

Exponential Lawson for the nonlinear Schrödinger equation

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Abstract

We explore the numerical properties of the the Exponential fourth order Lawson integrator on the nonlinear Schrödinger equation for varying regularity of the potential and the initial condition. Some estimates on the regularity dependency are presented.

(25 minute talk)

- 1 The Schrödinger equation.
- 2 Dependency on the regularity of the potential.
- 3 Dependency on the regularity of initial conditions.

The nonlinear Schrödinger equation

Our aim is to solve the nonlinear Schrödinger equation,

$$\begin{aligned}i \frac{\partial \psi}{\partial t} &= -\frac{\partial^2 \psi}{\partial x^2} + (V(x) + C_{\text{nl}}|\psi|^2)\psi, \quad x \in [-\pi, \pi] \\ \psi(x, 0) &= \psi_0(x), \quad x \in [-\pi, \pi] \\ \psi(-\pi, t) &= \psi(\pi, t), \quad t > 0.\end{aligned}$$

where $V(x)$ is some potential, C_{nl} is the nonlinearity constant and ψ_0 is some initial condition.

After a spectral discretisation, we have the system of equations

$$\begin{aligned}\frac{du}{dt} &= Lu + N(u), \quad \text{where} \\ N(u) &= -i \cdot \mathcal{F}((V(x) + C_{\text{nl}}|\mathcal{F}^{-1}(u)|^2)\mathcal{F}^{-1}(c)) \\ L &= \text{diag}(-ik^2)\end{aligned}$$

Fourth order Lawson scheme based on cRK4

In a RK-like format, we write the scheme as

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2}e^{z/2} & & & \\ \frac{1}{2} & & \frac{1}{2} & & \\ 1 & & & e^{z/2} & \\ \hline & \frac{1}{6}e^z & \frac{1}{3}e^{z/2} & \frac{1}{3}e^{z/2} & \frac{1}{6} \end{array}$$

In general, Lawson schemes may be written as

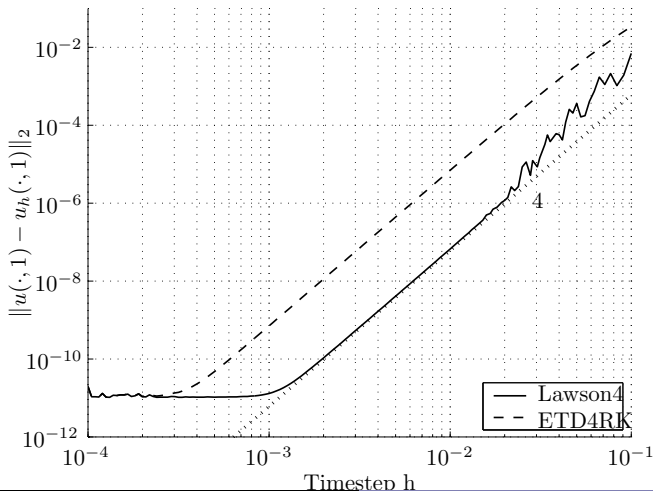
$$a_r^j(z) = \alpha_r^{j,0} e^{(c_r - c_j)z} \quad \text{and} \quad b^r(z) = \beta^{r,0} e^{(1 - c_r)z}.$$

where $\alpha_r^{j,0}$, $\beta^{r,0}$ and c_r are the coefficients from the underlying Runge–Kutta scheme.

Lawson is order 4

An introductory numerical test with smooth IC and smooth potential:

Global error, NLS, $N = 256$, IC: $\exp(\sin(2x))$, Pot: $1/(1 + \sin^2(x))$, $\lambda = 1$



The stiff order conditions

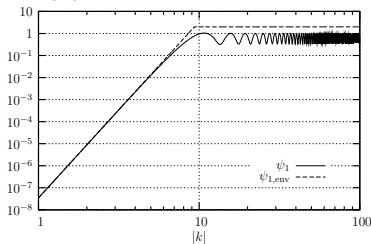
Hochbruck and Ostermann (2004) introduced stiff order conditions for analyzing exponential integrators.

- The first one reads

$$h\phi_1(z)N(u(t_0)) - h \sum_{r=1}^s b^r(z)N(u(t_0)) = h\psi_1(z)N(u(t_0))$$

so they require $\psi_1(z) = 0$.

- But for Lawson, $\psi_1(z)$ looks like



- For ETD-schemes, $\psi_1(z) = 0$, because they use $\phi_1(z)$.

Dependency on potential $V(x)$

From the first stiff order condition, we get a contribution less than order 4 to the error depending on the regularity of N . N does not have a higher regularity than the potential $V(x)$.

