Convergence of high-order time–splitting pseudospectral methods for Schrödinger equations

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Objectives

Gross–Pitaevskii equation (GPE). Nonlinear Schrödinger equation of the form

$$\mathrm{i}\,\hbar\,\partial_t\psi(x,t) = \big(-\tfrac{\hbar^2}{2\,m}\Delta + U(x) + g|\psi(x,t)|^2\big)\,\psi(x,t)\,.$$

Numerical solution.

- Space discretisation based on pseudospectral methods.
- Time discretisation based on exponential operator splitting methods.

Aims.

- Convergence analysis for linear Schrödinger equations.
- Comparison of high-order splitting methods regarding accuracy, efficiency and conservation of geometric properties (particle number, energy).

Linear Schrödinger equations

Time–dependent Schrödinger equations. Normalised linear Schrödinger equation

$$\mathrm{i}\,\partial_t \psi(x,t) = \left(-\tfrac{1}{2}\Delta + \tfrac{1}{2}V_{\mathrm{H}}(x) + W(x)\right)\psi(x,t)$$

with unbounded polynomial potential

$$V_{\mathrm{H}}(x) = \sum_{j=1}^{d} \gamma_j^4 x_j^2\,, \qquad W(x) = \sum_{m\in\mathbb{N}^d} \alpha_m x^m\,.$$

Characteristics.

- Partial differential equation separable into two parts.
- Solution for each part computable in an efficient way.

Abstract evolution equations

Abstract formulation. Interpret time-dependent linear Schrödinger equation as abstract evolution equation

$$u'(t) = (A + B)\, u(t)\,.$$

Numerical solution. Split right hand side into two parts

$$A = \mathrm{i}\,\tfrac{1}{2}\,(\Delta - V_{\mathrm{H}})\,, \qquad B = -\mathrm{i}\,W\,.$$

Numerical method relies on solution of subproblems

$$v'(t) = A\,v(t) \qquad w'(t) = B\,w(t)$$
$$v(0) = v_0 \text{ given} \qquad w(0) = w_0 \text{ given}$$

Exponential operator splitting methods

Problem class. Linear evolution equation

$$u'(t) = A\,u(t) + B\,u(t), \qquad t \geq 0, \quad u(0) \text{ given.}$$

Compute numerical approximation $u_n \approx u(t_n)$ at time $t_n = n\,h$.

Example method. Strang or symmetric Lie–Trotter splitting

$$u_{n+1} = \mathrm{e}^{\frac{h}{2}A}\,\mathrm{e}^{hB}\,\mathrm{e}^{\frac{h}{2}A}\,u_n,$$

see Trotter (1959) and Strang (1968).

Method class. Higher-order exponential operator splitting methods of the form

$$u_{n+1} = \prod_{j=1}^{s} \mathrm{e}^{a_j hA}\,\mathrm{e}^{b_j hB}\,u_n$$

with coefficients a_j, b_j $(1 \leq j \leq s)$.

Assumptions and hypothesis

Problem class. Linear initial value problem

$$u'(t) = A\,u(t) + B\,u(t), \qquad t \geq 0, \quad u(0) \text{ given.}$$

Assumptions

- **Purely imaginary eigenvalues.** $A : D(A) \to L^2(\mathbb{R}^d)$ generates $\mathscr{C}_0$-group of contraction
$$\|\mathrm{e}^{tA}\|_{L^2 \leftarrow L^2} = 1, \qquad \forall t \in \mathbb{R}.$$
- **Real potential.** $B : D(B) \to L^2(\mathbb{R}^d)$ generates $\mathscr{C}_0$-group of contraction
$$\|\mathrm{e}^{tB}\|_{L^2 \leftarrow L^2} = 1, \qquad \forall t \in \mathbb{R}.$$
- **Particle number preservation.** $A + B : D(A+B) \to L^2(\mathbb{R}^d)$ generates $\mathscr{C}_0$-group of contraction
$$\|\mathrm{e}^{t(A+B)}\|_{L^2 \leftarrow L^2} = 1, \qquad \forall t \in \mathbb{R}\,.$$

