Hamiltonian simulation and optimal control

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Applied and Computational Analysis (ACA) seminar
University of Cambridge

What is Hamiltonian simulation?

Solution of the Schrödinger equation,

$$\mathrm{i}\partial_t \psi \;=\; \mathrm{H}(t)\,\psi, \qquad \mathrm{H}(t)^* = \mathrm{H}(t), \qquad \psi(t) \in \mathscr{H}\,.$$

Feynman, R. P. Simulating physics with computers. *Int J Theor Phys* **21**, 467-488 (1982).

> the real difficulty is this: If we had many particles, we have R particles, for example, in a system, then we would have to describe the probability of a circumstance by giving the probability to find these particles at points $x_1, x_2, \ldots, x_R$ at the time t. That would be a description of the probability of the system. And therefore, you'd need a k-digit number for every configuration of the system, for every arrangement of the R values of x. And therefore if there are N points in space, we'd need N^R configurations.

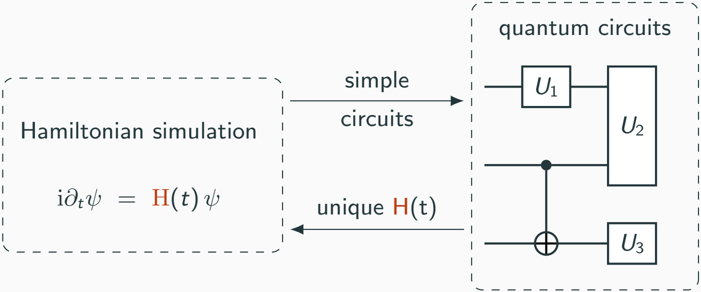
n-body problems

- PDE, $\psi \in \mathbb{C}^{N^{3n}}$ after spatial discretisation with N points in each direction,
- ODE, $\psi \in \mathbb{C}^{2^n}$ for 2-level systems (e.g. spin systems).

Why quantum algorithms for Hamiltonian simulation?

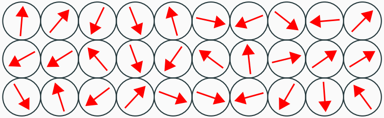
4. QUANTUM COMPUTERS—UNIVERSAL QUANTUM SIMULATORS

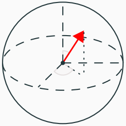
The first branch, one you might call a side-remark, is, Can you do it with a new kind of computer—a quantum computer? (I'll come back to the other branch in a moment.) Now it turns out, as far as I can tell, that you can simulate this with a quantum system, with quantum computer elements.



- Linear growth in number of qubits vs exponential in classical computing
- Simple circuits with Trotterisation (no auxiliary qubits)
- Subroutine in quantum algorithms – QPE (Kitaev 95), HHL (Harrow, Hassidim, Lloyd 09)
- Every gates has underlying Hamiltonian ⇒ every quantum circuit is HS

- A uniquely quantum phenomenon that has no classical counterpart.
- A type of *intrinsic angular momentum* - the particle is not rotating.
- Makes a quantum particle behave like a tiny magnet with a North pole and a South pole.





$$\rho = \frac{1}{2}(I + \boldsymbol{s} \cdot \boldsymbol{\sigma}) \in \mathbb{C}^{2\times 2},$$

$$\boldsymbol{s} \in \mathbb{R}^3,$$

and $\boldsymbol{\sigma} = (X, Y, Z)$

are 2×2 Pauli matrices.

- Responsible for ferromagnetism.
- The phenomenon that powers
  - magnetic resonance imaging (MRI)
  - spintronics
  - quantum computing
- Suspected to be involved in detection of Earth's magnetic field by birds (quantum biology).

For n interacting spins, state space is exponentially large, $\rho \in \mathbb{C}^{2^n \times 2^n}$.

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Resurgence of interest in quantum algorithms for Hamiltonian simulation.

Berry et al. 15, Low & Chuang 17, 19, Low & Wiebe 18, Smith et al. 19, Kieferova et al. 19, Berry et al. 20, Chen et al. 21, Haah et al. 21, Jin & Li 21, Jin et al. 21, Dong et al. 21,22, An et al. 22, Watkins et al. 22, Mizuta et al. 23,...

Hamiltonian simulation of two-level systems is among early candidates for demonstrating quantum advantage. (Childs et al. 18, Seetharam et al. 21).

Recent claim by IBM (using their Eagle processor, 14 June 2023):

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Used Trotter splitting for an Ising chain.

The Hamiltonian

$$\begin{aligned}\mathcal{H}(t) &= \underbrace{\mathbf{e}(t)^\top \mathbb{S}}_{\mathcal{H}_{\text{ss}}(t)} + \underbrace{\frac{1}{2}\mathbb{S}^\top C\, \mathbb{S}}_{\mathcal{H}_{\text{in}}} \\ &= \sum_{k=1}^{n} \sum_{\alpha\in\{X,Y,Z\}} \mathrm{e}_k^\alpha(t)\,\alpha_k + \frac{1}{2}\sum_{j,k=1}^{n} \sum_{\alpha,\beta\in\{X,Y,Z\}} C_{j,k}^{\alpha,\beta}\,\alpha_j\,\beta_k\end{aligned}$$

where α_k acts on kth spin only,

$$\alpha_k = \underbrace{I\otimes\cdots\otimes I}_{n-k\ \text{times}} \otimes \underbrace{\alpha}_{k\text{th}} \otimes \underbrace{I\otimes\cdots\otimes I}_{k-1\ \text{times}} \quad \in \mathbb{C}^{2^n\times 2^n},$$

and $\alpha = X, Y, Z$ are Pauli matrices,

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Two-level systems: Ising chains, Kitaev models, NMR/ESR, qubits (spin, superconducting, ...)

