Magnus, splitting and composition techniques for solving non-linear Schrödinger equations

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We analyse the numerical integration of several non-linear Schrödinger equations (NLSEs) of different nature and we explore if it would be interesting to look for efficient algorithms using algebraic technique in which many participants of the programme are familiar.

The equations (initial cond. $\psi(x, 0) = \varphi_0(x)$)

1. The Gross-Pitaevskii equation (GPE)

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\nabla^2 + V(x,t) + \beta|\psi(x,t)|^2\right)\psi(x,t)$$

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3. Quantum optimal control problems

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3. Magnus averaging: Mag. for non-linear + Comm. Free

$$i\frac{\partial}{\partial t}\psi = \left(-\frac{1}{2\mu}\nabla^2 + \widetilde{V}(x) + \beta|\psi|^2\right)\psi$$

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Can we find $\widetilde{\psi}(t) \sim \psi(t)$ such that

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This approximation would allow us to use algebraic techniques for the linear case.

- Kohn-Sham equation ($\rho = \sum_{m=1}^{N} |\psi_m|^2$)

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One procedure to solve it: To take ρ as a time-dependent function using

$$\rho_n \equiv \rho(t_n) = \rho(\psi(x,t_n)), \quad \rho_{n-1}, \quad \rho_{n-2}, \dots$$

and to build by extrapolation

$$\tilde{\rho}(t), \quad t \in [t_n, t_{n+1}]$$

4th-order CF methods using $\tilde{\rho}(t_n + c_1 h), \tilde{\rho}(t_n + c_2 h)$ showed a high performance.
Gómez-Pueyo, Marques, Rubio & Castro, JChemTheorComp (2018)

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QUESTION: Are there alternative procedures to find better approximations to $\tilde{\rho}(t), \; t \in [t_n, t_{n+1}]$?

1. Quantum optimal control problems

$$\boxed{i\frac{\partial}{\partial t}\psi(x,t) = \left(T + V(x) - \epsilon(t)\mu(x)\right)\psi(x,t)}$$

where $\epsilon(t)\mu(x)$ is an external field, e.g. a laser field, where we have a control on the intensity $\epsilon(t)$.

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We have to minimise:

$$\begin{aligned} J &= \langle\psi(T)|O|\psi(T)\rangle - \alpha_0 \int_0^T \epsilon(t)^2 dt \\ &\quad -2\mathrm{Re} \int_0^T \langle\chi(t)|\frac{\partial}{\partial t} + i(T + V - \mu\epsilon(t))|\psi(t)\rangle dt \end{aligned}$$

α_0: is a positive parameter chosen to weight the significance of the laser energy.
O: is the positive definite operator used to attract the solution.
$\chi(x,t)$: a Lagrange multiplier introduced to assure satisfaction of the Schrödinger equation.

Requiring $\delta J = 0$ will give the following value for the optimized laser field

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i\frac{\partial}{\partial t}\psi(t) &= \left(-\frac{1}{2\mu}\Delta + V + \mu_0\text{Im}\langle\chi(t)|\mu|\psi(t)\rangle\right)\psi(t) \\
\psi(0) &= \varphi_0 \\
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& \qquad\qquad \chi(T) = O\psi(T)
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with $\mu_0 = \mu/\alpha_0$.

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$$\chi(T) = O\psi(T)$$

with $\mu_0 = \mu/\alpha_0$.

This is a boundary value problem but, notice that $\chi(T)$ is NOT known.

Two steps are required:

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REMARK: for the first iterations, since one is far from the solution, high accuracy is NOT necessary.

To linearise and store some values from previous iterations to improve convergence (must be cheap to store)?

In all proposed problems we have to solve a differential equation that can be written as

$$\boxed{x' = M(t,x)x, \qquad\qquad x(0) = x_0}$$

and we analyse if it could be convenient to solve instead the non-autonomous linear equation

$$z' = A(t)z, \qquad\qquad z(0) = x_0$$

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If this is possible, we can then use Magnus, splitting and composition techniques to solve linear problems.
These techniques have shown to be very useful for solving many problems and they could also be useful in these cases.