Assumptions and hypothesis

Hypothesis

Commutator bounds on weighted sobolev space $D_{p+1} \subset L^2(\mathbb{R}^d)$

$$\Big\| \prod_{j=1}^{k} \left(\mathrm{ad}_A^{\mu_j}(B)\, \mathrm{e}^{\tau_j A} \right) v \Big\|_{L^2} \leq C \|v\|_{D_{p+1}} \quad |\mu| = p+1-k\,,\ 1 \leq k \leq p+1$$

where $\mathrm{ad}_A^0(B) = B$ and $\mathrm{ad}_A^j(B) = \left[A\,, \mathrm{ad}_A^{j-1}(B)\right]\,,\ j \geq 1.$

Reasonable assumptions for evolutionary Schrödinger equation with polynomial potential $B = x^m$ and

$$D_p = \Big\{ v = \sum_{\mu} v_\mu \mathscr{H}_\mu \in L^2(\mathbb{R}^d) : \sum_{\mu} (\mu + m\,p)^{m\,p} |v_\mu|^2 \leq \infty \Big\}.$$

In particular for Lie splitting

$$\left\| \left[A\,, B\right] \mathrm{e}^{\tau_1 A}\, v \right\|_{L^2} \leq C\, \|v\|_{D_2}\,, \quad \left\| B\, \mathrm{e}^{\tau_2 A}\, B\, \mathrm{e}^{\tau_1 A} v \right\|_{L^2} \leq C\, \|v\|_{D_2}\,.$$

Convergence result

Situation. Exponential operator splitting for linear evolutionary Schrödinger equation

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

$$u_{n+1} = \prod_{j=1}^{s} \mathrm{e}^{a_j h A}\,\mathrm{e}^{b_j h B}\,u_n\,, \qquad n \geq 0\,, \quad u_0 \text{ given.}$$

Theorem (N., Thalhammer (2009))

Suppose that the coefficients of the exponential operator splitting method satisfy the classical order conditions for $p \geq 1$. Then, provided that $u(0) \in D_{p+1}$, the following error estimate holds

$$\|u_n - u(t_n)\|_{L^2} \leq C\Big(\|u_0 - u(0)\|_{L^2} + h^p \max_{0\leq\tau\leq t_n} \|u(\tau)\|_{D_{p+1}}\Big).$$

Do's and Don'ts

Main tools.

- Variation-of-constants formula for expansion of exact solution

$$u(t) = \mathrm{e}^{t(A+B)}u_0 = \mathrm{e}^{tA}u_0 + \int_0^t \mathrm{e}^{(t-\tau)A} B\, u(\tau)\mathrm{d}\tau\,.$$

- Stepwise Taylor expansion of

$$\mathrm{e}^{hB} = I + h\,B + \int_0^1 \tau\,\mathrm{e}^{(1-\tau)hB}\, B^2 \mathrm{d}\tau$$

- Quadrature formulas, Taylor series expansions (commutator bounds).

Don'ts.

- Power series expansions of $\mathrm{e}^{tA} = \sum_{k=0}^{\infty} \frac{t^k}{k!} A^k$ and $\mathrm{e}^{tB} = \sum_{k=0}^{\infty} \frac{t^k}{k!} B^k$.

Local error estimate for Lie splitting

Expansion of exact solution. Variation-of-constant formula yields

$$u(h) = \mathrm{e}^{hA} u_0 \; + \int_0^h \mathrm{e}^{(h-\tau_1)A}\, B\, \mathrm{e}^{\tau_1 A}\, u_0 \, \mathrm{d}\tau_1 + R_2 \, .$$

Expansion of numerical solution. Stepwise expansion yields

$$u_1 = \mathrm{e}^{hA}\, u_0 + h\, \mathrm{e}^{hA}\, B\, u_0 + \|\hat{R}_2\|_{L^2} \, ,$$

with $\|\hat{R}_2\|_{L^2} + \|R_2\|_{L^2} \le C\, h^2 \, \max_{0\le\tau\le h} \|u(\tau)\|_{D_2}$.

Local error. Use rectangular rule for

$$\|u(h) - u_1\|_{L^2} \le \int_0^h \|\mathrm{e}^{(h-\tau_1)A}\, B\, \mathrm{e}^{\tau_1 A}\, u_0 - \mathrm{e}^{hA}\, B\, u_0\|_{L^2} \, \mathrm{d}\tau_1 + C\, h^2 \max_{0\le\tau\le h} \|u(\tau)\|_{D_2} \, .$$

and obtain finally $\|u(h) - u_1\|_{L^2} \le C\, h^2 \, \max_{0\le\tau\le h} \|u(\tau)\|_{D_2}$.

