerical experiments
Some usual schemes for GPE

- Splitting schemes
- Exponential Runge-Kutta
- Lawson methods
- IMEX schemes
**Splitting schemes**

Reference: see for example *Geometric Numerical Integration*, E. Hairer, C. Lubich & G. Wanner, Springer

We consider an arbitrary system of ODEs

\[ \dot{y} = f(y) = f^{[1]}(y) + f^{[2]}(y) \in \mathbb{R}^d, \quad y(0) = y_0. \]

The solution is given by the flow \( F_t: y(t) = F_t(y_0) \).

Assume we know the exact flows \( F_t^{[i]} \) of \( \dot{y} = f^{[i]}(y) \), \( i = 1, 2 \).

Numerical flow \( \Phi_h: y_n \mapsto y_{n+1} \) where \( y_n \approx y(t_n) \) and \( h = t_{n+1} - t_n \).

**Lie-Trotter** splitting scheme: \( \Phi_h = F_h^{[2]} \circ F_h^{[1]} \) or \( \Phi_h = F_h^{[1]} \circ F_h^{[2]} \)

Taylor expansion: \((F_h^{[1]} \circ F_h^{[2]})(y_0) = F_h(y_0) + \mathcal{O}(h^2)\).

**Strang** splitting scheme: \( \Phi_h^{[S]} = F_{h/2}^{[1]} \circ F_h^{[2]} \circ F_{h/2}^{[1]} = \Phi_{h/2} \circ \Phi_{h/2} \)

\( \Phi_h^{[S]}(y_0) = F_h(y_0) + \mathcal{O}(h^3) \).

**General Splitting Procedure:** look for coefficient \( a_1, b_1, a_2, \ldots, a_m, b_m \) such that

\[ \Phi_h = F_{b_m h}^{[2]} \circ F_{a_m h}^{[1]} \circ F_{b_{m-1} h}^{[2]} \circ \cdots \circ F_{a_2 h}^{[1]} \circ F_{b_1 h}^{[2]} \circ F_{a_1 h}^{[1]} \]

to get

\[ \Phi_h(y_0) = F_h(y_0) + \mathcal{O}(h^{s+1}), \quad s \geq 3. \]
**Splitting schemes**

**Application to cubic NLS:** \( \partial_t \varphi = i \frac{\Delta}{2} \varphi - i |\varphi|^2 \varphi \).

\[
f^{[1]}(\varphi) = -i|\varphi|^2 \varphi \quad \text{and} \quad f^{[2]}(\varphi) = i \frac{\Delta}{2} \varphi,
\]

and

\[
F^{[1]}_t(\varphi_0) = e^{-i|\varphi_0|^2} \varphi_0 \quad \text{and} \quad F^{[2]}_t(\varphi_0) = e^{i\Delta t/2} \varphi_0.
\]

The usual splitting preserves mass since

\[
\int_{\mathbb{R}^d} \left| F^{[1]}_t(\varphi_0) \right|^2 \, dx = \int_{\mathbb{R}^d} |\varphi_0|^2 \, dx \quad \text{and} \quad \int_{\mathbb{R}^d} \left| F^{[2]}_t(\varphi_0) \right|^2 \, dx = \int_{\mathbb{R}^d} |\varphi_0|^2 \, dx.
\]

**Properties:**

- **Numerical analysis results for NLS:** CB-Bidégaray-Descombes, Lubich, Thalhammer, Blanes-Casas-Murua, Faou, Bao *et al.*, ...
- **Time reversible, mass conservation, unconditional stability**
- **Explicit scheme:** high efficiency
- **Spatial accuracy:** usually pseudo-spectral methods
- **Time accuracy:** Lie (1st order), Strang (2nd order), it is possible to get higher order quite easily
- **does not preserve energy**
If we are interested in high time accuracy, some schemes based on RK method are available for PDE $u'(t) = Lu(t) + N(u(t))$

**ERK methods**


$u(t_{n+1}) = e^{hL}u(t_n) + \int_0^h e^{(h-\sigma)L} N(u(t_n + \sigma))d\sigma$ & interpolation polynomial of $N$

- high order but never preserve neither mass or energy
- superconvergence for Gauss points (order 2s for s nodes)
- high CPU usage

**Lawson method**

CB-Dujardin-Lacroix Violet (2017)

change of unknown: $v(t) = e^{-Lt}u(t) \implies v'(t) = e^{-Lt}N(e^{Lt}v(t))$

- preserve mass for well chosen Butcher tableau components (Cooper condition: $b_k a_{k,\ell} + b_\ell a_{\ell,k} = b_k b_\ell$)
- superconvergence for Gauss points (order 2s for s nodes)
- high CPU usage

**IMEX scheme**

Antoine-CB-Rispoli (2017)

- high order but never preserve neither mass or energy
- low CPU usage
Outline of the talk

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How to prove mass and energy conservation

Consider

\[ i \partial_t \varphi(t, x) + \frac{1}{2} \Delta \varphi(t, x) = \beta |\varphi(t, x)|^{p-1} \varphi(t, x), \quad \varphi(0, x) = \varphi_{\text{in}}(x). \]

Mass conservation: \( \text{Im} \int_{\mathbb{R}^d} (\text{NLS}) \overline{\varphi(t, x)} \, dx \)

