Controlling Quanta under Constraints

Quantum Compilation by Optimal Control of Open Systems

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includes joint work with
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Motivation: Control in Quantum Technology

We are currently in the midst of a second quantum revolution. The first quantum revolution gave us new rules that govern physical reality. The second quantum revolution will take these rules and use them to develop new technologies. DOWLING & MILBURN, 2003

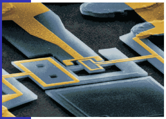
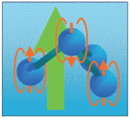
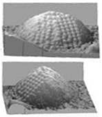
- economy

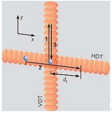
  currently some 30% of the GNP of industrial states depend on quantum effects (transistor, laser)

- technology ahead

  quantum & nano-technology rely on quantum control

  (solid-state devices, spintronics–NMR–EPR, quantum dots, ion-traps)



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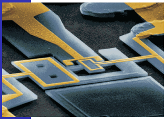
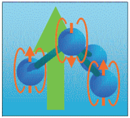
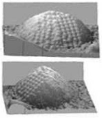
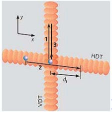






Outline

- assemble optimised medium-sized building blocks

Quantum Algorithm, Unitary Module

RISC−Compiler ↓ (**1**) | ↓ (**2**) | CISC−Compiler ↓ (**3**)

Universal Gates (RISC) | single CISC | Modular Controls (CISC)

Assembler ↓ | ↓ | scalable Assembler ↓

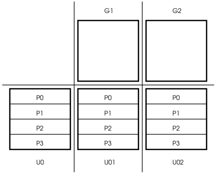
Machine Code of Quantum Evolutions under Drift and Controls

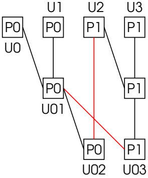
RISC-CISC analogy: G. Sanders *et al.* PRA **59**, 1098 (1999)

Parallelisation

Speed-Up on High-Performance Parallel Cluster with T. Gradl, T. Huckle

- Parallelising Matrix Operations
  1. slice-wise:
  2. tree-like:





- Resulting Speed-Ups: 10 spins 128 time slices

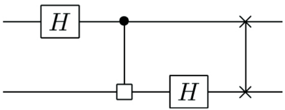
128 AMD *Opteron 850* CPU (2.4 GHz)

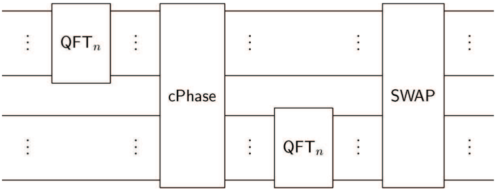
Subroutine	% of time	Speedup
optimizeCG	100	578
maxStepSize	90	709
getGradient	9.1	187
expm	7.5	879
propagation	1	31
gradient	0.6	81

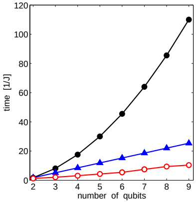
Gradl, Spörl, Huckle, Glaser, T.S.H., *Proceedings EUROPAR LNCS* **4128** (2006), 751

Assembling by Recursion
Ex.: QFT

- **Idea:** from 2-qubit QFT to $2n$-qubit QFT



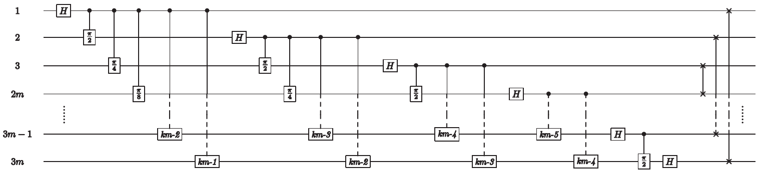




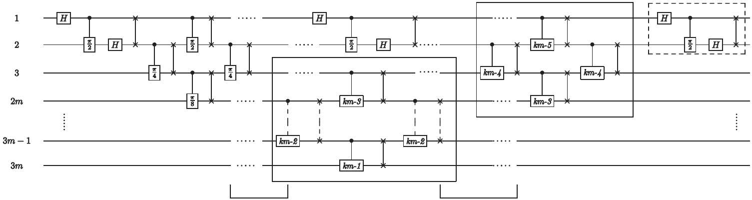
Assembling by Recursion

Ex.: Recursive QFT

- **Induction:** $k\,m$-qubit QFT to $(k+1)m$-qubit QFT ($m = 2$)