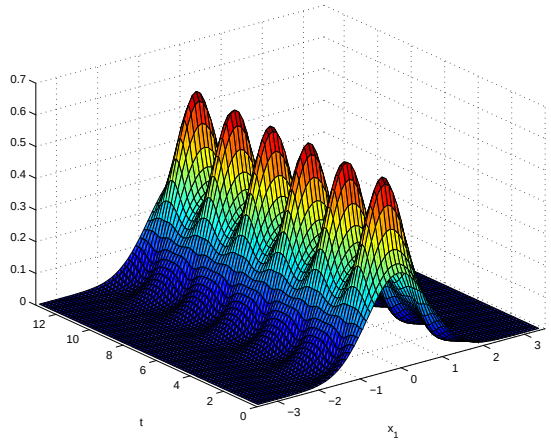
Gross–Pitaevskii equation

Gross–Pitaevskii equation (GPE). Normalised nonlinear Schrödinger equation

$$\mathrm{i}\,\partial_t \psi(x,t) = \big(-\tfrac{1}{2}\,\Delta + V(x) + \vartheta|\psi(x,t)|^2\big)\,\psi(x,t)$$

describes wave function of Bose–Einstein condensate.

Harmonic trap. Consider physically relevant case of harmonic potential $V(x) = \frac{1}{2}V_H(x) = \frac{1}{2}\sum_{j=1}^{d}\gamma_j^2\,x_j^2$.



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

$$E(\psi(\cdot,t)) = \Big(\Big(-\tfrac{1}{2}\,\Delta + V + \tfrac{1}{2}\,\vartheta\,|\psi(\cdot,t)|^2\Big)\,\psi(\cdot,t)\,\Big|\,\psi(\cdot,t)\Big)_{L^2}.$$

Evolutionary Schrödinger equations

Abstract formulation. Interpret time-dependent nonlinear Schrödinger equation as abstract evolution equation

$$u'(t) = \left(A + B(u(t))\right) u(t)\,.$$

Numerical solution. Split right hand side into two parts

Hermite	Fourier
$A = \mathrm{i}\,\frac{1}{2}\,(\Delta - V_{\mathrm{H}})$	$A = \mathrm{i}\,\frac{1}{2}\,\Delta$
$B(u) = -\mathrm{i}\,\vartheta\lvert u\rvert^2$	$B(u) = -\mathrm{i}\,(\frac{1}{2}\,V_{\mathrm{H}} + \vartheta\lvert u\rvert^2)$

Numerical method relies on solutions of evolution equations

$$v'(t) = A\,v(t) \qquad w'(t) = B(w(t))\,w(t)$$
$$v(0) = v_0 \text{ given} \qquad w(0) = w_0 \text{ given}$$

Pseudospectral methods

Hermite pseudospectral method.

- Compute transformation matrices in a preprocessing step.
- Hermite transform and inverse Hermite transform in 2D can be realised by two matrix–matrix multiplications.
- Complexity of Hermite transform in 2D is $\mathscr{O}(M^3)$.

Fourier pseudospectral method.

- Use Fast Fourier Transformation (FFT).
- Complexity of FFT in 2D is $\mathscr{O}(\log(M)\, M^2)$.

Numerical experiment (CPU-time)

Computation time of spectral methods.