Energy conservation: \( \text{Re} \int_{\mathbb{R}^d} (\text{NLS}) \partial_t \overline{\varphi(t, x)} \, dx \) leads to

\[ \text{Re} \int_{\mathbb{R}^d} i |\partial_t \varphi(t, x)|^2 - \frac{1}{2} \nabla \varphi(t, x) \cdot \nabla \partial_t \varphi(t, x) - \beta |\varphi(t, x)|^{p-1} \varphi(t, x) \partial_t \overline{\varphi(t, x)} \, dx = 0. \]

Thank to the identity

\[ \text{Re} \int_{\mathbb{R}^d} |\varphi(t, x)|^{p-1} \varphi(t, x) \partial_t \overline{\varphi(t, x)} \, dx = \frac{1}{p + 1} \frac{d}{dt} \int_{\mathbb{R}^d} |\varphi(t, x)|^p \, dx, \]

we obtain \( E(\varphi) = \frac{1}{2} \int_{\mathbb{R}^d} \frac{\|\nabla \varphi\|^2}{2} + \frac{\beta}{p + 1} |\varphi|^{p+1} \, dx \) is conserved.

The numerical scheme must be adapted to follow these two steps.
Consider the mid-point for the linear Schrödinger equation (2nd order scheme)

\[ i \frac{\varphi_{n+1} - \varphi_n}{h} = -\frac{1}{2} \Delta \frac{\varphi_{n+1} + \varphi_n}{2} \]

How to deal with nonlinearity $|\varphi|^{p-1} \varphi$?
The answer was given by M. Delfour, M. Fortin & G. Payre, 1981, following and idea by Strauss & Vasquez, 1978.

For $v \in \mathbb{R}$, $G(v) = \frac{|v|^{p+1}}{p+1}$, $G'(v) = |v|^{p-1}v$. The discretization of $G'(\varphi)$ is chosen such as

\[ \frac{G(\varphi_{n+1}) - G(\varphi_n)}{|\varphi_{n+1}|^2 - |\varphi_n|^2} (\varphi_{n+1} + \varphi_n) \]

Why this choice?

- If $(a, b) \in \mathbb{R}^2$, $\frac{G(b) - G(a)}{|b|^2 - |a|^2} (b + a) = \frac{G(b) - G(a)}{b - a} = G'(\frac{a + b}{2}) + \mathcal{O}((b - a)^3)$, second order approximation of $G'$. 

Crank-Nicolson scheme

- Energy conservation: mimic $|\varphi|^{p-1} \varphi \partial_t \varphi$

\[
(\varphi_{n+1} + \varphi_n) \frac{\varphi_{n+1} - \varphi_n}{h} = \frac{1}{h} \left( |\varphi_{n+1}|^2 - |\varphi_n|^2 + 2i \text{Im}(\varphi_n \bar{\varphi}_{n+1}) \right).
\]

\[
\text{Re} \int_{\mathbb{R}^d} \frac{G(\varphi_{n+1}) - G(\varphi_n)}{|\varphi_{n+1}|^2 - |\varphi_n|^2} (\varphi_{n+1} + \varphi_n) \frac{\varphi_{n+1} - \varphi_n}{h} \, dx = \int_{\mathbb{R}^d} \frac{G(\varphi_{n+1}) - G(\varphi_n)}{h} \, dx
\]

which corresponds to
\[
\frac{1}{p+1} \frac{d}{dt} \int_{\mathbb{R}^d} |u|^{p+1} \, dx.
\]

CN scheme

\[
i \frac{\varphi_{n+1} - \varphi_n}{h} = \left( -\frac{1}{2} \Delta + \frac{\beta}{\sigma + 1} \frac{|\varphi_{n+1}|^{2\sigma+2} - |\varphi_n|^{2\sigma+2}}{|\varphi_{n+1}|^2 - |\varphi_n|^2} \right) \frac{\varphi_{n+1} + \varphi_n}{2}
\]

- Preserves exactly mass and energy
- time reversible, implicit, nonlinear, high CPU usage
- Rmk: $\frac{|\varphi_{n+1}|^{2\sigma+2} - |\varphi_n|^{2\sigma+2}}{|\varphi_{n+1}|^2 - |\varphi_n|^2} = \sum_{k=0}^{\sigma} |\varphi_{n+1}|^{2k} |\varphi_n|^{2(\sigma-k)}$
**Relaxation method**

**Cubic NLS**

\[ i\partial_t \varphi(t, x) = -\frac{1}{2} \Delta \varphi(t, x) + \beta |\varphi(t, x)|^2 \varphi(t, x), \text{ with } \varphi(0, x) = \varphi_{in}. \]

**CB, SINUM 2004:** add a variable \( \Upsilon \), write

\[
\begin{align*}
\Upsilon &= |\varphi(t, x)|^2, \\
i\partial_t \varphi(t, x) &= -\frac{1}{2} \Delta \varphi(t, x) + \beta \Upsilon \varphi(t, x),
\end{align*}
\]

and discretize at times \( t_n \) and \( t_{n+1/2} \) (like in staggered grid method)

