# A numerical study of time-splitting spatial discretisations for nonlinear Schrödinger equations: Spectral approximation versus finite elements

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**Problem.** Time-dependent nonlinear Schrödinger equation for macroscopic wave function (order parameter) $\psi : \mathbb{R}^d \times [0,T] \to \mathbb{C}$

$$\begin{cases} \mathrm{i}\,\varepsilon\,\partial_t \psi(x,t) = \left(-\tfrac{1}{2}\varepsilon^2\Delta + V(x) + \vartheta\,|\psi(x,t)|^2\right)\psi(x,t)\,, \\ \psi(x,0) \text{ given}, \qquad x \in \mathbb{R}^d, \quad 0 \le t \le T\,, \end{cases} \tag{1}$$

subject to asymptotic boundary conditions.

**Aim.** Study accuracy and efficiency properties of full discretisations in dependence of critical parameter $0 < \varepsilon \ll 1$.

**Splitting.** Time integration of nonlinear evolution equation

$$\tfrac{\mathrm{d}}{\mathrm{d}t}u(t) = A\big(u(t)\big) + B\big(u(t)\big), \quad 0 \le t \le T, \qquad u(0) \text{ given},$$

by high-order exponential operator splitting method. For linear problems set

$$u_n = \prod_{j=1}^{s} \mathrm{e}^{b_j h_{n-1} B}\,\mathrm{e}^{a_j h_{n-1} A} u_{n-1} \approx u(t_n) = \mathrm{e}^{h_{n-1}(A+B)} u(t_{n-1}), \qquad 1 \le n \le N.$$

Extension to nonlinear problems by formal calculus of Lie-derivatives.

**Realisation.** Splitting results in numerical solution of two subproblems

$$\partial_t \psi(\cdot,t) = A\,\psi(\cdot,t) = \tfrac{\mathrm{i}\varepsilon}{2}\Delta\psi(\cdot,t)\,, \tag{2}$$

$$\partial_t \psi(\cdot,t) = B\big(\psi(\cdot,t)\big) = -\tfrac{\mathrm{i}}{\varepsilon}\left(V + \vartheta\,|\psi(\cdot,t)|^2\right)\psi(\cdot,t).$$

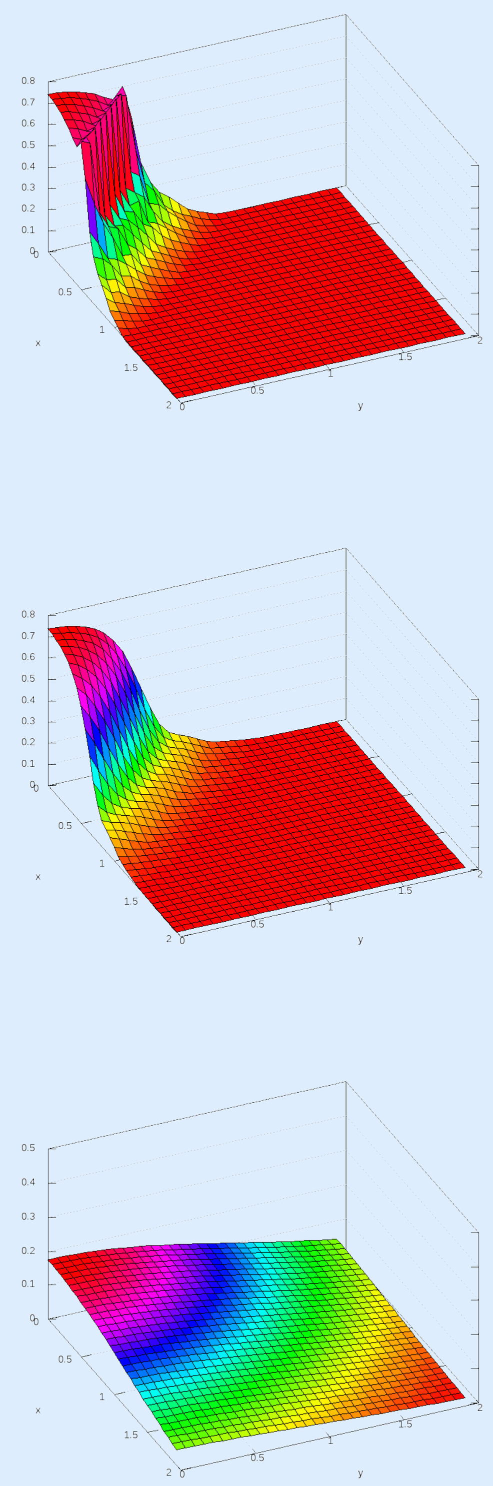
**Theorem ([3]).** *An exponential operator splitting method of (classical) order $p \ge 1$ applied to a linear Schrödinger equation satisfies the global error estimate*