$$\partial_t u = \mathcal{A}\, u, \quad u(0) = u_0,$$

exact solution given by matrix exponential

$$u(t) = \exp(t\mathcal{A})u_0 = \sum_{k=0}^{\infty} \frac{(t\mathcal{A})^k}{k!} u_0.$$

Hamiltonian simulation:

$$\mathcal{A} \quad = \quad -\mathrm{i}h \left(\ \mathbf{e}^\top \mathbb{S} \quad + \quad \frac{1}{2}\mathbb{S}^\top C \ \mathbb{S} \ \right) \tag{1}$$

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For non-interacting spins, since $\mathfrak{su}(2)$ is spanned by $\mathrm{i}X, \mathrm{i}Y, \mathrm{i}Z$ and

$$[X, Y] = \mathrm{i}Z, \quad [Y, Z] = \mathrm{i}X, \quad [Z, X] = \mathrm{i}Y,$$

can compute exponential analytically

$$\mathrm{e}^{t\mathcal{A}} = \bigotimes_{k=1}^{n} \mathrm{e}^{-\mathrm{i}t\mathbf{e}_k\cdot\boldsymbol{\sigma}} = \bigotimes_{k=1}^{n} \begin{pmatrix} \cos\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right) - \mathrm{i}e_k^z \frac{\sin\left(\frac{\|\boldsymbol{e}_k\|}{2}\right)}{\|t\boldsymbol{e}_k\|} & (-\mathrm{i}e_k^x - e_k^y)\frac{\sin\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right)}{\|\boldsymbol{e}_k\|} \\ (-\mathrm{i}e_k^x + e_k^y)\frac{\sin\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right)}{\|\boldsymbol{e}_k\|} & \cos\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right) + \mathrm{i}e_k^z \frac{\sin\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right)}{\|\boldsymbol{e}_k\|} \end{pmatrix},$$

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Trotterisation: For $-\mathrm{i}\mathrm{H} = A + B$ we need to split

$$\exp(h(A + B)) = \mathrm{e}^{hA}\mathrm{e}^{hB} + \mathcal{O}\left(h^2\right)$$

Trotterisation:

$$\mathrm{e}^{-\mathrm{i}h(\mathcal{H}^X+\mathcal{H}^Y+\mathcal{H}^Z)} = \mathrm{e}^{-\mathrm{i}h\mathcal{H}^X}\mathrm{e}^{-\mathrm{i}h\mathcal{H}^Y}\mathrm{e}^{-\mathrm{i}h\mathcal{H}^Z} + \mathcal{O}\left(h^2\right),$$

where

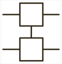
$$\mathcal{H}^\alpha = \mathbf{e}^\top \mathbb{S}^\alpha + \frac{1}{2}\mathbb{S}^{\alpha\top} C^{\alpha,\alpha}\,\mathbb{S}^\alpha, \qquad \alpha \in \{X, Y, Z\},$$

and

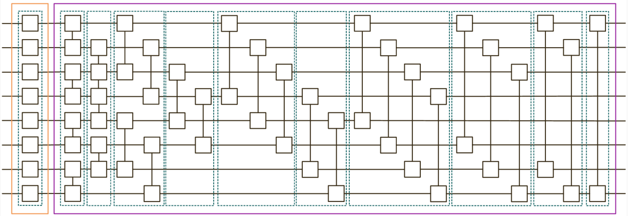
$$\mathrm{e}^{-\mathrm{i}h\mathcal{H}^\alpha} = \prod_{\ell=1}^{n} \mathrm{e}^{-\mathrm{i}h\mathbf{e}_\ell^\alpha \alpha_\ell} \prod_{j=1}^{n}\prod_{k=j+1}^{n} \mathrm{e}^{-\mathrm{i}hC_{j,k}^{\alpha,\alpha}\alpha_j\alpha_k},$$

computed exactly using n single-qubit gates and $\mathcal{O}\left(n^2\right)$ coupling gates.

(a)



(b)



(c)

If e^{hA} and e^{hB} are easier to compute, approximate $\mathrm{e}^{h(A+B)}$ by

splitting	error	name	stages
$\mathrm{e}^{hA}\mathrm{e}^{hB}$	$\mathcal{O}\left(h^2\right)$	Trotter	2

Trotterisation ↔ Splitting methods for matrix exponential

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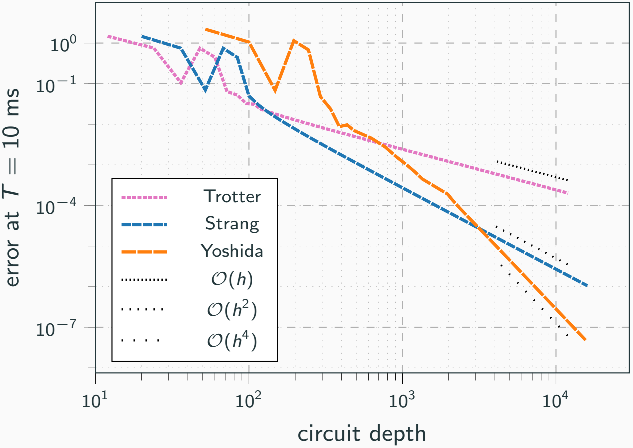
$\mathrm{e}^{\frac{1}{2}hB}\mathrm{e}^{hA}\mathrm{e}^{\frac{1}{2}hB}$	$\mathcal{O}\left(h^3\right)$	Strang	3
$\mathrm{e}^{a_1 hB}\mathrm{e}^{b_1 hA}\mathrm{e}^{a_2 hB}\ldots\mathrm{e}^{b_n hA}\ldots\mathrm{e}^{a_2 hB}\mathrm{e}^{b_1 hA}\mathrm{e}^{a_1 hB}$	$\mathcal{O}\left(h^{2p+1}\right)$	Classical	$\mathcal{O}(2^p)$
$\mathrm{e}^{\frac{h}{6}A}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{\frac{2}{3}(hA+\frac{h^3}{48}[[A,B],B])}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{\frac{h}{6}A}$	$\mathcal{O}\left(h^{2p+1}\right)$	Compact	$\mathcal{O}(2^p)$
$\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{\frac{h}{2}A}\mathrm{e}^{h^3 R}\mathrm{e}^{h^5 S}\mathrm{e}^{h^3 R}\mathrm{e}^{\frac{h}{2}A}\mathrm{e}^{\frac{h}{2}B}$	$\mathcal{O}\left(h^{2p+1}\right)$	Asymptotic	$\mathcal{O}(p)$