**Relaxation**

\[
\begin{align*}
\frac{\Upsilon_{n+1/2} + \Upsilon_{n-1/2}}{2} &= |\varphi_n|^2, \\
i \frac{\varphi_{n+1} - \varphi_n}{h} &= \left( -\frac{1}{2} \Delta + \beta \Upsilon_{n+1/2} \right) \frac{\varphi_{n+1} + \varphi_n}{2},
\end{align*}
\]

with \( \Upsilon_{-1/2} = |\varphi(-h/2)|^2 \) (or at worst \( \Upsilon_{-1/2} = |\varphi(-h/2)|^2 + O(h^2) \)).
Relaxation method

- time reversible
- linearly implicit method, “low” CPU usage
- preserves mass and the energy

\[
E_{rlx}(\varphi, \eta) = \int \frac{\|\nabla \varphi\|^2}{4} dx + \frac{\beta}{2} \int \eta |\varphi|^2 - \frac{\eta^2}{2} dx = \int \frac{\|\nabla \varphi\|^2}{4} dx + \frac{\beta}{2} \int \eta \left( |\varphi|^2 - \frac{\eta}{2} \right) dx
\]

Indeed

\[
\text{Re}(\eta_{n+1/2} \frac{\varphi_{n+1}}{2} + \frac{\varphi_n}{2} (\varphi_{n+1} - \varphi_n)) = \frac{\eta_{n+1/2}}{2} \left( |\varphi_{n+1}|^2 - |\varphi_n|^2 \right).
\]

But

\[
\eta_{n+1/2} \left( |\varphi_{n+1}|^2 - |\varphi_n|^2 \right) = \eta_{n+1/2} \left( |\varphi_{n+1}|^2 - |\varphi_n|^2 \right) + \eta_{n-1/2} \left( |\varphi_n|^2 - |\varphi_n|^2 \right)
\]

\[
= \left( \eta_{n+1/2} |\varphi_{n+1}|^2 - \eta_{n-1/2} |\varphi_n|^2 \right) - \left( \eta_{n+1/2} - \eta_{n-1/2} \right) |\varphi_n|^2.
\]

Using the definition of \(\eta_{+.1/2}\)

\[
\left( \eta_{n+1/2} - \eta_{n-1/2} \right) |\varphi_n|^2 = \frac{\left( \eta_{n+1/2} \right)^2 - \left( \eta_{n-1/2} \right)^2}{2}
\]

Consistency: \(E_{rlx}(\varphi, |\varphi|^2) = E(\varphi)\).
CB 2004: classical relaxation scheme: well-posedness and convergence results in $H^s(\mathbb{R}^d)$ ($s > d/2 + 4$), but no proof of 2nd-order consistency.

**Difficulty:** $\Upsilon = |\phi|^2$ is not an evolution equation.

Depending on the parity of $n$, we have

$$\Upsilon_{n+1/2} = \Upsilon_{-1/2} + 2 \sum_{k=1}^{p} |\phi_{2k}|^2 - |\phi_{2k-1}|^2 = \Upsilon_{-1/2} + 2 \sum_{k=1}^{p} h |\phi_{2k}|^2 - |\phi_{2k-1}|^2.$$

Discrete version of

$$\Upsilon(t, x) = \Upsilon(-\frac{h}{2}, x) + \int_{0}^{h/2} \partial_s |\phi(s, x)|^2 ds = \Upsilon(-\frac{h}{2}, x) + 2 \int_{0}^{h/2} \text{Re}(\overline{\phi} \partial_s \phi) ds.$$

or

$$\partial_t \Upsilon(t, x) = 2\text{Re}(\overline{\phi} \partial_t \phi).$$

Rewrite the continuous NLSE as the system ($v = \partial_t \phi$)

$$
\begin{align*}
    i \partial_t \phi &= -\Delta \phi / 2 + \beta \Upsilon \phi, \\
    \partial_t \Upsilon &= 2\text{Re}(v \phi), \\
    i \partial_t v &= -\Delta v / 2 + \beta(\partial_t \Upsilon \phi + \Upsilon \partial_t \phi).
\end{align*}
$$
The discrete system has a \textit{discrete augmented equivalent}. Let $v_{n+\frac{1}{2}} = \frac{\varphi_{n+1} - \varphi_n}{h}$ the discrete time derivative of $\varphi_n$ and define the nonlinearities as
\[
\begin{align*}
\Phi_{n+\frac{1}{2}} &= \Upsilon_{n+\frac{1}{2}} (\varphi_{n+1} + \varphi_n)/2, \\
\Xi_{n+\frac{1}{2}} &= \Re \left( v_{n+\frac{1}{2}} \varphi_{n+1} + \varphi_n \right), \\
V_{n+\frac{1}{2}} &= (\Upsilon_{n+\frac{3}{2}} + \Upsilon_{n-\frac{1}{2}}) (v_{n+\frac{3}{2}} + 2v_{n+\frac{1}{2}} + v_{n-\frac{1}{2}})/8 \\
&\quad + \Re \left( v_{n+\frac{1}{2}} \varphi_{n+1} + \varphi_n \right) (\varphi_{n+2} + \varphi_{n+1} + \varphi_n + \varphi_{n-1})/4.
\end{align*}
\]

