Splitting methods for quantum dynamics and control

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15th of November 2022

Complex Quantum Systems
Paderborn

Quantum Dynamics and Control

Quantum Dynamics:

$$\partial_t u = \mathcal{A}(t; \theta)\ u, \qquad u(0) = u_0$$

compute $u(T; \theta)$, where

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- $\theta \in \Omega$ are a set of controls.

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   Quantum Gates.

optimal control $\Longleftrightarrow$ (electric or magnetic) pulse design

Outline

- **The matrix exponential**
- The Magnus expansion
- Specialised splittings for Schrödinger equation under laser potential
- Spin dynamics and control
  - Dynamics
  - Computation of gradients
  - Optimization strategies

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If A is easily diagonalisable, $A = U\, \mathrm{diag}(\lambda_1, \ldots, \lambda_n)\, U^*$,

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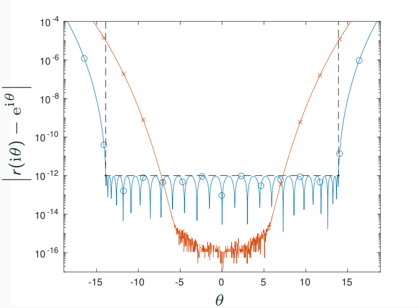

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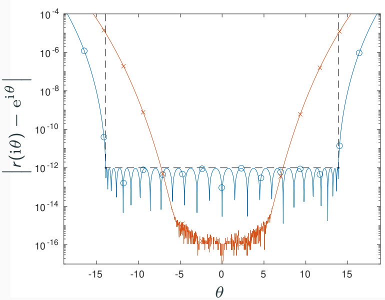

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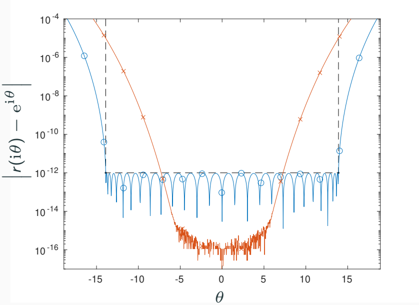

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Tobias Jawecki (TU Vienna). JS 23. Under review; JS 23. In preparation.

$$u(h) = \mathrm{e}^{hA} u_0$$

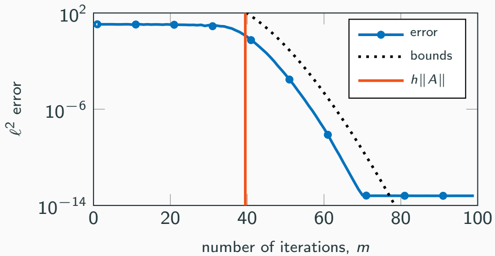
We need to approximate matrix-vector product $\exp(hA)u_0$. Krylov subspace:

$$\mathcal{K}_m(A, u_0) = \mathrm{span}\,\{u_0, Au_0, A^2 u_0, \ldots, A^{m-1} u_0\}, \qquad m \in \mathbb{N}.$$

Lanczos: power-iteration interspersed with Gram–Schmidt orthogonalisation. Produces basis $\mathcal{V}_m$ and tridiagonal $\mathcal{H}_m$.

$$\mathrm{e}^{hA} u_0 \approx \mathcal{V}_m \mathrm{e}^{h\mathcal{H}_m} \mathcal{V}_m^* \, u_0$$

Really effective if $m \ll N$ ($\mathcal{H}_m$ is $m \times m$, A is $N \times N$).



Lanczos approximations to $\exp(-\mathrm{i}h\mathrm{H})u_n$

$$u(h) = \mathrm{e}^{hA} u_0$$

We need to approximate matrix-vector product $\exp(hA)u_0$. Krylov subspace:

$$\mathcal{K}_m(A, u_0) = \mathrm{span}\{u_0, Au_0, A^2u_0, \ldots, A^{m-1}u_0\}, \qquad m \in \mathbb{N}.$$

Lanczos: power-iteration interspersed with Gram–Schmidt orthogonalisation.
Produces basis $\mathcal{V}_m$ and tridiagonal $\mathcal{H}_m$.

$$\mathrm{e}^{hA} u_0 \approx \mathcal{V}_m \mathrm{e}^{h\mathcal{H}_m} \mathcal{V}_m^* \, u_0$$

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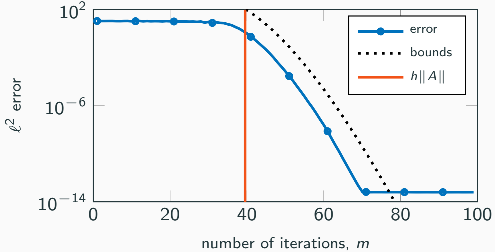

Need $m > h\|A\|$. Hochbruck & Lubich 97.

Approximating the matrix exponential

Different methods might be more efficient depending on the matrix structure.

C. Moler & C. V. Loan, *Nineteen dubious ways to compute the exponential of a matrix*, SIAM Review 78; *Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later*, SIAM Review 03.

