Adaptive Full Discretization of Nonlinear Schrödinger Equations

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joint with W. Auzinger, H. Hofstätter, and M. Thalhammer

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- Defect based error estimators.

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  - Backsolve for the estimator using a generalized (nonlinear!) Sylvester equation.
  - Hermite quadrature for integral solution representation
    (akin to Gröbner–Alexeev Lemma).

Lie Calculus

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Lie derivative D_F

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Define recursively iterated commutators

$$\mathrm{ad}_{D_A}^0(D_B)u := D_B u, \qquad \mathrm{ad}_{D_A}^j(D_B)u := [D_A, \mathrm{ad}_{D_A}^{j-1}(D_B)](u).$$

Higher-Order Splittings

$$u_{n+1} = \mathcal{S}(h, u_n) := \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, h D_A}\, \mathrm{e}^{b_{s+1-j}\, h D_B}\, u_n, \qquad n = 0, 1, \ldots$$

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Theorem: The local error of the splitting operator admits the expansion

$$\mathrm{e}^{hD_{A+B}} v - \mathcal{S}(h, v) \sim \sum_{k=1}^{p} \sum_{\substack{\mu \in \mathbb{N}^k \\ |\mu| \le p-k}} \frac{1}{\mu!}\, h^{k+|\mu|}\, C_{k\mu} \prod_{\ell=1}^{k} \mathrm{ad}_{D_A}^{\mu_\ell}(D_B)\, \mathrm{e}^{hD_A}\, v.$$

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The remainder term can be proven separately to be of higher order.

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\begin{aligned}
\varphi_0(tD_A) &= \mathrm{e}^{tD_A}, \\
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- Taylor expansion of the evolution operator.

TDSE

Time-dependent Schrödinger equation (TDSE)

$$\mathrm{i}\frac{\partial \psi}{\partial t}(x_1, \ldots, x_f, t) = H\psi(x_1, \ldots, x_f, t), \quad \psi(0) = \psi_0.$$

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Hamiltonian for a system of f electrons interacting by Coulomb force and subject to nuclear attraction,

$$H := \sum_{k=1}^{f} \left(-\frac{1}{2}\Delta^{(k)} - \frac{Z}{|x_k|} + \sum_{l<k} \frac{1}{|x_k - x_l|} \right) = T + V.$$

$\Delta^{(k)}$ …Laplace operator w. r. t. k-th particle.

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Fermions indistinguishable!

MCTDHF

MCTDHF ansatz: Model reduction of TDSE by

$$\psi(x_1, \ldots, x_f, t) \approx u := \sum_J a_J(t) \Phi_J(x, t)$$

$$= \sum_{j_1,\ldots,j_f} a_{j_1,\ldots,j_f}(t) \phi_{j_1}(x_1, t) \cdots \phi_{j_f}(x_f, t) \in \mathcal{M}.$$

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Dirac–Frenkel variational principle

$$\left\langle \delta u \middle| \mathrm{i}\frac{\partial u}{\partial t} - Hu \right\rangle = 0 \quad \forall \text{ variations } \delta u \in \mathcal{T}_u\mathcal{M}.$$

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Additional constraints for uniqueness

$$\langle \phi_j | \phi_k \rangle = \delta_{j,k}, \quad \left\langle \phi_j \,\middle|\, \frac{\partial \phi_k}{\partial t} \right\rangle = -\mathrm{i}\langle \phi_j | T | \phi_k \rangle.$$

Equations of Motion

This yields the equations of motion

$$\mathrm{i}\frac{da_J}{dt} = \sum_K \langle \Phi_J \, | V | \, \Phi_K \rangle \, a_K =: \mathcal{A}_V(\phi)a,$$

$$\mathrm{i}\frac{\partial \phi_j}{\partial t} = T\phi_j + (1-P)\sum_k \sum_l \rho^{-1}_{j,l}\overline{V}_{l,k}\phi_k =: T\phi + \mathcal{B}_V(a,\phi),$$

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where

$\psi_j := \langle \phi_j | u \rangle$, “single-hole functions”,

$\rho_{j,l} := \langle \psi_j | \psi_l \rangle$, “density matrix”,

$\overline{V}_{l,k} := \langle \psi_l \,|V|\, \psi_k \rangle$, “mean-field operator matrix”,

$P := \sum_j |\phi_j\rangle \langle \phi_j|$, (orthogonal projector).