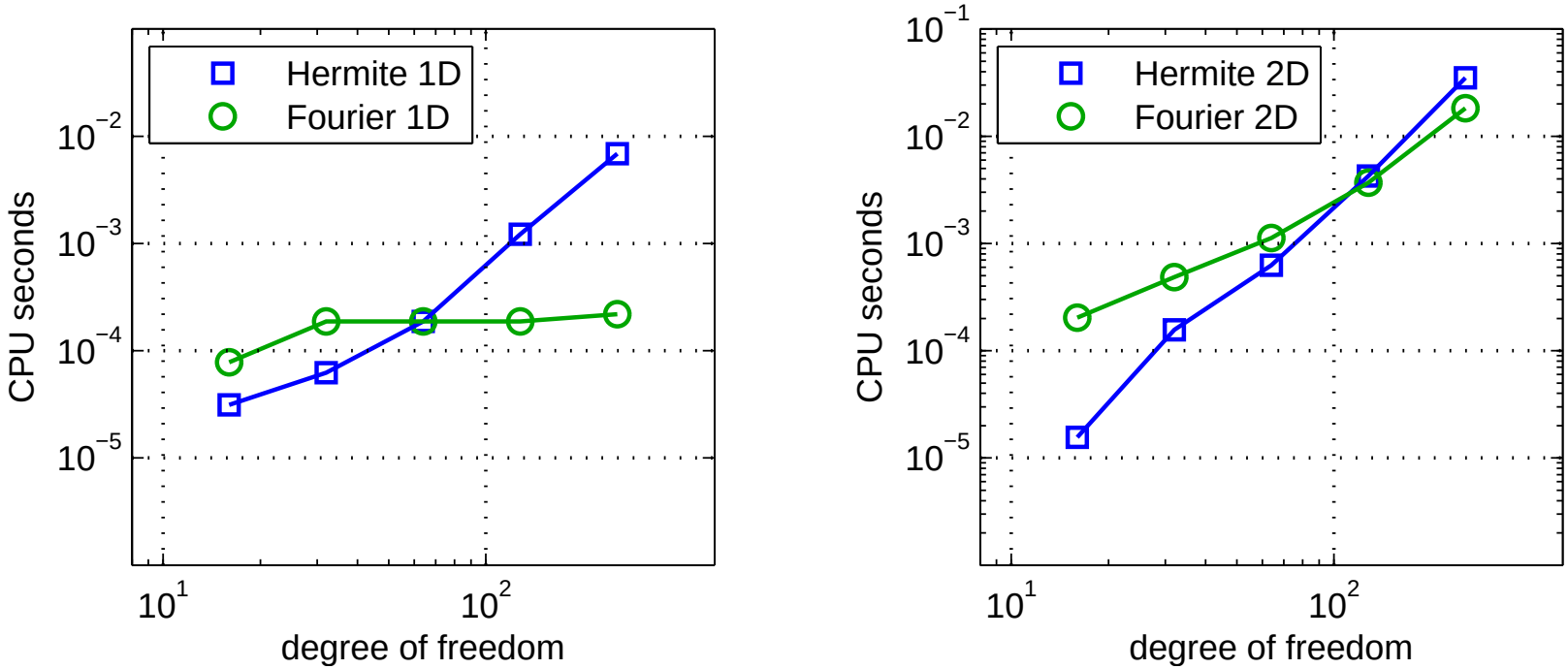


Figure: Computation time of the Hermite and Fourier spectral methods in one (left picture) and two (right picture) space dimensions using $M = 2^i$, $4 \leq i \leq 8$, basis functions in each space direction.

Numerical experiment (spatial error)