- Diagonalisation
- Padé
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- Scaling and squaring
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- Rational Krylov **(new)**

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- **Splitting**

Exponential splittings

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$\mathrm{e}^{\frac{h}{2}A}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{h^3 R}\mathrm{e}^{h^5 S}\mathrm{e}^{h^3 R}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{\frac{h}{2}A}$	$\mathcal{O}\left(h^{2p+1}\right)$	Asymptotic	$\mathcal{O}(p)$

Asymptotic (Zassenhaus) BIKS 14 Found. Comp. Math.

Outline

- The matrix exponential
- **The Magnus expansion**
- Specialised splittings for Schrödinger equation under laser potential
- Spin dynamics and control
    - Dynamics
    - Computation of gradients
    - Optimization strategies

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$\Theta(h)$ is the **Magnus expansion**,

$$\begin{aligned}\Theta(h) \quad = \quad & \int_0^h A(\xi)\,\mathrm{d}\xi - \tfrac{1}{2}\int_0^h \int_0^\xi [A(\zeta), A(\xi)]\,\mathrm{d}\zeta\,\mathrm{d}\xi \\ & + \tfrac{1}{12}\int_0^h \int_0^\xi \int_0^\xi [A(\chi), [A(\zeta), A(\xi)]]\,\mathrm{d}\chi\,\mathrm{d}\zeta\,\mathrm{d}\xi \\ & + \tfrac{1}{4}\int_0^h \int_0^\xi \int_0^\zeta [[A(\chi), A(\zeta)], A(\xi)]\,\mathrm{d}\chi\,\mathrm{d}\zeta\,\mathrm{d}\xi + \ldots\end{aligned}$$

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In practice: truncate series, discretise integrals, approximate matrix exponential.

Magnus–Lanczos methods

The exponentiation of the sixth-order Magnus expansion

$$\begin{aligned}\Theta_5(h) =& \tfrac{1}{18}(5A_1 + 8A_2 + 5A_3) - \tfrac{\sqrt{15}}{108}\left(2[A_1, A_2] + [A_1, A_3] + 2[A_2, A_3]\right) \\ &+ \tfrac{1}{27216}(94[A_1, [A_1, A_2]] + 45[A_1, [A_1, A_3]] + 194[A_1, [A_2, A_3]] - 152[A_2, [A_1, A_2]] \\ &\qquad + 152[A_2, [A_2, A_3]] - 194[A_3, [A_1, A_2]] - 45[A_3, [A_1, A_3]] - 94[A_3, [A_2, A_3]]),\end{aligned}$$

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- **Fewer commutators** Munthe–Kaas & Owren 99

$$\begin{aligned}\Theta_4(h) =& J_1 + \tfrac{1}{12}J_3 - \tfrac{1}{12}[J_1, J_2] + \tfrac{1}{240}[J_2, J_3] + \tfrac{1}{360}[J_1,[J_1,J_3]]\\ &- \tfrac{1}{240}[J_2,[J_1,J_2]] + \tfrac{1}{720}[J_1,[J_1,[J_1,J_2]]],\end{aligned}$$

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- **Commutator-free splittings**. Alvermann & Fehske 11,

$$\exp(\Theta_p) \approx \exp\left(\sum_{k=1}^{n} c_{1k}\, h\, A(t_k)\right) \ldots \exp\left(\sum_{k=1}^{n} c_{pk}\, h\, A(t_k)\right).$$

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- **Solve commutators** in algebra of differential operators.

$$\Theta_2(h) = \mathrm{i}\Delta t \partial_x^2 - \mathrm{i}\mu_{0,0}(h) - 2\left\langle \partial_x \mu_{1,1}(h)\right\rangle_1,$$
$$\Theta_3(h) = \Theta_2(h) + \mathrm{i}\Lambda\,[\psi]_{1,1}(h) + 2\mathrm{i}\left\langle \partial_x^2 \mu_{2,1}(h)\right\rangle_2$$

IKS 18. SIAM J. Num. Anal.

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Asymptotic Magnus–Zassenhaus schemes: $\mathrm{e}^{\frac{h}{2}A}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{h^3 R}\mathrm{e}^{h^5 S}\mathrm{e}^{h^3 R}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{\frac{h}{2}A}$.

BIKS 16. Proc. Roy. Soc. A.; IKS 19. J. Comp. Phys.

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BIKS 16. Proc. Roy. Soc. A.; IKS 19. J. Comp. Phys.

For the Schrödinger equation under influence of laser,

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$$\mathrm{e}^{-\frac{1}{2}\boldsymbol{s}^\top\nabla}\mathrm{e}^{\mathrm{i}h\varepsilon\Delta - \mathrm{i}\varepsilon^{-1}(hV_0 + \boldsymbol{r}^\top \boldsymbol{x})}\mathrm{e}^{-\frac{1}{2}\boldsymbol{s}^\top\nabla} \qquad \text{Strang}$$

$$\mathrm{e}^{-\frac{1}{6}\mathrm{i}h\varepsilon^{-1}\widetilde{V}}\mathrm{e}^{\frac{1}{2}\mathrm{i}h\varepsilon\Delta - \frac{1}{2}\boldsymbol{s}(t,h)^\top\nabla}\mathrm{e}^{-\frac{2}{3}\mathrm{i}h\varepsilon^{-1}\widehat{V}}\mathrm{e}^{\frac{1}{2}\mathrm{i}h\varepsilon\Delta - \frac{1}{2}\boldsymbol{s}(t,h)^\top\nabla}\mathrm{e}^{-\frac{1}{6}\mathrm{i}h\varepsilon^{-1}\widetilde{V}} \qquad \text{Compact}$$