Let us define the operators and the matrix of operators
\[
A = (i - h\Delta/4)^{-1}(i + h\Delta/4), \quad B = (i - h\Delta/4)^{-1},
\]
\[
C = \begin{pmatrix}
I & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & I & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & B & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & B & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & B & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & B & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & B
\end{pmatrix}.
\]
The discrete system involves a seven variable unknown vector

\[ X_n := (\Upsilon_{n-\frac{1}{2}}, \Upsilon_{n+\frac{1}{2}}, \varphi_{n-1}, \varphi_n, \varphi_{n+1}, v_{n-\frac{1}{2}}, v_{n+\frac{1}{2}}) . \]

The mapping \( X_n \mapsto X_{n+1} \) reads

\[
\begin{pmatrix}
\Upsilon_{n+\frac{1}{2}} \\
\Upsilon_{n+\frac{3}{2}} \\
\varphi_n \\
\varphi_{n+1} \\
v_{n+\frac{1}{2}} \\
v_{n+\frac{3}{2}}
\end{pmatrix}
= \begin{pmatrix}
0 & I & 0 & 0 & 0 & 0 & 0 \\
I & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & I & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & I & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & A & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & I
\end{pmatrix}
\begin{pmatrix}
\Upsilon_{n-\frac{1}{2}} \\
\Upsilon_{n+\frac{1}{2}} \\
\varphi_{n-1} \\
\varphi_n \\
v_{n-\frac{1}{2}} \\
v_{n+\frac{1}{2}}
\end{pmatrix}
+ hC
\begin{pmatrix}
0 \\
2\Xi_{n+\frac{1}{2}} \\
0 \\
\beta\Phi_{n+\frac{3}{2}} \\
0 \\
2\beta V_{n+\frac{1}{2}}
\end{pmatrix}.
\]

In a more compact form, we define \( B \) and \( M \) so that the mapping reads

\[ X_{n+1} = BX_n + hCM(X_n, X_{n+1}) . \]
Consistency analysis:

**Theorem B-Descombes-Dujardin-Lacroix**

There exists $C > 0$ and $h_0 > 0$ such that for all $\Upsilon_{-1/2} \in H^{s+4}(\mathbb{R}^d)$ with 

$$
\| \Upsilon_{-1/2} \|_{H^{s+4}(\mathbb{R}^d)} \leq R_1, \text{ all } n \in \mathbb{N} \text{ and all } h \in (0, h_0) \text{ with } nh \leq T,
$$

$$
\| X_n - X(t_n) \|_{(H^s(\mathbb{R}^d))^7} \leq C \left( \| \Upsilon_{-1/2} - |\varphi(-h/2)|^2 \|_{H^{s+2}(\mathbb{R}^d)} + h^2 \right).
$$

Remark: the result remains true for $x \in \mathbb{T}^d$ and for a smooth bounded domain $O \in \mathbb{R}^d$ homogeneous Dirichlet boundary conditions.
**Relaxation method**

**Generalization**

\[
i \partial_t \varphi(t, x) = -\frac{1}{2} \Delta \varphi(t, x) + \beta |\varphi(t, x)|^{2\sigma} \varphi(t, x), \quad \text{with } \varphi(0, x) = \varphi_{in}.
\]

Original relaxation method: add variable \( \Upsilon \) and write

\[
\begin{align*}
\Upsilon(t, x) &= |\varphi(t, x)|^{2\sigma}, \\
i \partial_t \varphi(t, x) &= -\frac{1}{2} \Delta \varphi(t, x) + \beta \Upsilon \varphi(t, x),
\end{align*}
\]

→ does not lead to energy preserving scheme.

Modification

\[
\begin{align*}
\gamma^{\sigma}(t, x) &= |\varphi(t, x)|^{2\sigma}, \\
i \partial_t \varphi(t, x) &= -\frac{1}{2} \Delta \varphi(t, x) + \beta \gamma^{\sigma} \varphi(t, x),
\end{align*}
\]

Approx. of Schrödinger equation

\[
i \frac{\varphi_{n+1} - \varphi_n}{h} = \left(-\frac{1}{2} \Delta + \beta \gamma^{\sigma}_{n+1/2}\right) \frac{\varphi_{n+1} + \varphi_n}{2}.
\]

Find an approximation of \( \gamma^{\sigma} = |\varphi|^{2\sigma} = \gamma^{\sigma-1} |\varphi|^2 \) that allows energy conservation.
As before \( \text{Re}(\gamma_{n+1/2}^\sigma \frac{\varphi_{n+1} + \varphi_n}{2} \varphi_{n+1} - \varphi_n) = \frac{\gamma_{n+1/2}^\sigma}{2} \left( |\varphi_{n+1}|^2 - |\varphi_n|^2 \right) \),

and

\[
\gamma_{n+1/2}^\sigma \left( |\varphi_{n+1}|^2 - |\varphi_n|^2 \right) = \gamma_{n+1/2}^\sigma \left( |\varphi_{n+1}|^2 - |\varphi_n|^2 \right) + \gamma_{n-1/2}^\sigma \left( |\varphi_n|^2 - |\varphi_n|^2 \right) \\
= \left( \gamma_{n+1/2}^\sigma |\varphi_{n+1}|^2 - \gamma_{n-1/2}^\sigma |\varphi_n|^2 \right) - \left( \gamma_{n+1/2}^\sigma - \gamma_{n-1/2}^\sigma \right) |\varphi_n|^2.
\]

Choice

\[
\left( \gamma_{n+1/2}^\sigma - \gamma_{n-1/2}^\sigma \right) |\varphi_n|^2 = \frac{\sigma}{\sigma + 1} \left( \gamma_{n+1/2}^\sigma - \gamma_{n-1/2}^\sigma \right).
\]

The following energy is preserved \((\gamma^\sigma = |\varphi|^{2\sigma})\)

\[
E_{\text{rlx}}(\varphi, \gamma) = \int \frac{\|\nabla \varphi\|^2}{4} dx + \frac{\beta}{2} \int \gamma^\sigma |\varphi|^2 - \frac{\sigma}{\sigma + 1} \gamma^{\sigma+1} |\varphi|^2 dx
\]

Consistency: \(E_{\text{rlx}}(\varphi, |\varphi|^2) = E(\varphi)\).