Variational Splitting

Time propagation by high-order splitting method

$$u_{n+1} = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, h D_A}\, \mathrm{e}^{b_{s+1-j}\, h D_B} u_n\,, \quad 0 \leq n \leq N-1\,.$$

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- $\mathrm{e}^{a_j h D_A} u_0$: Compute the solution at time $t_0 + a_j h$ of

$$\left\langle \delta u \,\middle|\, \mathrm{i}\frac{\partial}{\partial t} - T \,\middle|\, u \right\rangle = 0 \quad \forall \delta u \in \mathcal{T}_u\mathcal{M}, \qquad u(t_0) = u_0.$$

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Convergence of Splitting

Theorem (Koch, Lubich (2010); Koch (2010); Koch, Neuhauser, Thalhammer (2012)):
Consider the numerical approximation of the MCTDHF equations for a free electron gas ($Z = 0$) given by time semidiscretization based on an order p splitting.

Assume that $\|u(t)\|_{H^m} \le M_m$ for $0 \le t \le T$. Then

$$\big\|u_n - u(t_n)\big\|_{L^2} \le C\, h^p\,, \qquad C = C(M_m),$$

$$m = p = 2 \text{ or } m = 2\,p - 3,\ p \ge 3,$$

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Remark: For an atom, $p = 2$ if $u \in H^3$ and $u(0, t) = 0$.

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- Local error in L^2: $O(h^{p+1})$, constant depends on the H^m-norm of u (m as specified).
- Since $\|u_n\|_{H^1}$ is bounded, we conclude convergence order p in L^2.

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Proof: First H^2, then H^2-conditional stability in H^1 and L^2, respectively.

Full Discretization

Cubic NLS with *rotation term* in 2D:

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\begin{aligned}
\mathrm{i}\partial_t\psi(x,y,t) &= -\frac{1}{2}\Delta\psi(x,y,t) + \frac{\gamma^2}{2}(x^2+y^2)\psi(x,y,t) + \cdots \\
&\quad + \mathrm{i}\Omega(x\partial_y - y\partial_x)\psi(x,y,t) + V(x,y)\psi(x,y,t) + \cdots \\
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Spatial discretization in cylindrical coordinates: Laguerre(r)–Fourier(θ)–[Hermite(z)].

Theorem: Consider splitting of order p for full discretization. If $\psi \in H_{2p}$, then

$$
\|\psi_{n,M} - \psi(t_n)\|_{L^2} \le C\left(\|\psi_{0,M} - \psi(0)\|_{L^2} + M^{-q} + (\Delta t)^p\right),
$$

where $q>0$ and M^d . . . # of basis functions, $d = 2, 3$.

Proof Ingredients

- 4-term recursion holds in Cartesian coordinates for differential and multiplication operators applied to scaled generalized Laguerre functions $\mathcal{L}_{km}^{\gamma}$ (eigenfunctions of A)

$$\mathcal{L}_{km}^{\gamma}(r\cos\vartheta, r\sin\vartheta) = \widetilde{L}_{k,|m|}^{\gamma}(r)\,\mathrm{e}^{im\vartheta}$$

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- Asymptotical properties of Gauß–Laguerre nodes and weights.

Embedded Splittings

We use *embedded pairs* of splitting formulae for estimating the local error:

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j	a_j	j	b_j
1	0	1,7	0.0829844064174052
2,7	0.245298957184271	2,6	0.396309801498368
3,6	0.604872665711080	3,5	-0.039056304922349
4,5	$1/2-(a_2+a_3)$	4	$1-2\,(b_1+b_2+b_3)$

j	$\hat{a}_j$	j	$\hat{b}_j$
1	a_1	1	b_1
2	a_2	2	b_2
3	a_3	3	b_3
4	a_4	4	b_4
5	0.3752162693236828	5	0.4463374354420499
6	1.4878666594737946	6	-0.0060995324486253
7	-1.3630829287974774	7	0

Embedded Splittings (2)

Cubic NLS with blow-up solution:

$$\mathrm{i}\,\partial_t \psi(x,t) = -\frac{1}{2}\Delta\psi(x,t) - 2|\psi(x,t)|^2\psi(x,t), \qquad x \in \mathbb{R}^2.$$