Magnus expansion + Splittings

$$\partial_t \psi = \left(\mathrm{i}\varepsilon\Delta + \mathrm{i}\varepsilon^{-1} V(x,t)\right)\psi, \quad u(0) = u_0, \qquad A = \mathrm{i}h\Delta,\ B = -\mathrm{i}\int_0^h V(x,\xi)\,\mathrm{d}\xi$$

Asymptotic Magnus–Zassenhaus schemes: $\mathrm{e}^{\frac{h}{2}A}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{h^3R}\mathrm{e}^{h^5S}\mathrm{e}^{h^3R}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{\frac{h}{2}A}$.

BIKS 16. Proc. Roy. Soc. A.; IKS 19. J. Comp. Phys.

For the Schrödinger equation under influence of laser,

$$\partial_t \psi = \left(\mathrm{i}\varepsilon\,\Delta - \mathrm{i}\varepsilon^{-1}\left(V_0(\boldsymbol{x}) + \boldsymbol{e}(t)^\top \boldsymbol{x}\right)\right)\psi,$$

using $[\Delta, \boldsymbol{a}^\top \boldsymbol{x}] = 2\boldsymbol{a}^\top \nabla$, we can simplify the order four Magnus expansion to

$$\Theta_2(h) = \mathrm{i}h\varepsilon\Delta - \mathrm{i}\varepsilon^{-1}(hV_0 + \boldsymbol{r}^\top \boldsymbol{x}) - \boldsymbol{s}^\top \nabla,$$

where $\boldsymbol{r} = \mu_0^e = \int_0^h \boldsymbol{e}(\zeta)\,\mathrm{d}\zeta$, and $\boldsymbol{s} = 2\mu_1^e = 2\int_0^h \left(\zeta - \frac{h}{2}\right)\boldsymbol{e}(\zeta)\,\mathrm{d}\zeta$. Split:

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$$\mathrm{e}^{-\frac{1}{6}\mathrm{i}h\varepsilon^{-1}\widetilde{V}}\mathrm{e}^{\frac{1}{2}\mathrm{i}h\varepsilon\Delta - \frac{1}{2}\boldsymbol{s}(t,h)^\top\nabla}\mathrm{e}^{-\frac{2}{3}\mathrm{i}h\varepsilon^{-1}\widehat{V}}\mathrm{e}^{\frac{1}{2}\mathrm{i}h\varepsilon\Delta - \frac{1}{2}\boldsymbol{s}(t,h)^\top\nabla}\mathrm{e}^{-\frac{1}{6}\mathrm{i}h\varepsilon^{-1}\widetilde{V}} \qquad \text{Compact}$$

- Strang – reuse any existing fourth order method for the central exponent.

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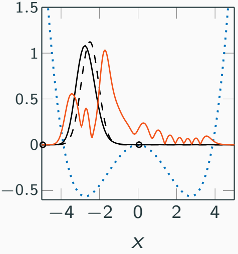
- Strang – reuse any existing fourth order method for the central exponent.
- Compact – same cost as time-independent Hamiltonian!

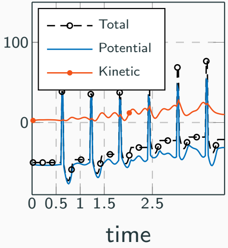
IKS 19. Comput. Phys. Commun.

Numerical examples

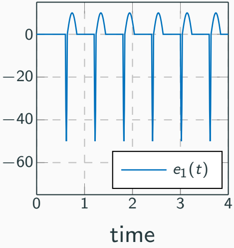
Wave functions ($\varepsilon = 1$)



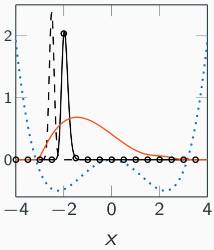
Energy



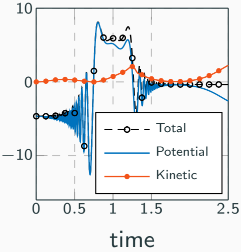
Laser profile



Wave functions ($\varepsilon = 0.01$)



Energy



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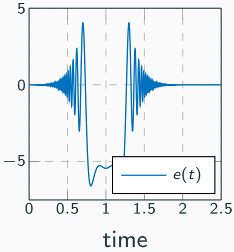
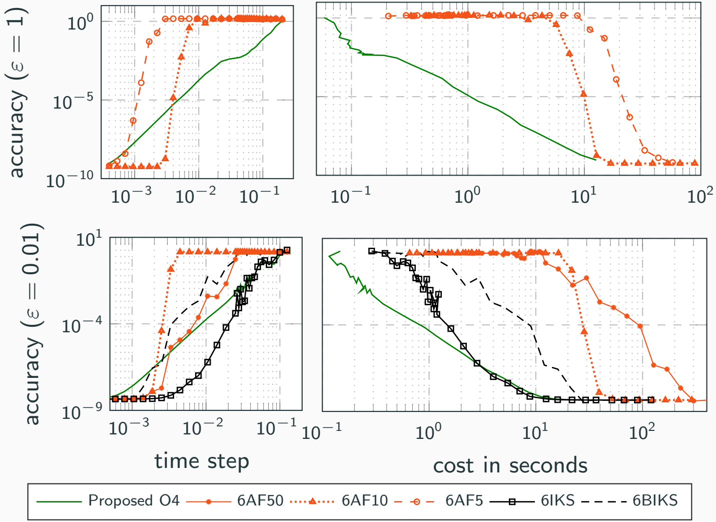