Rmk: \[
\frac{1}{\sigma + 1} \frac{\gamma_{n+1/2}^{\sigma+1} - \gamma_{n-1/2}^{\sigma+1}}{h} = \frac{1}{\sigma} \frac{\gamma_{n+1/2}^{\sigma} - \gamma_{n-1/2}^{\sigma}}{h} |\varphi_n|^2 \text{ is a 2}^{\text{nd}} \text{ order approx. of } \gamma^\sigma = \gamma^{\sigma-1} |\varphi|^2 \text{ at } t = t_n.
\]
**Relaxation method**

- Generalized relaxation for $\sigma \geq 1$

\[
\begin{aligned}
\begin{cases}
\frac{\gamma_{n+1/2}^{\sigma+1} - \gamma_{n-1/2}^{\sigma+1}}{\gamma_{n+1/2}^{\sigma} - \gamma_{n-1/2}^{\sigma}} = \frac{\sigma + 1}{\sigma} |\varphi_n|^2, \\
\frac{i\varphi_{n+1} - \varphi_n}{h} = \left(-\frac{1}{2} \Delta + \beta \gamma_{n+1/2}^{\sigma}\right) \frac{\varphi_{n+1} + \varphi_n}{2}.
\end{cases}
\end{aligned}
\]

- The first equation also reads

\[
\sigma_{n+1/2} = \left(\frac{\sigma + 1}{\sigma} |\varphi_n|^2 - \gamma_{n-1/2}\right) \left(\sum_{k=0}^{\sigma-1} \gamma_{n+1/2}^{k} \gamma_{n-1/2}^{\sigma-1-k}\right).
\]

- $\sigma = 1$ : $\gamma_{n+1/2} = 2|\varphi_n|^2 - \gamma_{n-1/2}$
- $\sigma = 2$ : $\gamma_{n+1/2}^2 - k_1 \gamma_{n+1/2} - k_1 \gamma_{n-1/2} = 0$, $k_1 = (3/2)|\varphi_n|^2 - \gamma_{n-1/2}$, explicit solutions
- Explicit solutions for $\sigma = 3$ and $\sigma = 4$
- fully implicit on its first stage (for $\sigma \geq 5$), and linearly implicit in its second stage
- time reversible
- 2nd order accuracy in time
Relaxation method

**Gross-Pitaevskii equation**

\[
i\partial_t \varphi = \left( -\frac{1}{2} \Delta + V(x) + \beta |\varphi|^{2\sigma} + \lambda (U * |\varphi(t, \cdot)|^2)(x) - \Omega.L \right) \varphi,
\]

the generalized relaxation reads

\[
\begin{cases}
\gamma_{n+1/2} = \left( \frac{\sigma + 1}{\sigma} |\varphi_n|^2 - \gamma_{n-1/2} \right) \left( \sum_{k=0}^{\sigma-1} \gamma_{n+1/2} \gamma_{n-1/2} \right), \\
\frac{\gamma_{n+1/2} + \gamma_{n-1/2}}{2} = |\varphi_n|^2, \\
\frac{i\varphi_{n+1} - \varphi_n}{\hbar} = \left( -\frac{1}{2} \Delta + V + \beta \gamma_{n+1/2} + \lambda (U * \gamma_{n+1/2}) - \Omega.R \right) \frac{\varphi_{n+1} + \varphi_n}{2},
\end{cases}
\]

that preserves the following energy

\[
E_{rlx}(\varphi, \gamma, \Upsilon) = \int_{\mathbb{R}^d} \left( \frac{1}{4} \|\nabla \varphi\|^2 + \frac{1}{2} V|\varphi|^2 + \frac{\beta}{2} \gamma^\sigma |\varphi|^2 - \beta \frac{\sigma}{2(\sigma + 1)} \gamma^{\sigma+1} \right) dx \\
+ \int_{\mathbb{R}^d} \left( \frac{\lambda}{2} (U * \Upsilon)|\varphi|^2 - \frac{\lambda}{4} (U * \Upsilon) \Upsilon - \frac{\Omega}{2} \varphi R \varphi \right) dx,
\]
Relaxation method

Let \( \varphi_{n+1/2} = (\varphi_{n+1} + \varphi_n)/2 \).

The last eq. of relaxation method reads

\[
\left( I - i \frac{\delta t}{2} \Delta \right) + i \frac{\delta t}{2} V + i \frac{\delta t}{2} \beta \gamma_{n+1/2}^\sigma + i \frac{\delta t}{2} \lambda (U \ast \Upsilon_{n+1/2}) - i \frac{\delta t}{2} \Omega \cdot R \right) \varphi_{n+1/2} = \varphi_n,
\]

or

\[
\mathcal{A} \varphi_{n+1/2} = \varphi_n.
\]

The computation of the solution depends on the space discretization method.