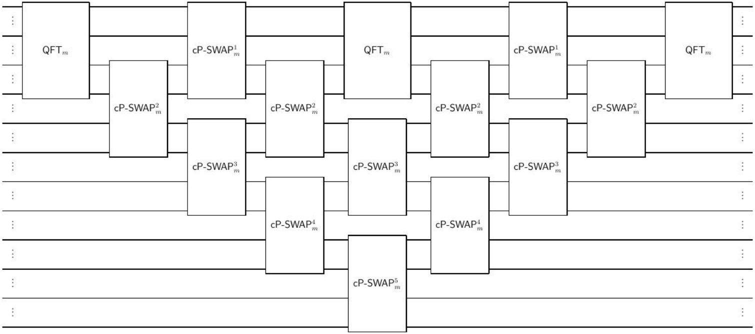
- **Induction:** km-qubit QFT to $(k+1)m$-qubit QFT $(m=2)$



Assembling by Recursion

Ex.: Recursive QFT

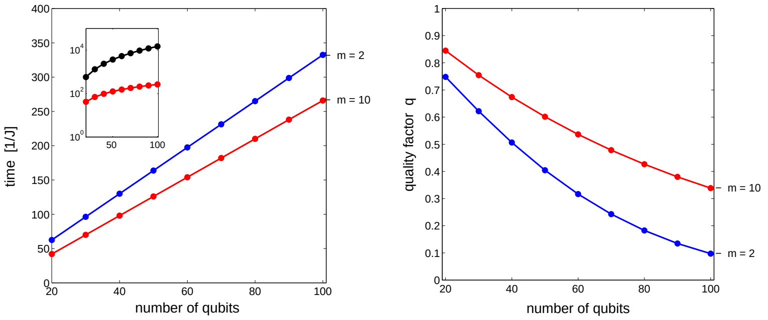
- **Induction:** km-qubit QFT to $k(m+2)$-qubit QFT (m even)



Results for Large Systems

Ex.: Recursive *km*-QFT

- quality gain by speed-up



Results for Large Systems

Ex.: Recursive 1, *n*-SWAP

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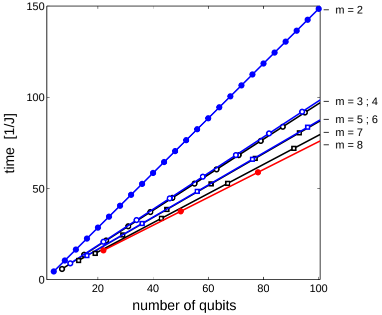
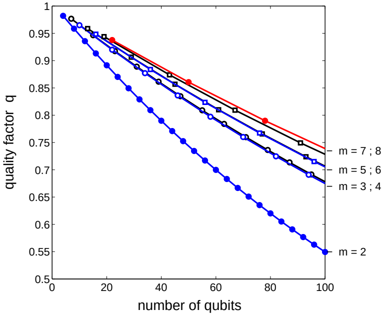
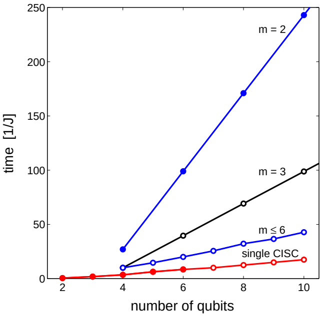