Magnus–Compact fourth-order



Proposed O4	Iserles, Kropielnicka & S., *Comput. Phys. Commun.* (2019).
6IKS	Iserles, Kropielnicka & S., *J. Comput. Phys.* (2019).
6BIKS	Iserles, Kropielnicka & S., *Proc. Roy. Soc. A* (2016).
6AF	Alvermann & Fehske, *J. Comput. Phys.* (2011).

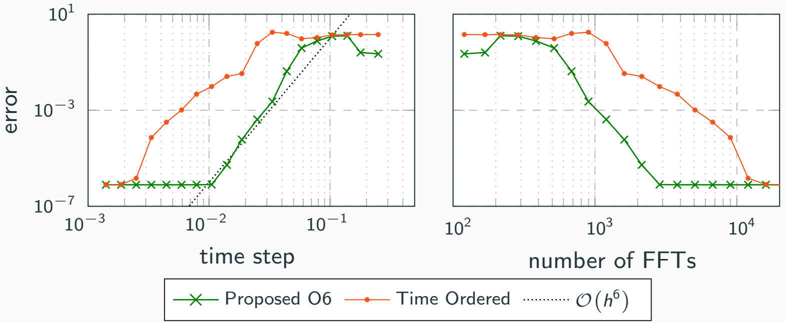
Magnus–Compact sixth-order

The sixth-order Magnus expansion

$$\Theta_4 = \mathrm{i}h\varepsilon\Delta - \mathrm{i}\varepsilon^{-1}(hV_0(\boldsymbol{x}) + \boldsymbol{r}^\top\boldsymbol{x}) - \boldsymbol{s}^\top\nabla + \mathrm{i}\varepsilon^{-1}\boldsymbol{q}^\top(\nabla V_0) + \left[\Delta, \boldsymbol{p}^\top(\nabla V_0)\right] + c,$$

can be split as

$$\mathrm{e}^{3\mathrm{i}h^{-2}\varepsilon^{-1}\boldsymbol{q}^\top\boldsymbol{x}}\,\mathrm{e}^{-6h^{-2}\boldsymbol{p}^\top\nabla}\,\mathrm{e}^{(\mathrm{i}h\varepsilon\Delta-\tilde{\boldsymbol{s}}^\top\nabla)+(-\mathrm{i}h\varepsilon^{-1}\widetilde{V}-6\mathrm{i}h^{-2}\varepsilon^{-1}\boldsymbol{q}^\top\boldsymbol{x}+\tilde{c})}\,\mathrm{e}^{-6h^{-2}\boldsymbol{p}^\top\nabla}\,\mathrm{e}^{3\mathrm{i}h^{-2}\varepsilon^{-1}\boldsymbol{q}^\top\boldsymbol{x}}$$



Proposed O6	S., *J. Chem. Phys.* (2019).
Time Ordered O6	Omelyan, Mryglod & Folk, *Comput. Phys. Commun.* (2003).

Outline

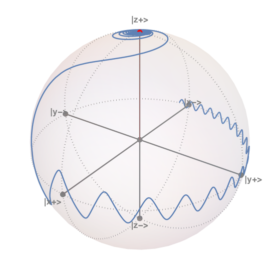
- The matrix exponential
- The Magnus expansion
- Specialised splittings for Schrödinger equation under laser potential
- **Spin dynamics and control**
    - **Dynamics**
    - Computation of gradients
    - Optimization strategies

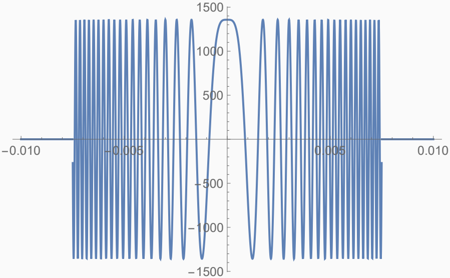
Spin dynamics

The Liouville–von Neumann equation,

$$\partial_t \rho = \mathcal{L}(t)\rho$$

describes the dynamics of spins under the influence of a changing magnetic field.





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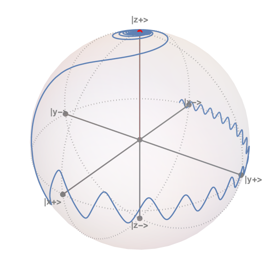

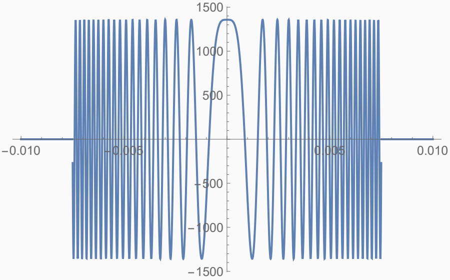

Initial assumption: no dissipation $\mathcal{L}(t) = -\mathrm{i}\,\mathrm{ad}_{\mathrm{H}(t)}$.