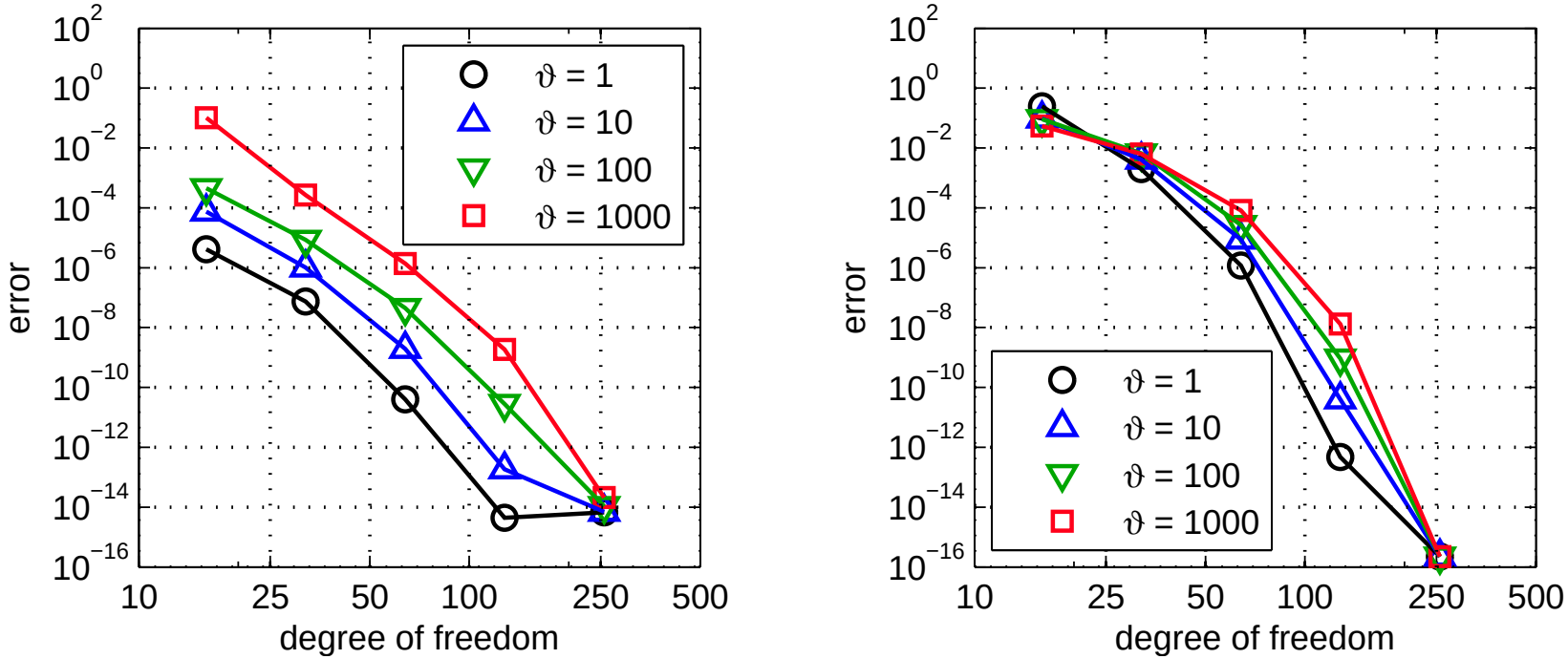


Figure: Spatial error of the Hermite (left picture) and Fourier (right picture) spectral method for different values of the coupling constant ϑ.

High-order exponential operator splitting methods

method		order	#compositions
McLachlan	McLachlan	$p = 2$	$s = 3$
Strang	Strang	$p = 2$	$s = 2$
BM4-1	Blanes & Moan PRKS$_6$	$p = 4$	$s = 7$
BM4-2	Blanes & Moan SRKN$_6^b$	$p = 4$	$s = 7$
M4	McLachlan	$p = 4$	$s = 6$
S4	Suzuki	$p = 4$	$s = 6$
Y4	Yoshida	$p = 4$	$s = 4$
BM6-1	Blanes & Moan PRKS$_{10}$	$p = 6$	$s = 11$
BM6-2	Blanes & Moan SRKN$_{11}^b$	$p = 6$	$s = 12$
BM6-3	Blanes & Moan SRKN$_{14}^a$	$p = 6$	$s = 15$
KL6	Kahan & Li	$p = 6$	$s = 10$
S6	Suzuki	$p = 6$	$s = 26$
Y6	Yoshida	$p = 6$	$s = 8$

Table: Splitting methods of order p involving s compositions.

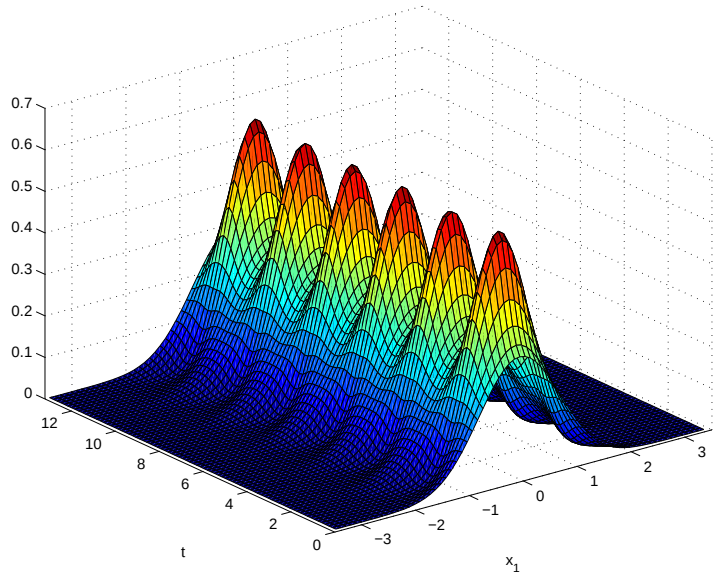
Numerical experiment (long-term integration)