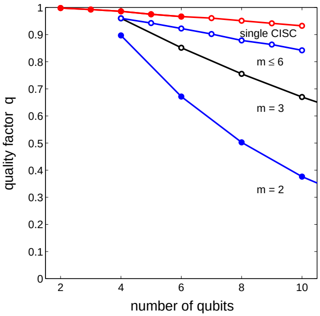


Results for Large Systems

Ex.: Recursive C^n-NOT

- quality gain by speed-up





Dynamical Systems and Flows

- dynamic systems on smooth manifolds M, e.g.:
  (1) all states on the (unitary) orbit of an initial state
  (2) group of unitary actions $\{Ad_U \mid U \in SU(N)\}$
  (3) vectors of piece-wise constant control amplitudes $(\overset{\text{iso}}{=} \mathbb{R}^n)$

- flow: smooth map $\mathbb{R} \times M \to M$

$$\Phi(0, X) = X$$
$$\Phi(\tau, \Phi(t, X)) = \Phi(t + \tau, X) \quad .$$

- flow acts as one-parameter semigroup for $\tau, t \geq 0$

$$\Phi_\tau \circ \Phi_t = \Phi_{t+\tau}$$

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- smooth quality function $f : M \to \mathbb{R}$ on M
- differential of f at $X \in M$ is Df: $M \to T^*M$ mapping to cotangent bundle T^*M
- gradient of f at $X \in M$ is grad f: $M \to TM$ mapping to tangent bundle TM

$$Df(X) \cdot \xi = \langle \text{grad}\, f(X) | \xi \rangle_X \quad \text{for all } \xi \in T_X M.$$

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- gradient flow $\Phi : \mathbb{R} \times M \to M$:
  solution to gradient system on M determined by ordinary differential equation

  $$\dot{X} = \operatorname{grad} f(X)$$

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- steepest ascent, special case:
  M coincides with T_M (as for $M = \mathbb{R}^n$)

  $$X_{k+1} = X_k + \alpha_k \operatorname{grad} f(X_k)$$

  $\alpha_k \geq 0$ appropriate step size

- steepest ascent for Riemannian manifolds M
  (M and T_M in general not identifiable):

  $$X_{k+1} := \exp_{X_k}(\alpha_k \operatorname{grad} f(X_k))$$

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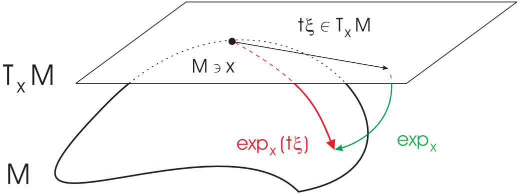
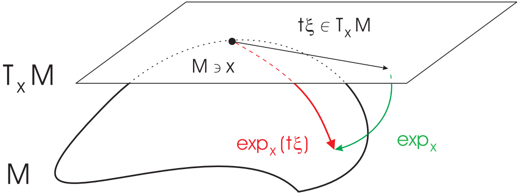
- $\exp_x : T_X M \to M$



- specially simple in Lie groups: $\exp_x : T_X \mathbf{G} \to \mathbf{G}$

$$\begin{array}{ccc} \xi = \Omega X \in T_X\mathbf{G} & \xrightarrow{\exp_X} & e^{t\Omega}X \in \mathbf{G} \\ R_{X^{-1}} \downarrow & & \uparrow R_X \\ \Omega \in \mathfrak{g} & \xrightarrow{\exp} & e^{t\Omega} \in \mathbf{G}\,. \end{array}$$

- $\exp_x : T_X M \rightarrow M$



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$$X_{k+1} := \exp_{X_k}\big(\alpha_k \operatorname{grad} f(X_k)\big) = \exp\big(\alpha_k \operatorname{grad} f(X_k)\, X_k^{-1}\big) X_k \,,$$

Brockett (1988)
Helmke, Moore (1994)