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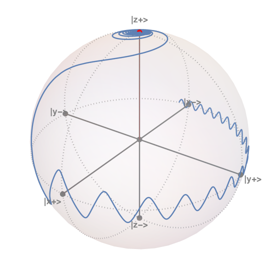

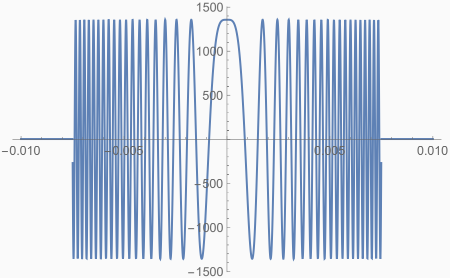

Initial assumption: no dissipation $\mathcal{L}(t) = -\mathrm{i}\,\mathrm{ad}_{\mathrm{H}(t)}$.

Later: relaxation $\mathcal{L}(t) = -\mathrm{i}\,\mathrm{ad}_{\mathrm{H}(t)} + \mathcal{R}$.

Single spin

Solution of

$$\rho(t)' = -\mathrm{i}[\mathrm{H}(t), \rho(t)], \qquad \rho(0) = \rho_0,$$

is given by

$$\rho(h) = \mathrm{Ad}_{\mathrm{e}^{\Theta(h)}} \rho_0 = \mathrm{e}^{\Theta(h)} \; \rho_0 \; \mathrm{e}^{-\Theta(h)}.$$

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$$\mathrm{H}(t) = \boldsymbol{e}(t) \cdot \boldsymbol{\sigma}, \quad \boldsymbol{e}(t) = (f(t), g(t), \Omega), \quad \boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z),$$

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Since $\mathfrak{su}(2)$ is a finite dimensional Lie algebra spanned by $\mathrm{i}\sigma_x, \mathrm{i}\sigma_y, \mathrm{i}\sigma_z$, with commutator identities

$$[\sigma_x, \sigma_y] = \mathrm{i}\sigma_z, \quad [\sigma_y, \sigma_z] = \mathrm{i}\sigma_x, \quad [\sigma_z, \sigma_x] = \mathrm{i}\sigma_y,$$

$\Theta(h) = -\mathrm{i}\boldsymbol{a}(h) \cdot \boldsymbol{\sigma}$ for some $\boldsymbol{a}(h) \in \mathbb{R}^3$.

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$\Theta(h) = -\mathrm{i}\boldsymbol{a}(h)\cdot\boldsymbol{\sigma}$ for some $\boldsymbol{a}(h) \in \mathbb{R}^3$. The exact solution should be expressible as

$$\rho(h) = \mathrm{e}^{-\mathrm{i}\boldsymbol{a}(h)\cdot\boldsymbol{\sigma}}\ \rho_0\ \mathrm{e}^{\mathrm{i}\boldsymbol{a}(h)\cdot\boldsymbol{\sigma}},$$

so long as one can find the correct $\boldsymbol{a}$.

Single spin

For single spin, the exponential can be computed exactly,

$$e^{-i\boldsymbol{a}\cdot\boldsymbol{\sigma}} = \begin{pmatrix} \cos(\|a\|/2) - i a_z \frac{\sin(\|a\|/2)}{\|a\|} & (-i a_x - a_y)\frac{\sin(\|a\|/2)}{\|a\|} \\ (-i a_x + a_y)\frac{\sin(\|a\|/2)}{\|a\|} & \cos(\|a\|/2) + i a_z \frac{\sin(\|a\|/2)}{\|a\|} \end{pmatrix},$$

provided we have a good approximation of $\boldsymbol{a}$.

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$$\mathrm{H}(t) = \boldsymbol{e}(t)\cdot\boldsymbol{\sigma}, \quad \boldsymbol{e}(t) = (f(t), g(t), \Omega),$$

Order 2 Magnus:

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Order 4 Magnus: $\boldsymbol{a} = \boldsymbol{r} + \boldsymbol{s}$ where

$$\boldsymbol{s} = \left(\Omega\mu_1^g, -\Omega\mu_1^f, -\tfrac{1}{2}\Lambda^{f,g}\right).$$

For multiple spins, only Ω changes, so integrals need to be computed once.

Multiple spins

For multiple isolated spins, the Hamiltonian is

$$\mathrm{H}(t) = \underline{\boldsymbol{e}}(t) \cdot \underline{\boldsymbol{L}}, \qquad \underline{\boldsymbol{e}}(t) = (f(t)\underline{1},\ g(t)\underline{1},\ \underline{\Omega}), \qquad \underline{\boldsymbol{L}} = (\underline{L}_x, \underline{L}_y, \underline{L}_z),$$

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Coupling between multiple interacting spins described by Hamiltonian H_J. The overall Hamiltonian for coupled spins is

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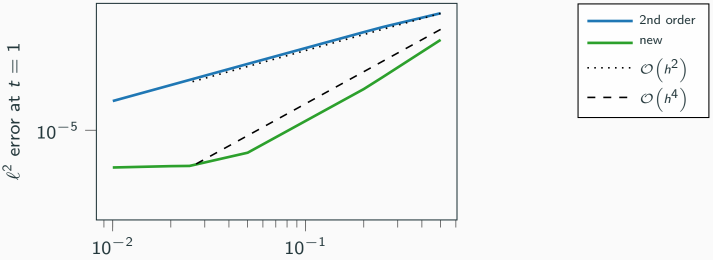
Order 4 Magnus expansion in MagPy (Danny Goodacre (MMath at Bath)). More efficient version coming soon. $N = 3$ spins, 3 qubits.