- Finite differences, finite element, finite volume: discretized operators are matrices. Simple linear system to solve.
- Fourier based discretization. The equation can also be written as

\[
\mathcal{L} \varphi_{n+1/2} = P^{-1} \varphi_n,
\]

where

\[
\mathcal{L} = \left( I + i \frac{\delta t}{2} P^{-1} \left( V + \beta \gamma_{n+1/2}^\sigma + \lambda (U \ast \Upsilon_{n+1/2}) - \Omega \cdot R \right) \right),
\]

and

\[
P = \left( I - i \frac{\delta t}{2} \Delta \right).
\]
Outline of the talk

1. Motivations

2. Not energy conservative schemes

3. Numerical schemes with preservation properties

4. Numerical experiments
1D simulations with local nonlinearity

We compute the numerical solution to the one-dimensional cubic NLS equation

\[ i \partial_t \varphi(t, x) = -\frac{1}{2} \Delta \varphi(t, x) - q|\varphi(t, x)|^{2\sigma} \varphi(t, x), \quad (t, x) \in [0, T] \times (x_\ell, x_r), \]

Two different spatial discretizations:
- **spectral methods** for periodic boundary conditions
- **finite differences** methods for homogeneous Dirichlet boundary conditions

Spectral discretization for periodic boundary conditions

- \( \delta x = (x_r - x_\ell)/J \) with \( J = 2^P, \ P \in \mathbb{N}^* \),
- \( x_j := x_\ell + j\delta x, \ t_n := n\delta t, \ j = 0, 1, \cdots, J, \ n = 0, 1, \cdots, N \)
- \( \varphi_{j,n} = \frac{1}{J} \sum_{k=0}^{J-1} \hat{\varphi}_{k,n} \omega_J^{jk}, \ j = 0, \cdots, J - 1, \)
- \( \hat{\varphi}_k^n = \sum_{q=0}^{J-1} \varphi_q^n \omega_J^{-jk}, \ k = -\frac{J}{2}, \cdots, \frac{J}{2} - 1, \) with \( \omega_J = \exp \left( \frac{2i\pi}{J} \right) \)
- discrete gradient and Laplace operators \( \nabla_d \) and \( \Delta_d \)

\[ (\nabla_d v)_k = i\mu_k \hat{v}_k, \quad (\Delta_d v)_k = -\mu_k^2 \hat{v}_k, \quad v \in \mathbb{C}^J, \quad k = -\frac{J}{2}, \cdots, \frac{J}{2} - 1, \]

where \( \mu_k = 2\pi k/(x_r - x_\ell) \).
We define the operator \( \mathcal{L}_d = I - \delta t \Delta_d/2 - i\delta t q \gamma_{n+1}^\sigma \) and we solve

\[
\mathcal{L}_d(\varphi_{n+1/2}) = P^{-1} \varphi_n
\]

with biconjugate gradient method. One computation of \( \mathcal{L}_d(\varphi) \) from a vector \( \varphi \) requires the computation of 2 discrete Fourier transforms.

For the Crank-Nicolson method, the solution \( \varphi_{n+1} \) is obtained by the following standard fixed point procedure:

We start with \( \varphi_{n+1}^0 = \varphi_n \) and we compute for \( n \in \mathbb{N} \), \( \varphi_{n+1}^{p+1} \) using the relation

\[
\left( I - i\delta t \frac{\Delta_d}{4} \right) \varphi_{n+1}^{p+1} = \left( I + i\delta t \frac{\Delta_d}{4} \right) \varphi_n + i\delta t \frac{q}{\sigma + 1} \frac{|\varphi_{n+1}^p|^{2\sigma+2} - |\varphi_n|^{2\sigma+2}}{|\varphi_{n+1}^p|^2 - |\varphi_n|^2} \left( \frac{\varphi_{n+1}^p + \varphi_n}{2} \right),
\]

and then we set \( \varphi_{n+1} = \lim_{p \to \infty} \varphi_{n+1}^p \).
Finite differences for homogeneous Dirichlet boundary conditions

\[(\nabla_d v)_j = \frac{v_{j+1} - v_j}{\delta x} \quad \text{and} \quad (\Delta_d v)_j = \frac{v_{j+1} - 2v_j + v_{j-1}}{\delta x^2},\]

for \( v \in \mathbb{C}^{J-1}, j \in \{1, \ldots, J - 1\} \), with the convention that \( v_0 = v_J = 0 \).

The solution of

\[A\varphi_{n+1/2} = \varphi_n\]

involves tridiagonal matrices and standard linear solvers can be used.