Yoshida 1990, Murua & Sanz-Serna 1999, Chin & Chen 2002, McLachlan & Quispel 2002, Blanes, Casas & Murua 2008, Chartier & Murua 2009, . . . Asymptotic (Zassenhaus) Bader, Iserles, Kropielnicka, & S. 2014, Found. Comp. Math.



No good reason to use Trotter instead of Strang, even for NISQ

Chen, Foroozandeh, Budd & S. 2023. *Quantum simulation of highly-oscillatory many-body Hamiltonians for near-term devices*, submitted

Quantum advantage in NISQ era?

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Dulwich Quantum Computing
@DulwichQuantum

At least 7 articles so far have reproduced the @IBM computation *classically*:
arxiv.org/abs/2306.14887
arxiv.org/abs/2306.15970
arxiv.org/abs/2306.16372
arxiv.org/abs/2308.01339
arxiv.org/abs/2308.03082
arxiv.org/abs/2308.05077
arxiv.org/abs/2308.09109

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What should we expect from quantum Hamiltonian simulation?

BQP (bounded-error quantum polynomial time)

Class of decision problems solvable by a quantum computer in polynomial time, with an error probability of at most 1/3 for all instances.

$$\mathrm{P} \subseteq \mathrm{BQP} \subseteq \mathrm{PSPACE}$$

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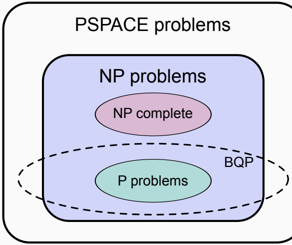
$$\mathrm{P} \stackrel{?}{=} \mathrm{BQP} \stackrel{?}{=} \mathrm{PSPACE} \qquad \text{is not known.}$$

The only ‘definitive’ proof of quantum ‘supremacy’ (in Hamiltonian simulation or otherwise) is to show BQP $\neq$ P.



Computing the matrix exponential

C. Moler & C. V. Loan, *Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later*, SIAM Review (2003).

Splitting, Diagonalisation, Scaling and Squaring

	Asymptotic $z \to 0$	Approximate e^z on spectrum $z \in [a, b] \subseteq \sigma(A)$	Iterative Use A and u_0
Polynomial	Taylor $\sum_{k=0}^{n} \frac{z^k}{k!}$	Chebyshev $J_0(\mathrm{i}) + 2\sum_{k=1}^{n} \mathrm{i}^k J_k(-\mathrm{i}) T_k(z)$	Lanczos
Rational	Padé $\frac{1+\frac{1}{2}z+\frac{1}{12}z^2}{1-\frac{1}{2}z+\frac{1}{12}z^2}$	?	Rational Krylov

Qubitization (Low & Chuang 2019) based on Chebyshev.

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Since $\sigma(\mathrm{iH}) \subseteq \mathrm{i}\mathbb{R}$,

$$|f(\mathrm{i}x)| = 1 \qquad x \in \mathbb{R} \qquad \Longrightarrow \qquad f(\mathrm{iH}) \text{ is unitary}$$

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No non-constant polynomial method can be unitary. Proof: coercivity.

Why care about unitarity?

Schrödinger equation

$$\partial_t u = -\mathrm{i}\mathrm{H}u, \qquad u(0) = u_0, \qquad \mathrm{H}^* = \mathrm{H},$$

$$\begin{aligned} u(t) &= \mathrm{e}^{-\mathrm{i}t\mathrm{H}} u_0 \\ E(t) := \langle u(t), \mathrm{H}u(t)\rangle &= \langle u(0), \mathrm{H}u(0)\rangle = E(0) \quad \text{energy conservation} \\ \underbrace{\langle u(t), v(t)\rangle = \langle u(0), v(0)\rangle}_{\text{unitary evolution}} &\implies \underbrace{\|u(t)\|_2 = \|u(0)\|_2 = 1}_{\text{mass or probability conservation}} \end{aligned}$$

exp maps Lie algebra $\mathrm{i}\mathrm{H} \in \mathfrak{su}(n)$ to Lie group $\mathrm{e}^{-\mathrm{i}t\mathrm{H}} \in \mathrm{U}(n)$.

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These properties are also desired from numerical approximations.

$e^z \approx 1 + z$	u_1	$=$	$(I - \mathrm{i}h\mathrm{H})u_0$	F.E.	$\|u_n\|_2 \to \infty$
$e^z \approx \frac{1}{1-z}$	$(I + \mathrm{i}h\mathrm{H})u_1$	$=$	u_0	B.E.	$\|u_n\|_2 \to 0$
$e^z \approx \frac{1+z/2}{1-z/2}$	$(I + \mathrm{i}(h/2)\mathrm{H})\, u_1$	$=$	$(I - \mathrm{i}(h/2)\mathrm{H})\, u_0$	T.R.	$\|u_n\|_2 = \|u_0\|_2$

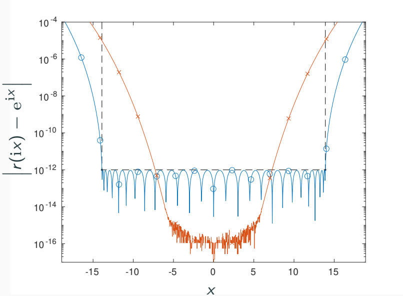
$\mathrm{cay}(z) = \frac{1+z/2}{1-z/2}$ maps Lie algebra $\mathrm{i}\mathrm{H} \in \mathfrak{su}(n)$ to Lie group $e^{-\mathrm{i}t\mathrm{H}} \in \mathrm{U}(n)$.