Numerical experiment (Caliari, N., Thalhammer (2009)).
Illustrates the accuracy of time–splitting Hermite and Fourier pseudospectral methods for the GPE

$$\mathrm{i}\,\partial_t \psi(x,t) = \big(-\tfrac{1}{2}\,\Delta + V(x) + |\psi(x,t)|^2\big)\,\psi(x,t)$$

involving the potential $V(x) = \frac{1}{2}\,(x_1^2 + x_2^2)$.

- Choose the ground state solution of the GPE involving the potential $V(x) = x_1^2 + x_2^2$ as initial value.
- Compute a reference solution at $T = 400$ (128×128 basis functions, 2^{17} time steps).



Numerical experiment (long-term integration)

Numerical experiment. Illustrates the temporal order of Hermite and Fourier pseudospectral splitting methods for the GPE

$$\mathrm{i}\,\partial_t \psi(x,t) = \big(-\tfrac{1}{2}\,\Delta + V(x) + |\psi(x,t)|^2\big)\,\psi(x,t)\,.$$

- Compute numerical approximations by time-splitting spectral methods with 2^i, $6 \le i \le 8$, basis functions in each space direction and 2^i, $6 \le i \le 15$, time steps.
- Compute numerical approximations by standard explicit Runge–Kutta methods of order four.
- Compute error in discrete L^2-norm.
- Measure the particle number and energy conservation.

Numerical experiment (long-term integration)

tol.	method	d.o.f.	#transf.	Δ_{pn}	Δ_E
$< 10^{-2}$	Hermite 2	32×32	16384	$2.6 \cdot 10^{-11}$	$4.2 \cdot 10^{-6}$
$< 10^{-2}$	Fourier 2	64×64	32768	$3.6 \cdot 10^{-13}$	$1.6 \cdot 10^{-6}$
$< 10^{-2}$	Hermite 4	32×32	6144	$9.7 \cdot 10^{-12}$	$1.1 \cdot 10^{-5}$
$< 10^{-2}$	Fourier 4	64×64	12288	$1.7 \cdot 10^{-13}$	$9.1 \cdot 10^{-7}$
$< 10^{-2}$	Hermite 6	32×32	14337	$2.3 \cdot 10^{-11}$	$3.2 \cdot 10^{-8}$
$< 10^{-2}$	Fourier 6	64×64	7169	$1.1 \cdot 10^{-13}$	$6.8 \cdot 10^{-6}$
$< 10^{-2}$	Hermite rk4	32×32	65532	$2.1 \cdot 10^{-5}$	$1.2 \cdot 10^{-4}$
$< 10^{-2}$	Fourier rk4	64×64	524284	$6.4 \cdot 10^{-10}$	$3.7 \cdot 10^{-9}$
$< 10^{-2}$	Hermite ode45	32×32	208376	$2.6 \cdot 10^{-8}$	$1.5 \cdot 10^{-7}$
$< 10^{-2}$	Fourier ode45	64×64	1132436	$5.6 \cdot 10^{-12}$	$3.1 \cdot 10^{-11}$

Observations

- The number of required Hermite basis functions resp. transforms are (in general) smaller than the number of Fourier basis functions resp. transforms.
- Splitting methods outperform explicit Runge–Kutta methods.
- The splitting methods of order four and six by Blanes and Moan are superior to the second order Strang splitting.

Conclusion and future work

Contents. High accuracy discretisations by time-splitting pseudospectral methods.

- Convergence analysis for linear evolutionary Schrödinger equations.
- Comparison of time-splitting methods regarding accuracy, efficiency, and geometric properties.

Future work.

- Provide convergence analysis of high-order time-splitting pseudospectral methods for nonlinear Schrödinger equations.
- Study other basis functions, well adapted for a certain potential.