The solution of the Crank-Nicolson scheme is still performed with fixed point procedure and also involves classical linear systems.
We define the discrete $\ell^r$ norm on $\mathbb{C}^M$ as
\[
\|v\|_{\ell^r} = \left( k \sum_{j=0}^{M-1} |v_j|^r \right)^{1/r}, \quad v \in \mathbb{C}^M, \ r \geq 1.
\]

We consider the following errors

- **Phase error**
  \[
  \mathcal{E}_{P,h} = \sup_{n \in \{0, \cdots, N\}} \|\varphi_{ex}(t_n, \cdot) - (\varphi^n_j)_j\|_{\ell^2},
  \]

- **Mass error**
  \[
  \mathcal{E}_{M,h} = \sup_{n \in \{0, \cdots, N\}} \left( \|\varphi_{ex}(t_n, \cdot)\|_{\ell^2} - \|(\varphi^n_j)_j\|_{\ell^2} \right) / \|\varphi_{ex}(0, \cdot)\|_{\ell^2}.
  \]

- **If we define the discrete energy**
  \[
  E_k(v) = \frac{1}{2} \|\nabla_k v\|_{\ell^2}^2 - \frac{q}{4} \|v\|_{\ell^4}^4,
  \]
  the energy error
  \[
  \mathcal{E}_{E,h} = \sup_{n \in \{0, \cdots, N\}} \left( E_k(\varphi_{ex}(t_n, \cdot)) - E_k((\varphi^n_j)_j) \right) / E_k(\varphi_{ex}(0, \cdot)).
  \]
For the first experiment, we compare the abilities of relaxation, CN and splitting numerical schemes to simulate the one-dimensional soliton

$$\varphi(t, x) = \rho(\sqrt{2}(x - x_0) - ct) \exp \left( \frac{ic}{2} \left( \sqrt{2}(x - x_0) - ct \right) \right) \exp \left( i \left( a + \frac{1}{4} c^2 \right) t \right),$$

where $a$, $c$ and $x_0$ are real parameters, and the profile $\rho$ is defined by

$$\rho(x) = \sqrt{\frac{2a}{q}} \text{sech}(\sqrt{a}x).$$

- Numerical parameters: $q = 10$, $c = 1$, $a = q^2/12$ and $x_0 = -1$.
- Computational domain: $(x_L, x_R) = (-12, 12)$.
- Spectral discretization: spectral accuracy → take $J = 2^{10}$
- Finite differences: $J = 2^{15}$
- The final time of simulation is $T = 5$. 

Legend

- Splitting
- Relaxation
- Crank-Nicolson
Figure: $\mathcal{E}_{P,h}$ as a function of $h$: spectral method (left) and finite differences (right)
**Figure:** Energy errors $\mathcal{E}_{E,h}$ and $\mathcal{E}_{E,h,rlx}$ as functions of $h$: spectral method (left) and finite differences (right)
**Figure:** CPU time as a function of $\mathcal{E}_{P,h}$: spectral method (left) and finite differences (right)
1D SIMULATIONS

Evolution of energy errors on long time simulations, spectral discretization
\( J = 256, \ a = 1, \ c = 0, \ x_0 = 0, \) and \((x_\ell, x_r) = (-\pi/S, \pi/S)\) with \( S = 0.11.\)
\( T = 1000 \) and we consider various \( \text{cfl} = hS^2 J^2/4 \)
cfl = 19.8 \((h = 0.1)\), cfl = 9.9 \((h = 0.05)\) and cfl = 1.9 \((h = 0.01)\).

**Figure:** Longtime behavior of energy errors (splitting) and (relaxation) for various cfl.
Evolution of $\mathcal{E}_{E,h}$ for other nonlinearities

Compute the numerical solution to the one-dimensional NLS equation

$$\partial_t \psi = \frac{i}{2} \partial_{xx} \psi + i|\psi|^{2\sigma} \psi, \quad (t, x) \in [0, T] \times \mathbb{R},$$

with $\psi(0, x) = \exp(-x^2)$.

$\sigma = 2$
Evolution of $\varepsilon_{E,h}$ for other nonlinearities

$\sigma = 3$

![Graph showing the evolution of $\varepsilon_{E,h}$ for different relaxation methods with $\sigma = 3$.]
Cubic-Quintic nonlinearities

Interactions of dark solitons under competing nonlocal cubic and local quintic nonlinearities

\[ \partial_t \varphi(t, x) = i \left( \frac{1}{2} \partial_x^2 + \alpha_1 U \ast |\varphi(t, x)|^2 + \alpha_2 |\varphi(t, x)|^4 \right) \varphi(t, x), \quad \varphi(0, x) = \varphi_{\text{in}}, \]

with kernels

\[ U_1(x) = \frac{1_{\{|x| \leq \mu\}}}{(2\mu)^d}, \quad \text{or} \quad U_2(x) = \frac{1}{(\mu\sqrt{\pi})^d} \exp \left( -|x|^2/\mu^2 \right), \quad x \in \mathbb{R}^d, \]

\( \mu \): control the width of the kernel.