BCFS 23. In preparation. MagPy 'pip install magpy'. git: github.com/brownadder/magpy

Outline

- The matrix exponential
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  - Dynamics
  - **Computation of gradients**
  - Optimization strategies

Optimal control for spin systems

Let solution of

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$$\mathcal{F}(\theta) = f(\mathbf{U}(T;\theta))$$

e.g.

$$f(X) = \Re\left[\mathrm{Tr}\left(\varrho^\dagger X \rho_0\right)\right] \qquad \text{state-to-state}$$

$$f(X) = \Re\left[\mathrm{Tr}\left(\mathbf{U}_{\mathrm{target}}^\dagger X\right)\right] \qquad \text{gate design}$$

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Local optimization: need gradients

$$\frac{\partial \mathcal{F}}{\partial \theta} = \mathbf{D}f(\mathbf{U}(T;\theta))\frac{\partial \mathbf{U}(T;\theta)}{\partial \theta},$$

and Hessians.

Gradients and Hessians – Single spin

Single spin $\mathrm{H}(t;\theta) = \boldsymbol{e}(t;\theta) \cdot \boldsymbol{\sigma}$.

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$$\mathrm{L}_n := \mathrm{U}_N \mathrm{U}_{N-1} \ldots \mathrm{U}_n, \qquad \mathrm{R}_n := \mathrm{U}_n \mathrm{U}_{n-1} \ldots \mathrm{U}_1, \qquad \mathcal{O}(N)$$

$$\frac{\partial \mathbf{U}}{\partial \theta_{n,k}} = \mathrm{L}_{n+1} \frac{\partial \mathrm{U}_n}{\partial \theta_{n,k}} \mathrm{R}_{n-1}, \qquad \frac{\partial \mathrm{U}_n}{\partial \theta_{n,k}} = -\mathrm{i}\mathrm{U}_n \left(\left[\boldsymbol{D}_n \frac{\partial \boldsymbol{s}_n}{\partial \theta_{n,k}} \right] \cdot \boldsymbol{\sigma} \right),$$

Gradients and Hessians – Single spin

Single spin $\mathrm{H}(t;\theta) = \boldsymbol{e}(t;\theta)\cdot\boldsymbol{\sigma}$. No dissipation $\mathcal{L}(t;\theta) = -\mathrm{i}\,\mathrm{ad}_{\mathrm{H}(t;\theta)}$. Piecewise constant $\boldsymbol{e}(t;\theta)$ (nth piece described by $\theta_{n,k}$, $k = 1, 2.$).

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where

$$\boldsymbol{D}_n = \sum_{p=0}^{\infty}\frac{(-\boldsymbol{S}_n)^p}{(p+1)!} = I + c_1\boldsymbol{S}_n + c_2\boldsymbol{S}_n^2, \qquad \boldsymbol{S}_n = \begin{pmatrix} 0 & -s_{n,z} & s_{n,y} \\ s_{n,z} & 0 & -s_{n,x} \\ -s_{n,y} & s_{n,x} & 0 \end{pmatrix}.$$

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Speedup: $\times 2 - 10$ fidelity, $\times 4 - 30$ gradient, $\times 20 - 600$ Hessian.

Foroozandeh & S. 22. Automatica. ESCALADE doi:10.17632/8zz84359m5
David L. Goodwin & Mads Sloth Vinding. arXiv:2207.09882 [math.OC]

Multiple spins & dissipation

Liouville–von Neumann equation

$$\partial_t \rho = \mathcal{L}(t; \theta)\, \rho$$

Multiple spins & dissipation

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$$\partial_t \rho = \mathcal{L}(t;\theta)\,\rho$$

In general,

$$\mathcal{L}(t;\theta) = \mathcal{L}^{[1]}(t;\theta) + \mathcal{L}^{[2]}, \quad \mathcal{L}^{[1]}(t;\theta) = -\mathrm{i}\,\mathrm{ad}_{\underline{\boldsymbol{e}}(t;\theta)\cdot\underline{\boldsymbol{L}}}, \quad \mathcal{L}^{[2]} = -\mathrm{i}\,\mathrm{ad}_{\mathrm{H}_J} + \mathcal{R}$$

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Compute nth propagator using splittings,

$$\mathrm{U}_n = \mathrm{e}^{h\mathcal{L}_n(\theta)} \approx \prod_{k=1}^{K} \mathrm{e}^{ha_k\mathcal{L}_n^{[1]}(\theta)}\mathrm{e}^{hb_k\mathcal{L}^{[2]}}$$

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GFS 22. Science Advances.