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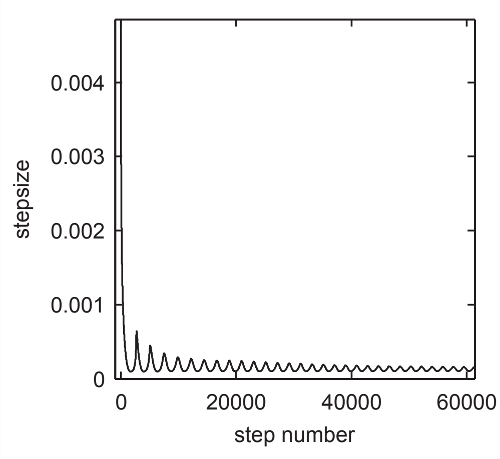
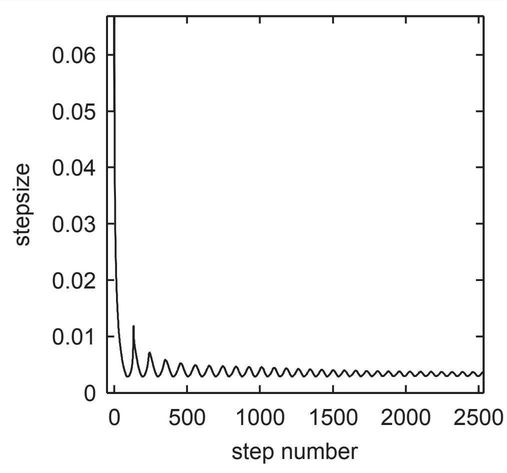
Time-stepping for pairs 2(1) (left) and 4(3) (right):





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Dissipative parabolic problem:

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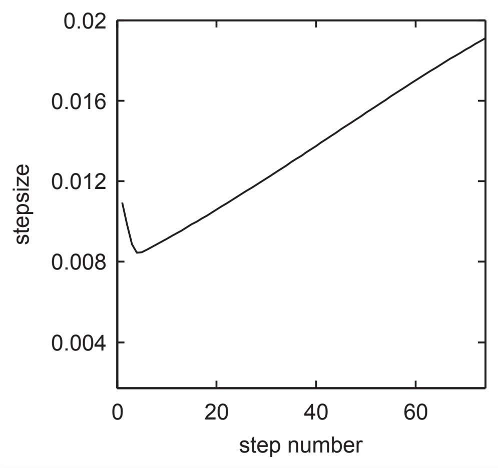

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We consider the linear case,

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The splitting flow satisfies Sylvester equation

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Defect and truncation error of splitting flow:

$$\begin{aligned}\mathcal{D}(t) &= \dot{\mathcal{S}}(t) - A\mathcal{S}(t) - B\mathcal{S}(t) = [\mathcal{S}(t), B],\\ \mathcal{T}(t) &= \dot{\mathcal{E}}(t) - A\mathcal{E}(t) - \mathcal{E}(t)B = [B, \mathcal{E}(t)].\end{aligned}$$

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- Local error $\varepsilon = \mathcal{E} - \mathcal{S}$ satisfies evolution equation

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- This is not computable in practice — approximate by trapezoidal quadrature:

$$\begin{aligned}\tilde{\varepsilon}(h) \approx \tilde{\varepsilon}_Q(h) \quad &:= \quad \frac{h}{2}\left(\mathrm{e}^{hA}\mathcal{D}(0)\mathrm{e}^{hB} + \mathrm{e}^0\mathcal{D}(h)\mathrm{e}^0\right) = \frac{h}{2}\mathcal{D}(h) \\ &= \quad \frac{h}{2}\left[\mathcal{S}(h), B\right] = \frac{h}{2}\left[\mathrm{e}^{hA}, B\right]\mathrm{e}^{hB}.\end{aligned}$$

Error Analysis

Rewrite

$$\tilde{\varepsilon}_Q(h) - \varepsilon(h) = \underbrace{\tilde{\varepsilon}_Q(h) - \tilde{\varepsilon}(h)}_{\tilde{\delta}_Q \ldots \text{quadrature error}} + \underbrace{\tilde{\varepsilon}(h) - \varepsilon(h)}_{\tilde{\delta} = \tilde{\delta}(\mathcal{D} + \mathcal{T})} .$$

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$$\frac{d^2}{ds^2} \mathrm{e}^{(h-s)A} B \, \mathrm{e}^{sA} \leadsto$$

critical dependence on $[[B, A], A] \Longrightarrow \tilde{\delta}_Q(h) = O(h^3)$.