Associated energy

\[ E(\varphi)(t) = \frac{1}{2} \int_{\mathbb{R}^d} \frac{1}{2} \| \nabla \varphi \|^2 - \frac{\alpha_1}{2} (U \ast |\varphi|^2)|\varphi|^2 - \frac{\alpha_2}{3} |\varphi|^6 \, dx. \]
The numerical scheme reads

\[
\begin{align*}
\gamma_{n+1/2} &= 2|\varphi_n|^2 - \gamma_{n-1/2}, \\
\gamma_{n+1/2}^2 &= \left(\frac{3}{2}|\varphi_n|^2 - \gamma_{n-1/2}\right)\left(\gamma_{n-1/2} + \gamma_{n+1/2}\right), \\
i\frac{\varphi_{n+1} - \varphi_n}{h} &= -\frac{1}{2} \Delta \frac{\varphi_{n+1} + \varphi_n}{2} - \left(\alpha_1 U \ast \gamma_{n+1/2} + \alpha_2 \gamma_{n+1/2}^2\right) \frac{\varphi_{n+1} + \varphi_n}{2},
\end{align*}
\]

and energy

\[
E_{rlx}(\varphi, \gamma, \Upsilon) = \frac{1}{2} \int_{\mathbb{R}^d} \frac{1}{2} \|
abla \varphi \|^2 - \alpha_1 U \ast \Upsilon(|\varphi|^2 - \frac{\gamma}{2}) - \alpha_2 \gamma^2(|\varphi|^2 - \frac{2}{3} \varphi) \, dx.
\]

Parameters:

- 1D \cite{Wei et al., Opt. Lett. 2014}
- kernel \(U_1, \alpha_1 = -1\).
- \(x \in [-256\pi, 256\pi]\) discretized with \(J = 2^{14} + 1\) nodes.
- \(h = 5 \cdot 10^{-3}\) and the final time is \(T = 30\)
- \(\varphi_{\text{in}}(x) = \tanh(D(x - x_0))\tanh(D(x + x_0))\), where \(D\) is the positive root of the equation

\[
\frac{\coth(D\mu)}{D\mu} \left[ \frac{1}{D^2} - \mu^2 \csch^2(D\mu) \right] - \frac{11}{15} \frac{2\alpha_2}{3D^2} = \frac{1}{3}.
\]
Cubic-Quintic nonlinearities

Case $\alpha_2 = -0.5$

$\mu = 0.5$

$\mu = 2.5$
Cubic-Quintic nonlinearities

Case $\alpha_2 = 0.1$

$\mu = 0.5$

$\mu = 2.5$
Evolution of the relative energy error

\[ \alpha_2 = -0.5 \]

\[ \alpha_2 = 0.1 \]

$$\varphi_{\text{in}}(x, y) = Ar^m e^{-r^2/2} e^{im\phi},$$

where $r = \sqrt{x^2 + y^2}$, $m$ is the topological charge, $\phi$ s.t. $x^2 + y^2 = re^{i\phi}$ and $A = 5.8$

- $m = 1$
- $(x, y) \in [-8, 8]^2$, 256 Fourier modes in each directions
- $T = 10$ and $h = 5 \cdot 10^{-3}$
- $\mu = 0.4$. 

Cubic-Quintic nonlinearities
2D case

$|\varphi|^2$ at $t = 0$
Cubic-Quintic nonlinearities
2D case

![Graphs showing cubic-quintic nonlinearities in 2D case]
Evolution of the relative energy error
We present here the simulation of a BEC subject to dipolar interaction and rotation.

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

\[ \psi(t, x) = -\frac{3}{2} (\partial n_\perp n_\perp - n_3^2 \Delta) \left( \frac{1}{2\pi |x|} * |\varphi|^2 \right)(t, x), \]

\[ \varphi(0, x) = \varphi_{\text{in}}(x), \quad x \in \mathbb{R}^2. \]

- \( L_z = -i(x_1 \partial_{x_2} - x_2 \partial_{x_1}) \)
- **Trapping potential** \( V(x) = (\gamma_{x_1} x_1^2 + \gamma_{x_2} x_2^2)/2 \)
- \( \lambda \): strength of the dipole
- \( n = (n_1, n_2, n_3)^T \), dipole axis, \( n_\perp = (n_1, n_2)^T \), \( \partial n_\perp = n_\perp \cdot \nabla \)
- **Energy** \( E(\varphi) = \frac{1}{2} \int |\nabla \varphi|^2 + V(x) |\psi|^2 + \frac{\beta}{2} |\varphi|^4 + \frac{\lambda}{2} |\psi| |\varphi|^2 - \Omega \varphi L_z \varphi dx \)
- **Initial datum**: ground state \( \phi_g = \underset{\|\phi\|^2 = 1}{\text{arg min}} E(\phi) \), computed thank to nonlinear conjugate gradient method

[Antoine, Levitt, Tang, JCP 2017, Danaila, Protas, SiSC 2017]

- Computation of nonlocal term \( \psi \): [Vico, Greengard, Ferrando, JCP 2016, Fast convolution with free-space Green’s functions]
Parameters

- $\Omega = 0.97, \gamma_x = \gamma_y = 1$
- $\lambda = 175, \beta = (250 - \lambda)\sqrt{\frac{5}{\pi}}$
- The computational domain is $(-16, 16)^2$ with $2^8 = 256$ Fourier modes in each direction.
- Initially, $n = (1, 0, 0)^T$. At $t = 0$, change it to $n = (\cos(\pi/3), \sin(\pi/3), 0)^T$.
- Computational time $T = 25$, $h = 10^{-3}$. 

2D rotating dipolar BEC
2D rotating dipolar BEC

\( t = 0 \)
\( t = 2.5 \)
\( t = 5.0 \)
\( t = 7.5 \)
\( t = 10 \)
\( t = 12.5 \)
\( t = 15 \)
\( t = 17.5 \)
\( t = 20 \)
2D rotating dipolar BEC

$|\varphi|^2 \text{ at } t = 0$
Energy evolution

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