We focus on the sixth-order Gauss-Legendre quadrature rule with nodes

$$c_1 = \frac{1}{2} - \frac{\sqrt{15}}{10}, \quad c_2 = \frac{1}{2}, \quad c_3 = \frac{1}{2} + \frac{\sqrt{15}}{10}.$$

The Lagrange polynomials through these nodes are defined by

$$\begin{aligned}
\mathcal{L}_1(\sigma) &= \frac{\sigma - c_2}{c_1 - c_2}\,\frac{\sigma - c_3}{c_1 - c_3}, \\
\mathcal{L}_2(\sigma) &= \frac{\sigma - c_1}{c_2 - c_1}\,\frac{\sigma - c_3}{c_2 - c_3}, \\
\mathcal{L}_3(\sigma) &= \frac{\sigma - c_1}{c_3 - c_1}\,\frac{\sigma - c_2}{c_3 - c_2}
\end{aligned}$$

Magnus and Magnus-composition methods

Let us consider the interpolating Lagrange matrix polynomial

$$\boxed{\widetilde{A}(t) = \mathcal{L}_1(\frac{t}{h})A_1 + \mathcal{L}_2(\frac{t}{h})A_2 + \mathcal{L}_3(\frac{t}{h})A_3}$$

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then we have $(z' = A(t)z, \ z(0) = x_0)$

$$y(h) = z(h) + \mathcal{O}(h^7)$$

(Iserles & Nørsett (1999), Munthe-Kaas & Owren (1999), **B** (2018))

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Notice also that

$$\begin{aligned}
A^{(0)} &= \int_0^h A(t)dt = \frac{h}{18}(5A_1 + 8A_2 + 5A_3) + \mathcal{O}(h^7) \\
A^{(1)} &= \int_0^h \left(t - \frac{h}{2}\right) A(t)dt = \frac{h^2\sqrt{15}}{36}(A_3 - A_1) + \mathcal{O}(h^7) \\
A^{(2)} &= \int_0^h \left(t - \frac{h}{2}\right)^2 A(t)dt = \frac{h^3}{24}(A_1 + A_3) + \mathcal{O}(h^7)
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QUESTION: In which cases is this advantageous?

To build efficient methods it is convenient to work with graded Lie algebras ($\tau = t - \frac{h}{2}$) (Munthe-Kaas & Owren (1999))

$$\widetilde{A}(\tau + \tfrac{h}{2}) = \frac{1}{h}\left(\alpha_1 + \alpha_2 \frac{\tau}{h} + \alpha_3 \frac{\tau^2}{h^2}\right), \qquad \tau \in \left[-\frac{h}{2}, \frac{h}{2}\right],$$

$$\alpha_1 = h A_2 = \mathcal{O}(h),$$

$$\alpha_2 = h \frac{\sqrt{15}}{3}\left(A_3 - A_1\right) = \mathcal{O}\left(h^2\right),$$

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Magnus expansion

$$y(h) = \mathrm{e}^{\Omega(h)} x_0,$$
$$\Omega(h) = \int_0^h \widetilde{A}(t)\, dt + \frac{1}{2}\int_0^h \int_0^t \left[\widetilde{A}(t), \widetilde{A}(s)\right] ds\, dt + \ldots$$

The integrals can be computed analytically.

$$\begin{aligned}\Omega^{[6]} &= \alpha_1 + \frac{1}{12}\alpha_3 - \frac{1}{12}[\alpha_1, \alpha_2] \\ &+ \frac{1}{240}[\alpha_2, \alpha_3] + \frac{1}{360}[\alpha_1, [\alpha_1, \alpha_3]] - \frac{1}{240}[\alpha_2, [\alpha_1, \alpha_2]] \\ &+ \frac{1}{720}[\alpha_1, [\alpha_1, [\alpha_1, \alpha_2]]]\end{aligned}$$

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We can take this as the formal solution.