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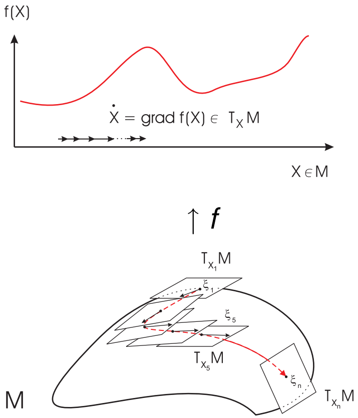
f(X)
Ẋ = grad f(X) ∈ T_X M
X ∈ M
↑ f
T_{X_1} M
ξ_1
ξ_5
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ξ_n
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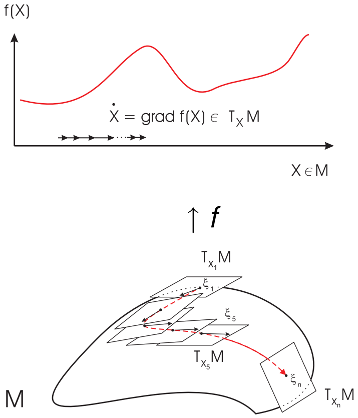
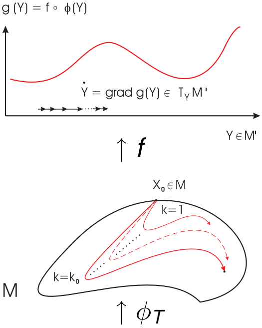
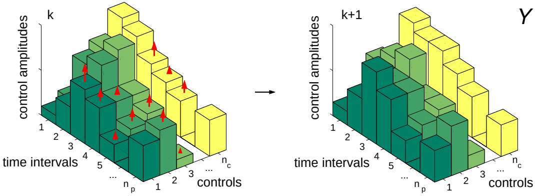
M



- quality function $f : M \to \mathbb{R}\, , X \mapsto f(X)$ drives into (local) maximum by gradient flow to $\dot{X} = \mathrm{grad}\, f(X)$ on M



$X(t, Y)$ solves control system $\dot{X} = F(X_0, Y)$



$Y \in \mathrm{M}' \cong \mathbb{R}^{n_p \cdot n_c}$

- **Bilinear Control System**

$$\dot{X}(t) = \Big(A + \sum_{j=1}^{m} u_j(t) B_j\Big)\; X(t)$$

- Hamiltonian dynamics (Schrödinger equation)

$$|\dot{\psi}(t)\rangle = -i\Big(H_d + \sum_{j=1}^{m} u_j(t) H_j\Big)\; |\psi(t)\rangle$$

$$\dot{U}(t) = -i\Big(H_d + \sum_{j=1}^{m} u_j(t) H_j\Big)\; U(t)$$

- H_d: drift term
- H_j: controls
- $u_j(t)$: control amplitudes

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Controllability of Quantum Systems

Definition

A system is *operator controllable*, if to any set of basis states its unitary image can be reached (in finite time).

Corollary (Jurdjevic and Sussmann, 1972)

The bilinear system (vide supra) is operator controllable if drift and controls are a generating set of $\mathfrak{su}(2^n)$ *by way of commutation, i.e.* $\langle H_d, H_j \,|\, j = 1, 2, \ldots, m \rangle_{\text{Lie}} \overset{\text{rep}}{=} \mathfrak{su}(2^n)$.

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Controllability and Coupling Topology

- Example: n weakly coupled spins-$\frac{1}{2}$.

  Which conditions suffice for

$$\langle H_d, H_j \,|\, j = 1, 2, \ldots, m \rangle_{\mathrm{Lie}} \stackrel{\mathrm{rep}}{=} \mathfrak{su}(2^n) \quad ?$$

Lemma (Diss. ETH 12752)

A system of n qubits is operator controllable, if e.g. the control Hamiltonians H_j comprise $\{\sigma_{kx}, \sigma_{ky} \,|\, k = 1, 2, \ldots n\}$ on every single qubit selectively and the drift Hamiltonian H_d encompasses the Ising pair interactions $\{J_{k\ell}\,(\sigma_{kz} \otimes \sigma_{\ell z})/2 \,|\, k < \ell = 2, \ldots n\}$, where the coupling topology of $J_{k\ell} \neq 0$ may take the form of any connected graph.