Proposition

If the regularity of N is ≤ 8 , assuming smooth initial conditions, we have an error contribution from the first stiff order condition

$$\|h\psi_1 N\|_2 = Ch^{1+\frac{r}{2}-\frac{1}{4}}$$

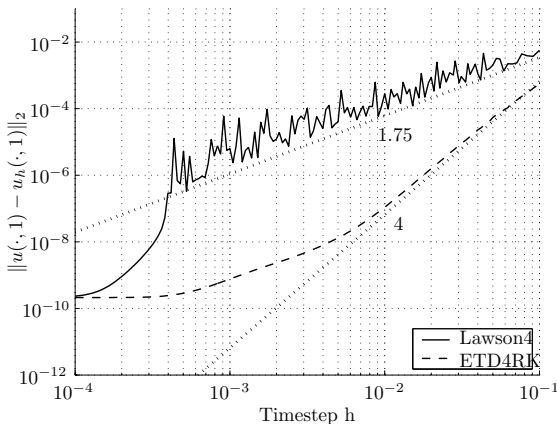
The proof is done by using the $\psi_{1,\text{env}}$ -function to bound ψ_1 , and then summing over each Fourier coefficient, where Fourier coefficients of N decays by r .

- With regard to dependency on potential-regularity, we have that local order *equals* global order (seen numerically).

Numerical experiment with varying potential

Setting $V(x)$ to be a random function with Fourier decay k^{-2} , we get the following result

Global error, NLS, $N = 256$, IC: $\exp(\sin(2x))$, Pot: Reg2, $\lambda = 1$

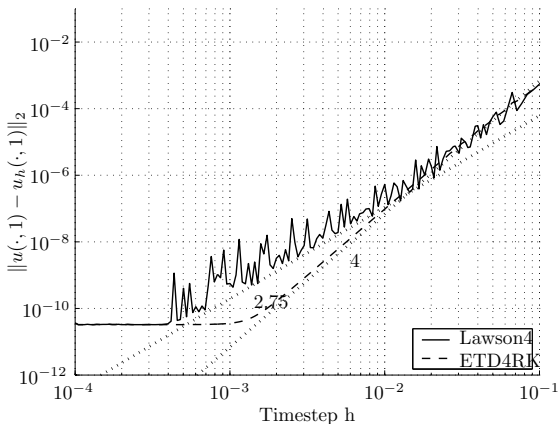


and the formula $Ch^{1+\frac{r}{2}-\frac{1}{4}}$ gives exactly order 1.75.

Numerical experiment with varying potential

Setting $V(x)$ to be a random function with Fourier decay k^{-4} , we get the following result

Global error, NLS, $N = 256$, IC: $\exp(\sin(2x))$, Pot: Reg4, $\lambda = 1$

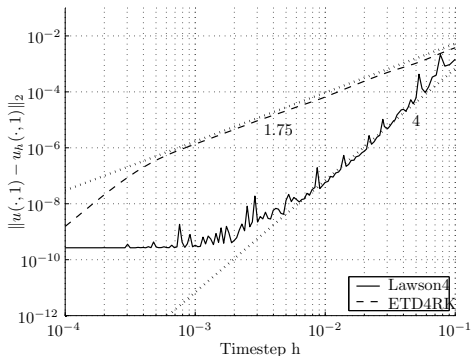


and the formula $Ch^{1+\frac{r}{2}-\frac{1}{4}}$ gives exactly order 2.75.

Dependency on the initial condition

- ETD has a local error depending on the IC-regularity equal to the dependency Lawson has on the potential-regularity.
- Lawson is less sensitive to the regularity of the initial condition. At regularity 4 we almost regain classical order:

Global error, NLS, $N = 256$, IC: Reg4, Pot: $1/(1 + \sin^2(x))$, $\lambda = 1$



- *This is unfinished research.*

Linear problem, $C_{nl} = 0$

We observe numerically that most of the dependency on the IC-regularity is still present for Lawson when we set $C_{nl} = 0$. Then the problem is linear.

- Applying the Lawson4 stepper to the simpler equation

$$\dot{u} = Lu + Vu$$

yields the following expression

$$u_{n+1} = \left[EE + \frac{h}{6}(EEV + 4EVE + VEE) + \frac{h^2}{6}(EVEV + EVVE + VEVE) + \frac{h^3}{12}(EVVEV + VEVVE) + \frac{h^4}{24}VEVVVEV \right] u_n$$

where $E = e^{hL/2}$.