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For a given problem we should look for the elements that can be computed efficiently and to approximate the formal solution using a composition of these terms if possible.

For example, given the linear SE

$$\boxed{i\frac{\partial}{\partial t}\psi(x,t) = (T + V(t))\psi(x,t)}$$

we have that

$$\begin{aligned} \alpha_1 &= h(T + V_2), \\ \alpha_2 &= h\frac{\sqrt{15}}{3}(V_3 - V_1) \\ \alpha_3 &= h\frac{10}{3}(V_3 - 2V_2 + V_1) \end{aligned}$$

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then

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is diagonal, but in addition

$$[\alpha_2, \alpha_3] = 0$$

$$[\alpha_2, [\alpha_1, \alpha_2]] = -h^3\frac{5}{3}(V_3' - V_1')^2$$

For example, to 4th-order we have

$$\boxed{e^{\Omega^{[4]}} = e^{\alpha_1 - \frac{1}{12}[\alpha_1, \alpha_2]}}$$

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$$e^{\alpha_1 - \frac{1}{12}[\alpha_1,\alpha_2]} = e^{\frac{1}{2}\alpha_1}\, e^{-\frac{1}{12}[\alpha_1,\alpha_2]}\, e^{\frac{1}{2}\alpha_1} + \mathcal{O}(h^5)$$

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$$\begin{aligned} e^{\alpha_1 - \frac{1}{12}[\alpha_1, \alpha_2]} &= e^{\frac{1}{2}\alpha_1}\, e^{-\frac{1}{12}[\alpha_1, \alpha_2]}\, e^{\frac{1}{2}\alpha_1} + \mathcal{O}(h^5) \\ &= e^{\frac{1}{12}\alpha_2}\, e^{\alpha_1}\, e^{-\frac{1}{12}\alpha_2} + \mathcal{O}(h^5) \end{aligned}$$

For example, to 4th-order we have

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To 6th-order we have

$$
\begin{aligned}
e^{\Omega^{[6]}} = &\exp\left(-x_{1,2}\alpha_2 + x_{1,3}\alpha_3 + y\,[\alpha_2,\alpha_1,\alpha_2]\right)\\
&\times \exp\left(x_{2,1}\alpha_1 - x_{2,2}\alpha_2 + x_{2,3}\alpha_3\right)\\
&\times \exp\left(x_{2,1}\alpha_1 + x_{2,2}\alpha_2 + x_{2,3}\alpha_3\right)\\
&\times \exp\left(x_{1,2}\alpha_2 + x_{1,3}\alpha_3 + y\,[\alpha_2,\alpha_1,\alpha_2]\right).
\end{aligned}
$$

$$
x_{1,2} = -x_{1,3} = -\frac{1}{60},\; x_{2,1} = \frac{1}{2},\; x_{2,2} = -\frac{2}{15},\; x_{2,3} = \frac{1}{40},\; y = \frac{1}{43200}.
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&\times \exp\left(x_{2,1}\alpha_1 + x_{2,2}\alpha_2 + x_{2,3}\alpha_3\right) \\
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This scheme has been used to solve the linear SE, the non-linear GPE and the Kohn-Sham equation.

Conclusions

1. The Gross-Pitaevskii equation (GPE)

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\nabla^2 + V(x,t) + \beta|\psi(x,t)|^2\right)\psi(x,t)$$

2. Kohn-Sham equation ($\rho = \sum_{m=1}^{N} |\psi_m(x,t)|^2$)

$$i\frac{\partial}{\partial t}\psi_m(x,t) = \left(-\frac{1}{2\mu}\nabla^2 + V(x,t) + v_{Hxc}(\rho)\right)\psi_m(x,t),$$

3. Quantum optimal control problems

$$i\frac{\partial}{\partial t}\psi(x,t) = (T + V(x) - \mu(x)\epsilon(t))\,\psi(x,t)$$

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QUESTION: Can we use the Magnus-composition techniques to build new algorithms with a proper linearisation?

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Thank You