Corollary

The following are equivalent:

1. *in a quantum system drift H_d and controls H_j form a generating set of $\mathfrak{su}(2^n)$;*
2. *every unitary transformation in $SU(2^n)$ can be realised on that quantum hardware;*
3. *there is a set of universal quantum gates for the quantum system;*
4. *reachability set for generalised expectation value $\langle C\rangle(t) := \text{tr}\{C^\dagger A(t)\}$ coincides with C-numerical range $W(C, A)$ $\forall A, C$.*

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1. *in a quantum system drift H_d and controls H_j form a generating set of $\mathfrak{su}(2^n)$;*
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Controllability and Quantum Gates

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Principles: Optimal Quantum Control

Scope in Optimal Control:

maximise quality function **subject to** equation of motion

Scenarios:

- Hamiltonian dynamics

  notation: $U := e^{-itH}$; $\mathrm{Ad}_U(\cdot) := U(\cdot)U^{-1}$; $\mathrm{ad}_H(\cdot) := [H, \ \cdot]$

  1. pure state $\quad |\dot\psi\rangle = -iH\,|\psi\rangle \quad \in \mathcal{H}$
  2. gate $\quad \dot U = -iH\,U \quad \in \mathcal{U}(\mathcal{H})$
  3. non-pure state $\quad \dot\rho = -i\,\mathrm{ad}_H\,(\rho) \quad \in \mathcal{B}_1(\mathcal{H})$
  4. projective gate $\quad \dot{\mathrm{Ad}}_U = -i\,\mathrm{ad}_H \circ \mathrm{Ad}_U \quad \in \mathcal{U}\big(\mathcal{B}_1(\mathcal{H})\big)$

- Master equations of dissipative dynamics

  3'. non-pure state $\quad \dot\rho = -(i\,\mathrm{ad}_H + \Gamma)\,(\rho)$

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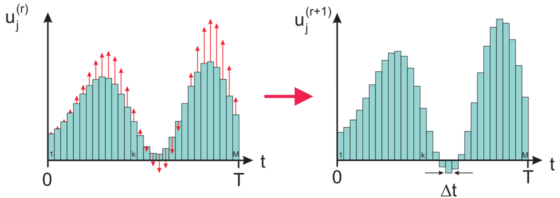
Gradient Ascent Algorithm GRAPE

J. Magn. Reson. **172** (2005), 296 and *Phys. Rev. A* **72** (2005), 042331



1. Define scalar-valued HAMILTON function
$$h(U) = \mathrm{Re}\,\mathrm{tr}\{\lambda^\dagger(-i(H_d + \textstyle\sum_j u_j H_j))U\}$$
2. with adjoint system satisfying
$$\dot\lambda(t) = -i(H_d + \textstyle\sum_j u_j H_j)\lambda(t) \quad .$$
3. Then PONTRYAGIN's maximum principle requires
$$\frac{\partial h}{\partial u_j} = \mathrm{Re}\,\mathrm{tr}\{\lambda^\dagger(-iH_j)U\} \overset{!}{=} 0$$
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$$u_j(t_k^{(r+1)}) = u_j(t_k^{(r)}) + \varepsilon \frac{\partial h}{\partial u_j}\Big|_{t=t_k}$$

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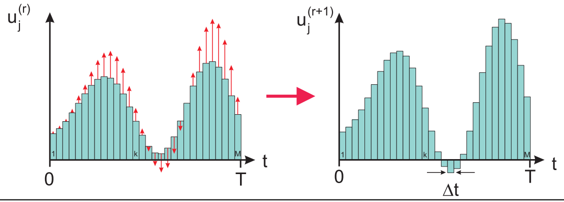