Wave, KdV, NLS, Pauli, Dirac, Liouville–von Neumann, Linblad, MCTDHF, CCSD, TDDFT, . . .

Uniform approximation with AAA & AAA–Lawson

- AAA. Nakatsukasa, Sète & Trefethen. *The AAA algorithm for rational approximation*, SIAM J. Sci. Comput., Vol. 40, Iss. 3 (2018).
- AAA–Lawson. Nakatsukasa & Trefethen. *An algorithm for real and complex rational minimax approximation*, SIAM J. Sci. Comput., Vol. 4, Iss. 5 (2020).

Error in approximation of $\mathrm{e}^{\mathrm{i}x}$
(Padé vs AAA–Lawson)



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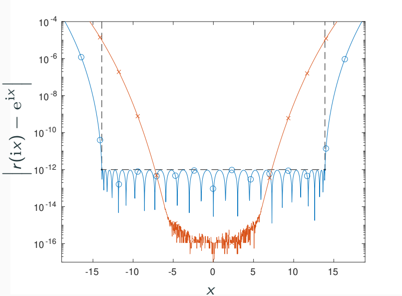
Error in approximation of e^{ix}
(Padé vs AAA–Lawson)



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$$r(x) = \underbrace{\sum_{j=1}^{m} \frac{e^{iy_j} w_j}{x - y_j}}_{n(x)} \Big/ \underbrace{\sum_{j=1}^{m} \frac{w_j}{x - y_j}}_{d(x)} \approx e^{ix},$$

linearize and minimize

$$\|Lw\|_2 = \left(\sum_{k=1}^{n} \mu_k |n(x_k) - e^{ix_k} d(x_k)|^2 \right)^{1/2}$$

Computed using SVD of Loewner matrix, $L_{kj} = \mu_k^{1/2} \frac{e^{ix_k} - e^{iy_j}}{x_k - y_j}$, and picking w as the right singular vector corresponding to the smallest singular value.

Loewner matrix based rational approximations and interpolations are unitary.

Jawecki & S 2023. *Unitarity of some barycentric rational approximants*, IMA J. Num. Anal.

Includes Antoulas & Anderson 1986, Mayo & Antoulas 2007, NST 2018 (AAA), NT 2020 (AAA–Lawson), JS (*submitted*) (interpolation at Chebyshev nodes, modified BRASIL algorithm, modified AAA–Lawson), ...

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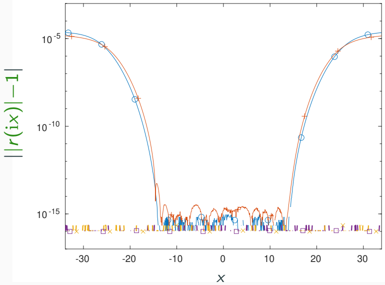


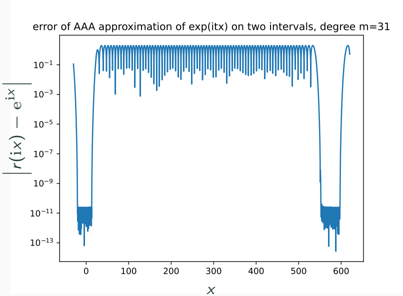
Modified AAA and AAA–Lawson (JS 23) ensures unitarity to machine precision.

Non-uniform and split spectrum approximation

Wavefunction centred around two different energy levels

$$u_0(x) = \psi_1(x) + \psi_2(x), \qquad \psi_j(x) = \sum_{k=0}^{n} c_{j,k} v_k(x), \quad c_{j,k} = \mathrm{e}^{-(\mu_j - \lambda_k)^2/2\sigma_j^2}$$

Error in approximation of $\mathrm{e}^{\mathrm{i}x}$
(AAA–Lawson)



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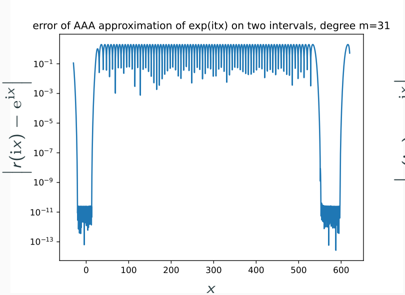
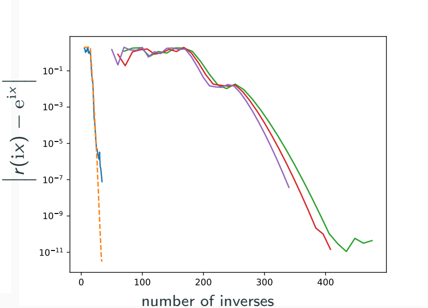


Error in matrix approximation $r(-\mathrm{i}h\mathrm{H})u_0$
((31,31) AAA–Lawson vs Padé)



Jawecki & S. *in preparation*

Best approximation

Approximating $f \in \mathrm{C}([a, b]; \mathbb{R})$ in $\mathcal{P}_n[a, b]$

- Best approximant $p^* \in \mathcal{P}_n$ exists & unique

$$\|f - p^*\|_\infty = \inf\{\|f - p\|_\infty : \ p \in \mathcal{P}_n\},$$

- Chebyshev equioscillation theorem

$$f(x_j) - p^*(x_j) = (-1)^{j+\iota}\|f - p\|_\infty, \qquad \iota \in \{0, 1\}$$

- Remez minimax algorithm
  - Find points $\{x_j\}$ of local maximum error $|f(x) - p^{[k]}(x)|$.
  - Stop if equioscillation property satisfied.
  - Otherwise, solve for $f(x_j) - p^{[k+1]}(x_j) = (-1)^j E$

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Motivates AAA–Lawson minimax algorithm [NT20] for approximating $f \in \mathrm{C}(I \subseteq \mathbb{C};\mathbb{C})$ in $\mathcal{R}_n[I] = \left\{\frac{p}{q} : p,q \in \mathcal{P}_n\right\}$ (or in Barycentric forms).