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- If commutators are bounded $\Longrightarrow \tilde{\delta} = O(h^3)$.

Linear Schrödinger equation

$$\mathrm{i}\,\partial_t \psi(x,t) = -\tfrac{1}{2}\,\Delta\,\psi(x,t) + V(x)\,\psi(x,t)\,, \qquad x \in \mathbb{R}^3\,.$$

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- For $V \in C^4,\ \|\psi_0\|_{H^2} \le M_2$,

$$\|(\mathcal{P}-\mathcal{L})(h)\psi_0\|_{L^2} \le Ch^3, \qquad C = C(M_2).$$

Nonlinear Defect Estimate

Define defect

$$
\begin{aligned}
\mathcal{D}(t) &= \partial_t \mathcal{S}(t,\psi_0) - A\mathcal{S}(t,\psi_0) - B(\mathcal{S}(t,\psi_0)) \\
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Asymptotically correct in nonlinear semi-discrete and fully-discrete setting! (in preparation)

Numerical example (1)

For $\Omega = \gamma = V = 0$ and $\beta = -1$ in 1D
(512 Fourier modes, spatial error negligible),

an exact solution is

$$\psi(x,t) = \frac{2\mathrm{e}^{\frac{3}{2}\mathrm{i}t - \mathrm{i}x}}{\cosh(2t + 2x)}.$$

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k	Δt	err	p	err_{est}	p_{est}
8	3.9062×10^{-3}	1.5560×10^{-4}	2.00	1.1997×10^{-6}	3.03
9	1.9531×10^{-3}	3.8906×10^{-5}	2.00	1.4902×10^{-7}	3.01
10	9.7656×10^{-4}	9.7267×10^{-6}	2.00	1.8597×10^{-8}	3.00
11	4.8828×10^{-4}	2.4317×10^{-6}	2.00	2.3237×10^{-9}	3.00
12	2.4414×10^{-4}	6.0792×10^{-7}	2.00	2.9044×10^{-10}	3.00
13	1.2207×10^{-4}	1.5198×10^{-7}	2.00	3.6304×10^{-11}	3.00

Numerical example (2)

2D example: $V = 0.4\,y^2,\ \Omega = 0.5,\ \beta = 100,\ \gamma = 0.8.$

The movie shows $|\psi|^2$ for

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100 Laguerre, 128 Fourier, Strang splitting ($\Delta t = 0.02$).

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[density_fourier_laguerre_strang.avi]

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We plot the functional “condensate width”,

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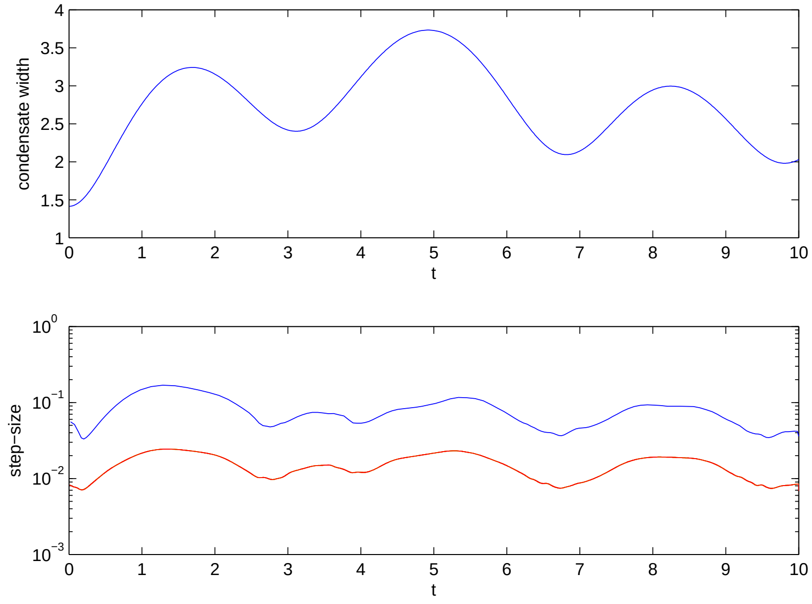
Plot of width and step-sizes for embedded 4(3) and defect based Lie–Trotter (tolerance $= 10^{-3}$):



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Use third-order Hermite quadrature
$\rightsquigarrow$ asymptotically correct local error estimator

$$\tilde{\varepsilon}_Q(h) = \frac{h}{3} \mathcal{D}(h) = \varepsilon(h) + O(h^4).$$

(error analysis uses higher order commutators).