Outline

- The matrix exponential
- The Magnus expansion
- Specialised splittings for Schrödinger equation under laser potential
- **Spin dynamics and control**
  - Dynamics
  - Computation of gradients
  - **Optimization strategies**

Optimal control for spin systems

Let solution of

$$\partial_t \rho = \mathcal{L}(t;\theta)\,\rho$$

at time t be given by $\rho(t) = \mathbf{U}(t;\theta)\rho_0$.

Fidelity functions

$$\mathcal{F}(\theta) = f(\mathbf{U}(T;\theta))$$

e.g.

$$f(X) = \Re\left[\mathrm{Tr}\left(\varrho^\dagger X \rho_0\right)\right] \qquad \text{state-to-state}$$

$$f(X) = \Re\left[\mathrm{Tr}\left(\mathbf{U}_{\mathrm{target}}^\dagger X\right)\right] \qquad \text{gate design}$$

Aim: Maximize fidelity:

$$\theta^* = \underset{\theta}{\mathrm{argmax}}\ \mathcal{F}(\theta)$$

Local optimization: need gradients

$$\frac{\partial \mathcal{F}}{\partial \theta} = \mathbf{D}f(\mathbf{U}(T;\theta))\frac{\partial \mathbf{U}(T;\theta)}{\partial \theta},$$

and Hessians.

Adaptive optimal control

Numerical solvers $\mathcal{S}_{(1)}, \mathcal{S}_{(2)}, \ldots, \mathcal{S}_{(L)}$ with increasing costs and accuracies.

$$\mathbf{U}(T;\theta) \approx \mathcal{S}_{(\ell)} := \mathcal{S}_{(\ell),N}\,\mathcal{S}_{(\ell),N-1}\,\cdots\,\mathcal{S}_{(\ell),2}\,\mathcal{S}_{(\ell),1}, \qquad \text{with} \quad \mathcal{S}_{(\ell),n} \approx \mathrm{U}_n,$$

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$$\mathcal{F}_{(\ell)}(\theta) := f(\mathcal{S}_{(\ell)}(\theta)) \quad \approx \quad f(\mathbf{U}(T;\theta)) = \mathcal{F}(\theta).$$

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Method for computing gradients of these solvers with respect to θ.

$$\frac{\partial \mathcal{F}_{(\ell)}(\theta)}{\partial \theta_n} = \mathbf{D}f(\mathcal{S}_{(\ell)}(\theta)) \frac{\partial \mathcal{S}_{(\ell)}(\theta)}{\partial \theta_n},$$

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Adaptively moving to higher accuracy solver as we approach optima.

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Adaptively moving to higher accuracy solver as we approach optima.

Assume $\mathcal{F}(\theta^*) = 1$.

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Adaptively moving to higher accuracy solver as we approach optima.

Assume $\mathcal{F}(\theta^*) = 1$. Let $\mathrm{tol}_{\mathcal{F}}$ be terminating threshold for $\mathcal{F}$,

$$|1 - \mathcal{F}| \quad \leq \quad |1 - \mathcal{F}_{(\ell)}| + |\mathcal{F}_{(\ell)} - \mathcal{F}| \quad \leq \quad (1 + \kappa_{\mathcal{F}})|1 - \mathcal{F}_{(\ell)}| \quad \leq \quad \mathrm{tol}_{\mathcal{F}},$$

Move from $\mathcal{S}_{(\ell)}$ to $\mathcal{S}_{(\ell+1)}$ when the following is violated:

$$|\mathcal{F}_{(\ell)} - \mathcal{F}| \quad \leq \quad \kappa_{\mathcal{F}}|1 - \mathcal{F}_{(\ell)}|.$$

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$$\frac{\partial \mathcal{F}_{(\ell)}(\theta)}{\partial \theta_n} = \mathbf{D}f(\mathcal{S}_{(\ell)}(\theta))\frac{\partial \mathcal{S}_{(\ell)}(\theta)}{\partial \theta_n},$$

Adaptively moving to higher accuracy solver as we approach optima.

Assume $\mathcal{F}(\theta^*) = 1$. Let $\mathrm{tol}_\mathcal{F}$ be terminating threshold for $\mathcal{F}$,

$$|1-\mathcal{F}| \quad \leq \quad |1-\mathcal{F}_{(\ell)}| + |\mathcal{F}_{(\ell)} - \mathcal{F}| \quad \leq \quad (1+\kappa_\mathcal{F})|1-\mathcal{F}_{(\ell)}| \quad \leq \quad \mathrm{tol}_\mathcal{F},$$

Move from $\mathcal{S}_{(\ell)}$ to $\mathcal{S}_{(\ell+1)}$ when the following is violated:

$$|\mathcal{F}_{(\ell)} - \mathcal{F}| \quad \leq \quad \kappa_\mathcal{F}|1-\mathcal{F}_{(\ell)}|.$$

This system of inequalities enforces the termination criteria

$$|1-\mathcal{F}_{(\ell)}| \quad \leq \quad \frac{\mathrm{tol}_\mathcal{F}}{1+\kappa_\mathcal{F}}.$$

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Numerical solvers $\mathcal{S}_{(1)}, \mathcal{S}_{(2)}, \ldots, \mathcal{S}_{(L)}$ with increasing costs and accuracies.