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- Gives *good* approximants in practice (typically), but ...
- No best approximation results for complex-valued rational approximation,
- $\{p \in \mathcal{P}_n : \|p\|_\infty = 1\}$ is compact, $\{r \in \mathcal{R}_n : \|r\|_\infty = 1\}$ is not compact,
- No equioscillation property in $\mathbb{C}$.

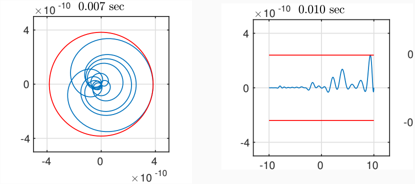
Equioscillation

Figures from [NT20]

(left) $f(z) = e^z$ on $\{z \in \mathbb{C} \ : |z| = 1\}$
(right) $f(z) = \mathrm{Ai}(z)$ on $z \in [-10, 10]$

deviation $f(z) - r(z)$ & max error $\|f - r\|$

No equioscillation!



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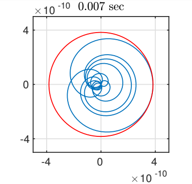
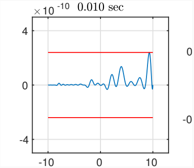
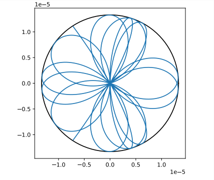


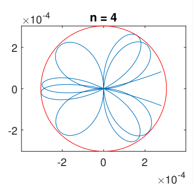


$$f(\mathrm{i}x) = \mathrm{e}^{\mathrm{i}\omega x}, \quad x \in [-1, 1]$$

18 June (left), T. Jawecki
28 June (right), N. Trefethen

Rose curves with $2n$ petals. equioscillation?





Equioscillation

Figures from [NT20]

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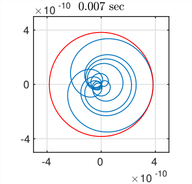

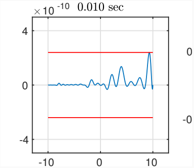

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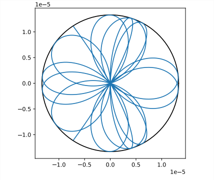
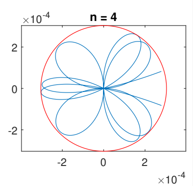


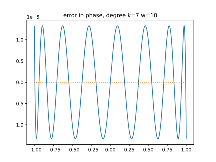


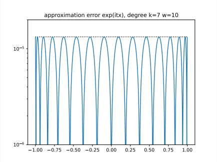
Let $r(\mathrm{i}x) = \mathrm{e}^{\mathrm{i}g(x)}$, where $g(x)$ is phase
Optimality $\Longleftrightarrow$ phase equioscillates

$$g(x_j) - \omega x_j = (-1)^{j+\iota} \max_{x \in [-1,1]} |g(x) - \omega x|.$$

$$|r(\mathrm{i}x_j) - \mathrm{e}^{\mathrm{i}\omega x_j}| = \|r - \exp(\omega \cdot)\|$$

Zeros of phase & approx error coincide.





Best (unitary rational) approximation

Jawecki & S 2023. *Unitary rational best approximations to the exponential function*, submitted.

Theorem. For $\omega \in (0, (n+1)\pi)$, there exists a unique unitary best approximation $r \in \mathcal{U}_n$, i.e.,

$$\|r - \exp(\omega\cdot)\| = \inf_{u \in \mathcal{U}_n} \|u - \exp(\omega\cdot)\|, \qquad \|f\| := \sup_{x \in [-1,1]} |f(\mathrm{i}x)|,$$

whose phase error equioscillates at $2n+2$ points, where max approx error is achieved. Moreover, r has minimal degree n, and distinct poles.

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Superlinear convergence. For $\omega < 1.47(n + 1/2)$,

$$\min_{u \in \mathcal{U}_n} \|u - \exp(\omega\cdot)\| \leq \frac{(n!)^2 \omega^{2n+1}}{(2n)!\,(2n+1)!}.$$

(proof via Padé),

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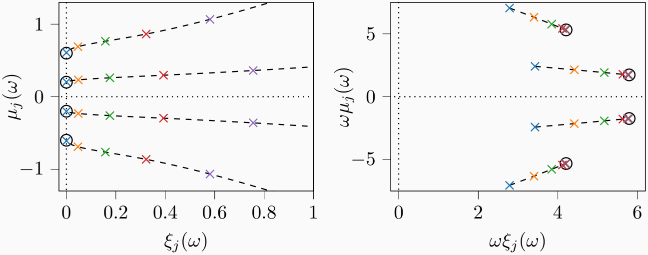
(proof via Padé), and in the limit $\omega \to 0^+$,

$$\min_{u \in \mathcal{U}_n} \|u - \exp(\omega\cdot)\| = \frac{2(n!)^2}{(2n)!\,(2n+1)!} \left(\frac{\omega}{2}\right)^{2n+1} + \mathcal{O}(\omega^{2n+2}), \quad \omega \to 0^+.$$

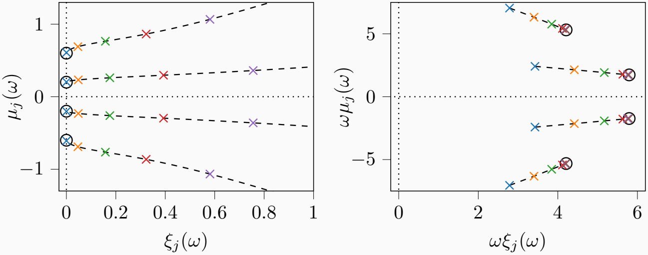
(proof via interpolation at Chebyshev points), twice as fast as Padé.