Extensions (2)

Extension of defect–based approach to higher-order splittings,

$$\mathcal{P}(h) = \frac{h}{p+1}\,\mathcal{D}(h) \approx \mathcal{L}(h)$$

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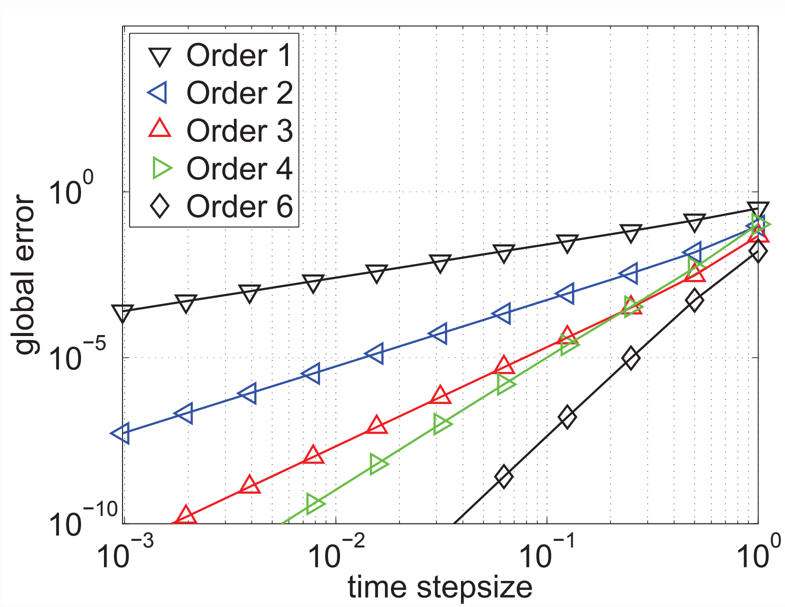

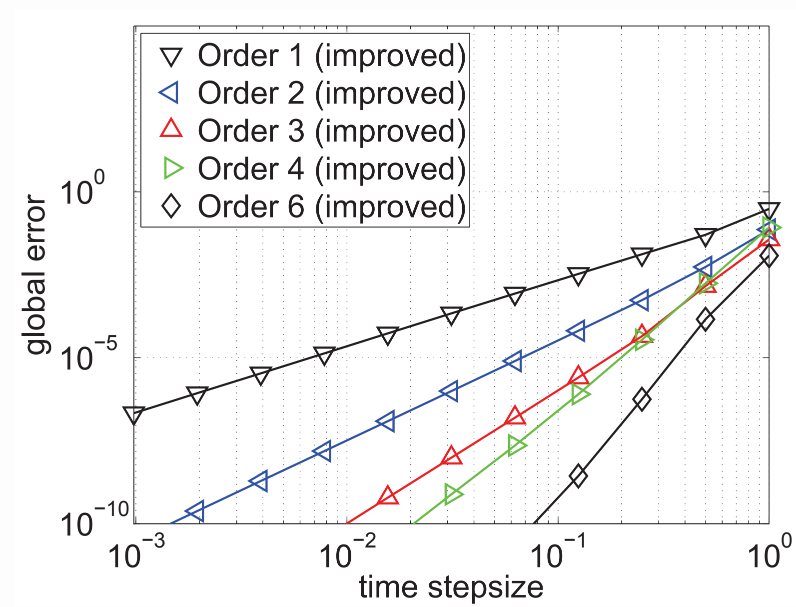

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- Construction of higher–order (complex) embedded splitting methods is a highly nontrivial optimization problem.
- Defect based approach may be iterated to obtain higher-order approximation. Convergence?
- Comparisons of error estimators.
- Time stepping strategies for splitting methods.
- Alternative spatial discretizations — FEM: Adaptivity, evaluation of nonlocal operators.

Adaptive Full Discretization of Nonlinear Schrödinger Equations

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