The exact solution of the linear problem

Following Jahnke and Lubich (2000), we write the exact solution of $\dot{u} = (L + V)u$ as given by the variation of constants formula;

$$e^{h(L+V)}u_0 = e^{hL}u_0 + \int_0^h e^{sL}V e^{(h-s)(L+V)}u_0 ds$$

and we may recursively apply this formula to the red part above. This yields

$$\begin{aligned} e^{h(L+V)}u_0 &= e^{hL}u_0 \\ &+ \int_0^h e^{s_1L}V e^{(h-s_1)L}u_0 ds_1 \\ &+ \int_0^h e^{s_1L}V \int_0^{h-s_1} e^{s_2L}V e^{(h-s_1-s_2)(L+V)}u_0 ds_2 ds_1 \end{aligned}$$

and this should be done three more times.

The Lawson approximation

Lawson solves each of these multi-dimensional integrals to a sufficient degree of accuracy, for example:

$$\int_0^h e^{s_1 L} V e^{(h-s_1)L} u_0 ds_1 = \frac{h}{6} (VE^2 + 4EVE + E^2V) u_0 + \frac{h^5}{2880} f^{(4)}(\xi) u_0$$

which is the Simpson rule, exact for cubic polynomials.

- The error term is

$$f^{(4)}(\xi) = e^{\xi L} [L, [L, [L, [L, V]]]] e^{(h-\xi)L} = e^{\xi L} \text{ad}_L^4(V) e^{(h-\xi)L}.$$

- Regarding $\bar{u} = e^{(h-s)L} u$ as a continuous function and $L = \frac{d^2}{dx^2}$ and V as operators on functions, we find the error term to be

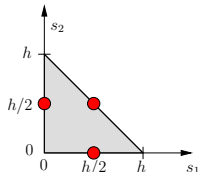
$$e^{sL} \left(V^{(8)} \bar{u} + 4V^{(7)} \bar{u}^{(1)} + 6V^{(6)} \bar{u}^{(2)} + 4V^{(5)} \bar{u}^{(3)} + V^{(4)} \bar{u}^{(4)} \right)$$

(in general, we have $\text{ad}_L^m(V) u = \sum_{i=0}^m 2^i \binom{m}{i} V^{(2m-i)} u^{(i)}$)

The Lawson approximation

The double integral

$$\int_0^h e^{s_1 L} V \int_0^{h-s_1} e^{s_2 L} V e^{(h-s_1-s_2)L} u_0 ds_2 ds_1$$



is approximated in the points in the figure by the quadrature rule

$$\frac{h^2}{6} (EVEV + EVVE + VEVE)$$

with degree of precision 2. The error term is

$$\int_0^h \int_0^{h-s_1} g(s_1, s_2) ds_1 ds_2 = \frac{h^2}{6} (EVEV + EVVE + VEVE) + CM_3 h^5$$

where the third derivatives of g is bounded by M_3 .

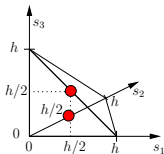
The Lawson approximation

The triple integral

$$\int_0^h e^{s_1 L} V \int_0^{h-s_1} e^{s_2 L} V \int_0^{h-s_1-s_2} e^{s_3 L} V e^{(h-s_1-s_2-s_3)L} u_0 ds_3 ds_2 ds_1$$

is approximated in the two points

$$(s_1, s_2, s_3) = \left\{ \left(\frac{h}{2}, 0, \frac{h}{2} \right), \left(0, \frac{h}{2}, 0 \right) \right\}$$



by $\frac{h^3}{12}(EVVEV + VEVVE)$ with degree of precision 1 (exact on linear functions).

The last quadruple integral is evaluated at one point, $\frac{h^4}{24} VEVVEV$ and is exact for constant functions.

- The error formula for the Simpson quadrature requires u_0 to be 4 times differentiable for order 4 of Lawson (and also the potential to be 8 times differentiable).
- The error terms from the double, triple and quadruple integral requires less regularity.
- Lawson on a constant potential shows no dependency on the initial condition, then $[L, V] = 0$.
- When mixing low regularity potential and low regularity initial condition, the differences in performance between Lawson and ETD are small.

- ETD-schemes are good on low-regularity potential and Lawson-schemes are good on low-regularity initial condition.
- Are the properties mutually exclusive?
- *Thank you for your attention*

- Cox and Matthews: *Exponential time differencing for stiff systems*, J. Comp. Physics, 2002.
- Hochbruck and Ostermann: *Explicit exponential Runge–Kutta methods for semilinear parabolic problems*, 2004.
- Jahnke and Lubich: *Error bounds for exponential operator splittings*, BIT 2000.
- Lawson: *Generalized Runge–Kutta Processes for Stable Systems with Large Lipschitz Constants*, SIAM J. Num. Anal., 1967.