Poles, $\omega \to 0^+$, $\omega \to (n+1)\pi^-$



In the limit $\omega \to 0^+$, poles converge to poles of Padé.

In the limit $\omega \to (n+1)\pi^-$, poles approach $\mathrm{i}\xi_j$, where $\xi_j = -1 + 2j/(n+1)$ for $j = 1, \ldots, n$, within the right-half complex plane.



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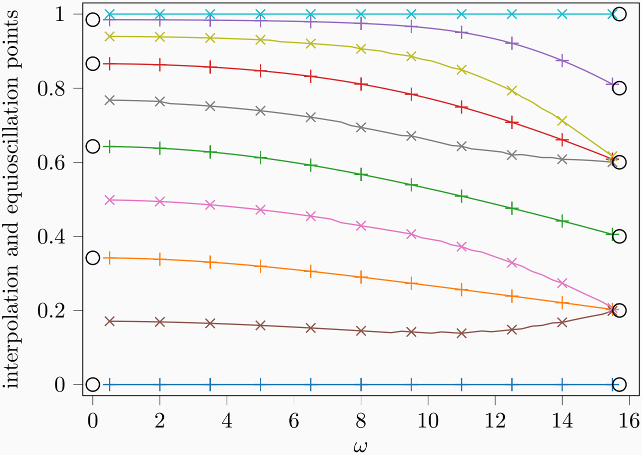
A-stability. Poles of best approximants are in right half plane and

$$|r(z)| < 1, \qquad \text{for } z \in \mathbb{C} \text{ with } \mathrm{Re}(z) < 0.$$

Relevant for non-Hermitian matrices/operators (e.g. open systems).

Time-symmetric.

$$r(-\mathrm{i}x) = r(\mathrm{i}x)^{-1}, \quad x \in \mathbb{R}.$$



In the limit $\omega \to 0^+$, interpolation points converge to Chebyshev nodes.

In the limit $\omega \to (n+1)\pi^-$, interpolation points and equioscillation points converge to uniformly distributed points. Phase error approaches sawtooth function.

Three new algorithms. Interpolation at Chebyshev points, modified AAA–Lawson and BRASIL algorithms – latter two candidates for best approximation (seem to display equioscillatory behaviour).

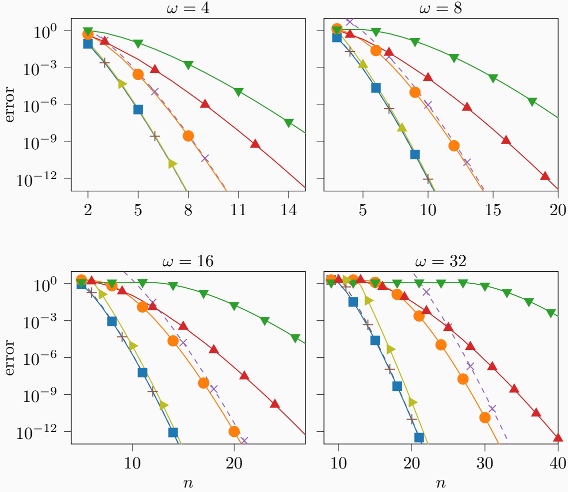


Figure 1: [new] unitary best approximation (■), error estimate (dashed, +), [new] rational interpolant at Chebyshev nodes (▷), Padé approximation (○), Padé error bound (dashed, ×), polynomial Chebyshev approximation (∇), rational Chebyshev approximation (△), .

How to compute the matrix exponential?

C. Moler & C. V. Loan, *Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later*, SIAM Review (2003).

	Asymptotic $z \to 0$	Approximate e^z on spectrum $z \in [a, b] \subseteq \sigma(A)$	Iterative Use A and u_0
Polynomial	Taylor $\sum_{k=0}^{n} \frac{z^k}{k!}$	Chebyshev $J_0(\mathrm{i}) + 2\sum_{k=1}^{n} \mathrm{i}^k J_k(-\mathrm{i})\, T_k(z)$	Lanczos
Rational	Padé $\frac{1+\frac{1}{2}z+\frac{1}{12}z^2}{1-\frac{1}{2}z+\frac{1}{12}z^2}$	unitary best approximations	Rational Krylov

Other techniques: Diagonalisation, Spectral methods, Scaling and Squaring, Splitting

AAA [NST 18], AAA–Lawson [NT 20], their unitary modifications [JS 23], and three new algorithms [JS *submitted*].

- Jawecki & S. 2023. *Unitarity of some barycentric rational approximants*, IMA J. Num. Anal.
- Jawecki & S. 2023. *Unitary rational best approximations to the exponential function*, submitted.
- Jawecki & S., in preparation.

Driven systems – Is Magnus expansion DoA?