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Adaptively moving to higher accuracy solver as we approach optima.

Assume $\mathcal{F}(\theta^*) = 1$. Let $\mathrm{tol}_{\mathcal{F}}$ be terminating threshold for $\mathcal{F}$,

$$|1-\mathcal{F}| \;\leq\; |1-\mathcal{F}_{(\ell)}| + |\mathcal{F}_{(\ell)} - \mathcal{F}| \;\leq\; (1+\kappa_{\mathcal{F}})|1-\mathcal{F}_{(\ell)}| \;\leq\; \mathrm{tol}_{\mathcal{F}},$$

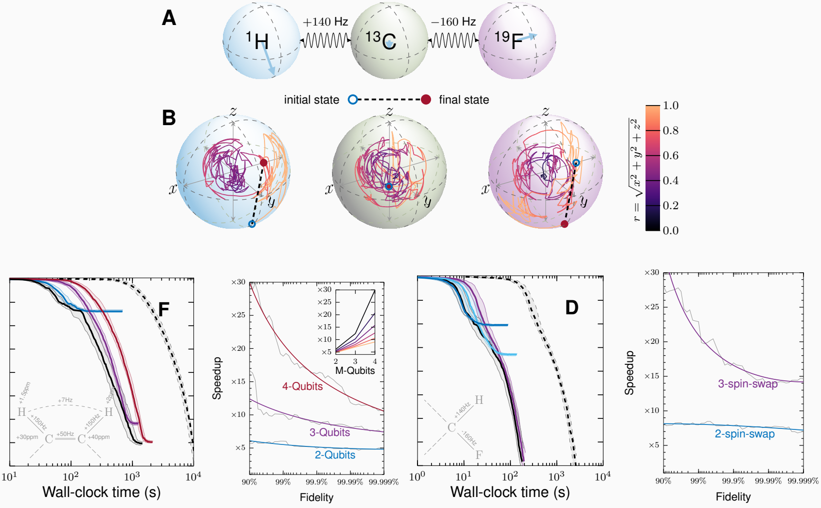
Move from $\mathcal{S}_{(\ell)}$ to $\mathcal{S}_{(\ell+1)}$ when the following is violated:

$$|\mathcal{F}_{(\ell)} - \mathcal{F}_{(\ell+1)}| \;\leq\; \kappa_{\mathcal{F}}|1-\mathcal{F}_{(\ell)}|.$$

This system of inequalities enforces the termination criteria

$$|1-\mathcal{F}_{(\ell)}| \;\leq\; \frac{\mathrm{tol}_{\mathcal{F}}}{1+\kappa_{\mathcal{F}}}.$$

Numerical results



State-to-state transfer (left two) and swap gate (right two)

GFS 22. Science Advances. QOALA github.com/superego101/qoala

Take aways

Optimal Control

- Do not need the most accurate method far from optima
- Compute gradients of the solver (discretise then optimise)
- Can compute exact gradients and Hessians efficiently using Lie algebraic techniques

Quantum Dynamics

- Need methods with different accuracies and costs
- Would like to conserve physical properties
- Magnus expansion for time-dependent controls
- Lanczos applies generally but struggles in many applications
- Magnus + Splittings specialised for individual systems much more efficient
- Can take steps larger than wavelength of oscillatory driving pulse

Based on joint works with

- Quantum dynamics
  - Rational approximations. PDE or ODE.

    Tobias Jawecki (TU Vienna). JS 23. Under review; JS 23. In preparation.
  - Magnus expansion-based methods. PDE. Schrödinger .

    Philipp Bader (Jaume I), Arieh Iserles (Cambridge), Karolina Kropielnicka (Gdansk + IMPAN).
    - Magnus–Lanczos. electrons. IKS 18. SIAM J. Num. Anal.
    - Magnus–Zassenhaus splittings. nuclei. BIKS 16. Proc. Roy. Soc. A.; IKS 19. J. Comp. Phys.
    - Magnus–Compact splittings. electrons. IKS 19. Comput. Phys. Commun.; S 19. J. Chem. Phys.
  - Commutator-free. ODE. Hubbard. W. Auzinger, J. Dubois, K. Held, H. Hofstätter, T. Jawecki, A. Kauch, O. Koch, K. Kropielnicka, P. S., C. Watzenbäck 22. J. Comput. Math. Dat. Sci..
  - Quantum circuits. ODE. LvN. Spins.

    Chris Budd (Bath), Guannan Chen (Bath), Mohammadali Foroozandeh (Oxford → Zurich Instruments).

    BCFS 23. In preparation.
- Optimal control. ODE. LvN. Spins.

  David Goodwin (Oxford), Mohammadali Foroozandeh (Oxford → Zurich Instruments), Ali Sherzod (Oxford).
  - Computation of gradients. FS 22. Automatica. GFS 22. Science Advances.
  - Optimization strategies. GFS 22. Science Advances.; FSS 23. In preparation.

Packages: MagPy 'pip install magpy'; git: github.com/brownadder/magpy;

ESCALADE doi:10.17632/8zz84359m5; QOALA github.com/superego101/qoala