$$\|\psi_N - \psi(\cdot,t_N)\|_{L^2} \le \|\psi_0 - \psi(\cdot,0)\|_{L^2} + C\sum_{n=1}^{N} \frac{h_{n-1}^{p+1}}{\varepsilon} \sum_{j=0}^{p} \varepsilon^j\,\|\psi(\cdot,0)\|_{H^j}$$

*with constant $C > 0$ depending on* $\max\{\|\partial_{x_j} U\|_{L^\infty} : 0 \le j \le 2p\}$ *and* $t_N \le T$.

**Theorem ([4]).** *The Lie–Trotter splitting method applied to the Gross–Pitaevskii equation under a regular initial condition with derivatives bounded independent of $\varepsilon > 0$ satisfies the local error estimate*

$$\|\mathscr{L}\big(h,\psi(\cdot,0)\big)\|_{L^2} \le P\big(\tfrac{h}{\varepsilon}\big)\,h^2, \qquad P(\xi) = \sum_{j=0}^{3} C_j\,\xi^j.$$



Numerical solution of (1) for $\varepsilon = 0.01$ (top), $\varepsilon = 0.1$ (middle), $\varepsilon = 1$ (bottom), $V = 0$, $\vartheta = 1$ at time $T = 1$ with initial value $\psi(x,0) = A_0(x)\,\mathrm{e}^{\mathrm{i}S_0(x)/\varepsilon}$, $A_0(x) = \mathrm{e}^{-\sum x_k^2}$, $S_0(x) = -\log(\mathrm{e}^{\sum x_k} + \mathrm{e}^{-\sum x_k})$ by Strang splitting and Fourier spectral method.

**Spectral approximation.** Fourier basis functions

$$\mathscr{F}_m(x) = \prod_{\ell=1}^{d} \frac{\mathrm{e}^{\mathrm{i}\pi m_\ell\left(\frac{x_\ell}{a_\ell}+1\right)}}{\sqrt{2a_\ell}}, \qquad x \in \Omega = \prod_{\ell=1}^{d}[-a_\ell, a_\ell], \quad m \in \mathbb{Z}^d,$$

satisfy eigenvalue relation

$$A\mathscr{F}_m = \lambda_m \mathscr{F}_m, \quad \lambda_m = \sum_{\ell=1}^{d} \frac{\pi^2 m_\ell^2}{a_\ell^2}, \qquad m \in \mathbb{Z}^d.$$

Hence, for $\psi(\cdot,t_{n-1}) = \sum_m c_m \mathscr{F}_m$ analytical solution of (2) given by

$$\psi(\cdot,t_n) = \mathrm{e}^{h_{n-1}A}\psi(\cdot,t_{n-1}) = \sum_m c_m\,\mathrm{e}^{h_{n-1}\lambda_m}\mathscr{F}_m.$$

Truncation of Fourier series and computation of $v_m(t_{n-1})$ by Trapezoidal rule.