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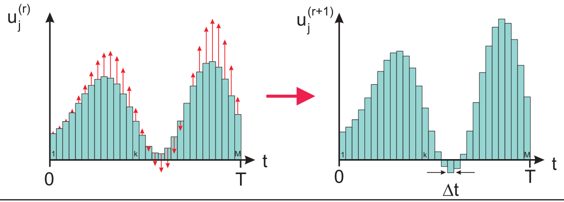

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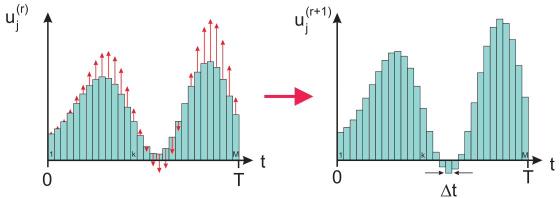

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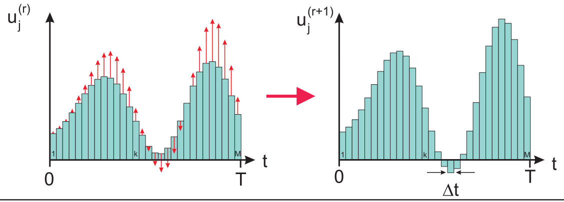

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Goal: realise *timeoptimal* CNOT on 2 coupled charge qubits

- pseudospin Hamiltonian: $H = H_{\text{drift}}$

$$
\begin{aligned}
H_{\text{drift}} = &-\left(\frac{E_m}{4} + \frac{E_{c1}}{2}\right)(\sigma_z^{(1)} \otimes \mathbb{1}) - \frac{E_{J1}}{2}(\sigma_x^{(1)} \otimes \mathbb{1}) \\
&-\left(\frac{E_m}{4} + \frac{E_{c2}}{2}\right)(\mathbb{1} \otimes \sigma_z^{(2)}) - \frac{E_{J2}}{2}(\mathbb{1} \otimes \sigma_x^{(2)}) \\
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$$

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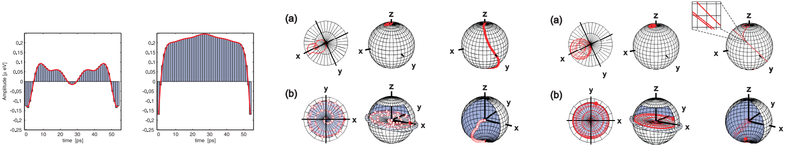
$$H_{\mathrm{control}} = \left(\frac{E_m}{2} n_{g2} + E_{c1} n_{g1}\right)(\sigma_z^{(1)} \otimes \mathbb{1}) + \left(\frac{E_m}{2} n_{g1} + E_{c2} n_{g2}\right)(\mathbb{1} \otimes \sigma_z^{(2)})$$

NB: components $\{H_d + H_d, H_c\}$ form minimal generating set of $\mathfrak{su}(4)$.

Examples of Quantum Control

2. Realising Quantum Gates in Minimal Time

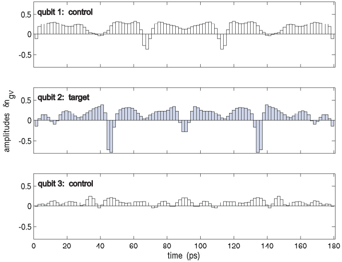


$\Rightarrow$ timeopt. CNOT: some 5 times faster than NEC group

- Quality $q := Fe^{-\tau_{\rm op}/\tau_Q}$
  so $1 - q = 1 - 0.999999999\, e^{-55\mathrm{ps}/10\mathrm{ns}} = 0.0055$
  (NEC: $1 - q = 1 - 0.4188\, e^{-250\mathrm{ps}/10\mathrm{ns}} = 0.5917$)

PRA **75**, 012302 (2007)