The solution to $u'(t) = \mathcal{A}(t)u(t)$, $\quad \mathcal{A}(t) = -\mathrm{i}\mathrm{H}(t)$,

$$u(h) = \exp\left(\Theta(h)\right) u_0,$$

where $\Theta(h)$ is the **Magnus expansion** [Magnus 54],

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

$$\mathcal{A}(t) = -\mathrm{i}\mathrm{H}(t), \quad \mathrm{H}(t) = \underbrace{\sum_{k=1}^{n} \sum_{\alpha\in\{X,Y,Z\}} \mathrm{e}_k^\alpha(t)\ \alpha_k}_{\mathcal{O}(n)\ \text{terms}} + \underbrace{\frac{1}{2}\sum_{j,k=1}^{n} \sum_{\alpha,\beta\in\{X,Y,Z\}} C_{j,k}^{\alpha,\beta}\ \alpha_j\ \beta_k}_{|C|\leq\mathcal{O}\left(n^2\right)\ \text{terms}}$$

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Issue: $\mathcal{A}$ has $\mathcal{O}(|C|) = \mathcal{O}\left(n^2\right)$ terms. Does Θ_2 have $\mathcal{O}\left(|C|^2\right) = \mathcal{O}\left(n^4\right)$ terms?

A standard method for classical computers, infeasible for quantum computers.

Instead, other approaches used: Dyson series (Kieferova et al. 2019), time-ordered operators (Watkins et al. 2022), L1 norm scaling (Berry et al. 2020), permutation expansion (Chen et al. 2021), slowly varying Hamiltonians (Haah et al. 2021), interaction picture (Low & Wiebe 2018), Floquet approach (Mizuta et al. 2023).

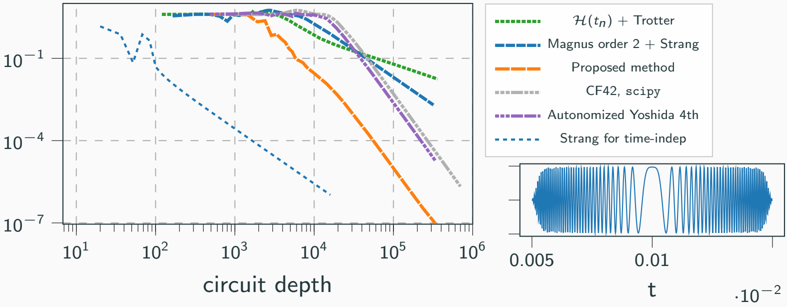
Driven systems – Is Magnus expansion DoA? No!

Theorem (Fourth order Magnus based circuit)

$$e^{\mathrm{i}\frac{2}{h}\mathbf{u}^\top \mathbb{S}} \underbrace{e^{-\mathrm{i}\tilde{\mathbf{r}}^\top \mathbb{S} - \mathrm{i}\frac{h}{2}\mathbb{S}^\top C\ \mathbb{S}}}_{\textit{reuse 4th order Trotterised circuit}} \underbrace{e^{-\mathrm{i}\frac{2}{h}\mathbf{u}^\top \mathbb{S}}}_{\textit{two single-gate layers}} = e^{\Theta_2} + \mathcal{O}\left(h^5\right)$$

Chen, Foroozandeh, Budd & S. 2023. submitted

For two controls: Ikeda, Abrar, Chuang & Sugiura 2023. Quantum.



In fact, Magnus is much better than all other methods!

Time-dependent problems of practical interest are **MUCH** harder!

Driven systems – optimal control

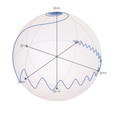
Maximize fidelity:

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

Fidelity functions

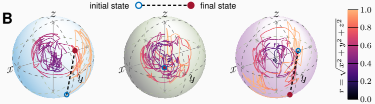
$$\mathcal{F}(\theta) = f(\mathbf{U}(T;\theta))$$

where state of system is $\rho(t) = \mathbf{U}(t;\theta)\rho_0$.



state-to-state

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



gate design

$$f(X) = \mathrm{Re}\left[\mathrm{Tr}\left(\mathbf{U}^\dagger_{\mathrm{target}} X\right)\right]$$

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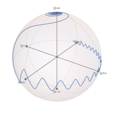

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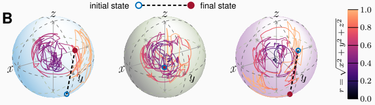

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$$f(X) = \mathrm{Re}\left[\mathrm{Tr}\left(\mathbf{U}^\dagger_{\mathrm{target}} X\right)\right]$$

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.

- No dissipation
- Piecewise constant

$$\mathbf{U}(T;\theta) = \mathrm{U}_N \mathrm{U}_{N-1} \cdots \mathrm{U}_2 \mathrm{U}_1, \qquad \text{with} \quad \mathrm{U}_n = \mathrm{e}^{-\mathrm{i}\boldsymbol{s}_n \cdot \boldsymbol{\sigma}}, \quad \boldsymbol{s}_n := \boldsymbol{he}(t_n).$$

We can store intermediate propagators

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

to compute gradients cheaply and exactly

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

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

The typical approach for computing the Hessian involves computing and storing

$$\mathrm{M}_{n,m} := \mathrm{U}_n \mathrm{U}_{n-1} \dots \mathrm{U}_{m+1} \mathrm{U}_m. \qquad \mathcal{O}\left(N^2\right)$$

and use for computing $\frac{\partial^2 \mathbf{U}}{\partial \theta_{m,j} \partial \theta_{n,k}} = \mathrm{L}_{n+1} \frac{\partial \mathrm{U}_n}{\partial \theta_{n,k}} \mathrm{M}_{n-1,m+1} \frac{\partial \mathrm{U}_m}{\partial \theta_{m,j}} \mathrm{R}_{m-1}$.