**Theorem ([2]).** *Let $c_m$ denote the analytical Fourier coefficients and $\tilde{c}_m$ the quadrature formula approximations. Then*

$$\Big|\sum_{m\in\mathbb{Z}} c_m\mathscr{F}_m - \sum_{-M\le m\le M-1} \tilde{c}_m\mathscr{F}_m\Big| \le 2\,|c_M - c_{-M}| + 4\sum_{|m|\ge M+1}|c_m|.$$

**Finite Elements.** Let $\phi_A$, $\phi_B$ denote numerical solution operators and set

$$U_{0,r} = \prod_{j=1}^{r} \phi_A(a_j h_j)\phi_B(b_j h_j)\,u(0) = V_{0,r} + \mathrm{i}\,W_{0,r}\,,$$

$$U_{0,r}^B = \phi_B(b_{r+1}h_{r+1})\,U_{0,r} = V_{0,r}^B + \mathrm{i}\,W_{0,r}^B\,.$$

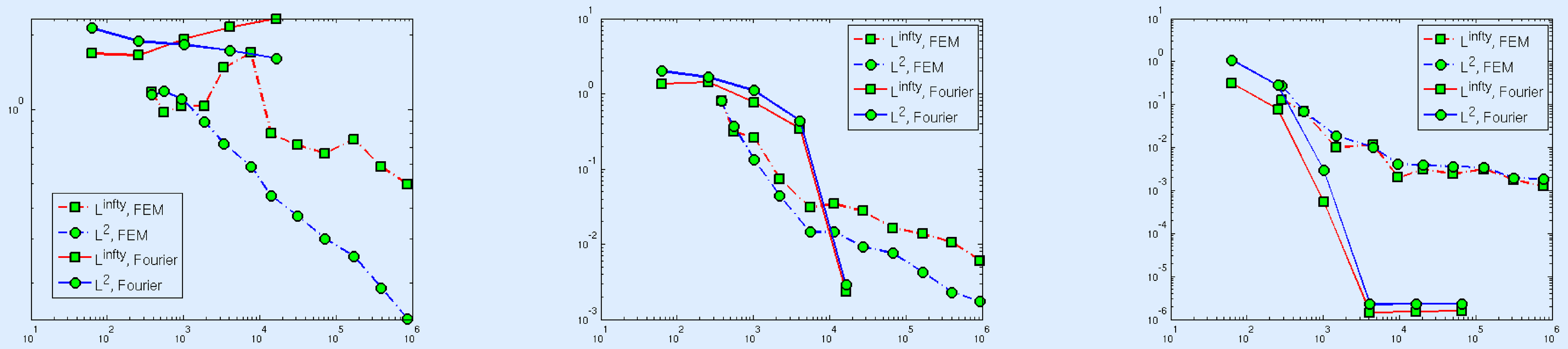
Approximate solution of real-valued PDE system ($\kappa \in [0,1]$)

$$\frac{V_{0,r+1} - V_{0,r}^B}{h_{r+1}} = -\tfrac{\varepsilon}{2}\left(\kappa\Delta W_{0,r+1} + (1-\kappa)\,\Delta W_{0,r}^B\right),$$

$$\frac{W_{0,r+1} - W_{0,r}^B}{h_{r+1}} = \tfrac{\varepsilon}{2}\left(\kappa\Delta V_{0,r+1} + (1-\kappa)\,\Delta V_{0,r}^B\right),$$

subject to homogeneous Dirichlet boundary conditions on rectangular grid with piecewise polynomial basis functions.

Comparison of the approximation error for $\varepsilon = 0.01$ (left), $\varepsilon = 0.1$ (middle), $\varepsilon = 1$ (right) of finite elements and the Fourier spectral method. The deal.II library was utilized for finite element computations.




**References.**

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[3] **S. Descombes, M. Th.**, *An exact local error representation of exponential operator splitting methods for evolutionary problems and applications to linear Schrödinger equations in the semi-classical regime.* BIT Numer. Math. 50 (2010), 729–749.

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