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$$\mathrm{M}_{n,m} = (\mathrm{U}_N \dots \mathrm{U}_{n+1})^* \mathrm{U}_N \dots \mathrm{U}_{n+1} \mathrm{M}_{n,m} \mathrm{U}_{m-1} \dots \mathrm{U}_1 (\mathrm{U}_{m-1} \dots \mathrm{U}_1)^*$$

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so that entries of the Hessian can be computed as $\mathrm{L}_{n+1} \frac{\partial \mathrm{U}_n}{\partial \theta_{n,k}} \mathrm{L}_n^* \mathbf{U} \mathrm{R}_m^* \frac{\partial \mathrm{U}_m}{\partial \theta_{m,j}} \mathrm{R}_{m-1}$.

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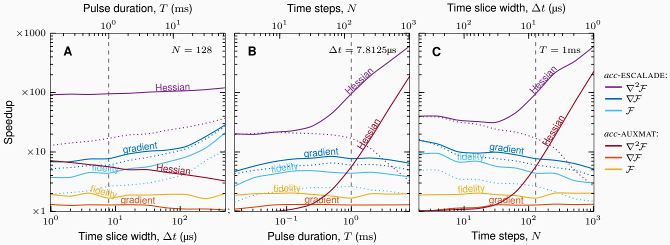


Speedup: $\times 2 - 10$ fidelity, $\times 4 - 30$ gradient, $\times 20 - 600$ Hessian.

Foroozandeh & S. 2022. Automatica. ESCALADE doi:10.17632/8zz84359m5
Goodwin & Vinding 2023. Phys. Rev. Res.

Coupling, dissipation & adaptive optimal control

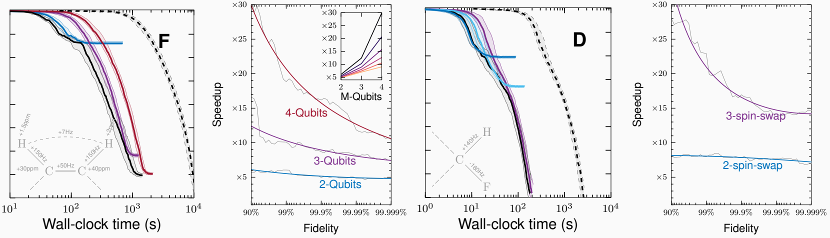
Liouville–von Neumann equation, piecewise constant,

$$\partial_t \rho = \mathcal{L}(t;\theta)\,\rho, \qquad \mathcal{L}_n(\theta) = \underbrace{-\mathrm{i}\,\mathrm{ad}_{\mathbf{e}(t_n;\theta)^\top \mathbb{S}}}_{\mathcal{L}_n^{[1]}(\theta)} \quad \underbrace{-\mathrm{i}\,\mathrm{ad}_{\mathrm{H}_{\mathrm{in}}+\mathcal{R}}}_{\mathcal{L}^{[2]}}$$

Splittings $\mathcal{S}_{(1)}, \mathcal{S}_{(2)}, \ldots, \mathcal{S}_{(L)} \approx \mathbf{U}(T;\theta)$ with increasing accuracies,

$$\mathrm{U}_n = \mathrm{e}^{h\mathcal{L}_n(\theta)} \quad \approx \quad \prod_{k=1}^{K} \underbrace{\mathrm{e}^{ha_k \mathcal{L}_n^{[1]}(\theta)}}_{\text{uncoupled, analytic grad}} \quad \mathrm{e}^{hb_k \mathcal{L}^{[2]}}$$

Move from $\mathcal{S}_{(\ell)}$ to $\mathcal{S}_{(\ell+1)}$ when $|\mathcal{F}_{(\ell)} - \mathcal{F}_{(\ell+1)}| \quad \leq \quad \kappa_{\mathcal{F}} |1 - \mathcal{F}_{(\ell)}|$



Goodwin, Foroozandeh & S. 2022. Science Advances. `QOALA` `github.com/superego101/qoala`

Takeaways & Open Problems

- **Quantum Computing.** [1] Chen, Foroozandeh, Budd & S. 2023. *Quantum simulation of highly-oscillatory many-body Hamiltonians for near-term devices*, submitted
  - No good reason to use Trotter (used in IBM paper) instead of Strang.
  - Practical time-dependent problems are much harder, high order methods required.
  - Magnus methods are not DoA, in fact, lead to shortest circuits even for 10^{-1} accuracy.
  - * Better splittings? Better commutator-free methods?
- **Approximation Theory.** [2] Jawecki & S. 2023. *Unitarity of some barycentric rational approximants*, IMA J. Num. Anal. [3] Jawecki & S. 2023. *Unitary rational best approximations to the exponential function*, submitted. [4] Jawecki & S., in prep.
  - Loewner based algorithms (incl. AAA) conserve unitarity, energy, norm
  - Unitary rational best approximations exist, unique & phase equioscillates
  - Three new algorithms (Cheb. interp., AAA–Lawson at Cheb., modified BRASIL), AAA/AAA–Lawson, all superior to existing rational approximations.
  - * Rational best approximations to $e^{i\omega x}$ = Unitary rational best approximations?
  - * Observed twice faster convergence than Padé. Proof for non-asymptotic ω?
  - * Does modified BRASIL converge to best approximation?
- **Optimal Control.** [5] Foroozandeh & S. 2022. *Optimal control of spins by Analytical Lie Algebraic Derivatives*, Automatica. `ESCALADE` doi:10.17632/8zz84359m5. [6] Goodwin, Foroozandeh & S. 2022. *Adaptive optimal control of entangled qubits*, Science Advances. `QOALA` `github.com/superego101/qoala`. [7] Sherzad, Chen, Foroozandeh & S., in prep.
  - Compute analytic gradients using Lie algebraic techniques.
  - Hessian factorization reduces cost from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$, $x20 - 600$ speedup.
  - Use cheaper method far from optima, switch adaptively.
  - * Are pulses robust under timing and amplitude imperfections?

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