Goal: TOFFOLI gate on 3 linearly coupled charge qubits



13 times faster than NEC

- error rates cut by two orders of magnitude ($T_2 \simeq 10$ ns):

1. direct gate by optimal control
$$1 - q = 1 - 0.99999\, e^{-180\mathrm{ps}/10\mathrm{ns}} = 0.0178$$
2. by 9 CNOT's from optimal control
$$1 - q = 1 - (0.999999999\, e^{-55\mathrm{ps}/10\mathrm{ns}})^9 = 0.0483$$
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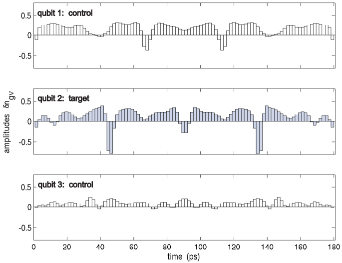

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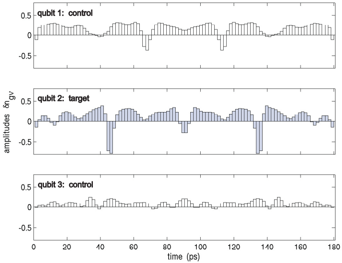

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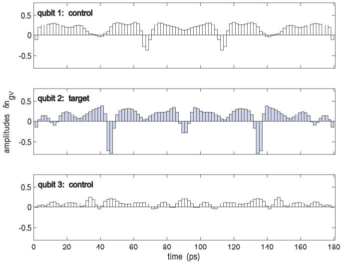

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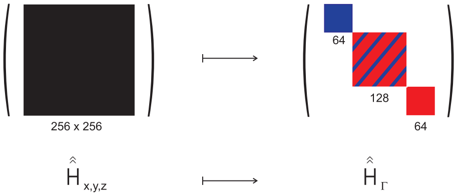
Principle:

Code *logical* qubits in decoherence-free *physical* levels

- Master equation: $\dot{\rho} = -(i\,\mathrm{ad}_H + \Gamma)\,\rho$
- DFS: eigenspace to Γ with eigenvalue =0
- Express $\widehat{H} \equiv \mathrm{ad}_H$ in eigenbasis of Γ (here 4 qubits)



- Idea: perform calculation (e.g. CNOT) within DFS

Zanardi, Rasetti, *Phys. Rev. Lett.* **79** (1997), 3309.

Lidar, Chuang, Whaley, *Phys. Rev. Lett.* **81** (1998), 2594.

Examples of Quantum Control

3. Decoherence Control: Idea of Decoherence-Free Subspaces (DFS)

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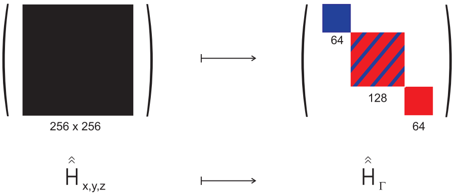

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- 1 logical qubit coded by 2 physical qubits in Bell states

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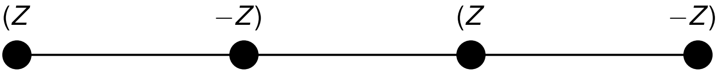
- protection against T_2 relaxation (Redfield: $\Gamma \sim [ZZ,[ZZ,\rho]]$)

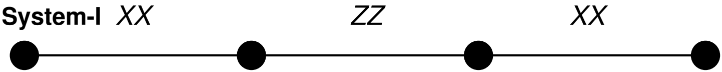
because $[\rho, ZZ] = 0 \quad \forall \quad \rho \in \mathcal{B} \otimes \mathcal{B}$

- controls

- controls



- drift: Ising (ZZ) and Heisenberg (XX) interactions



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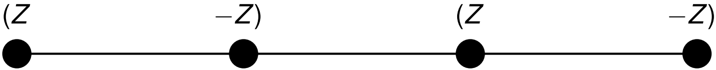

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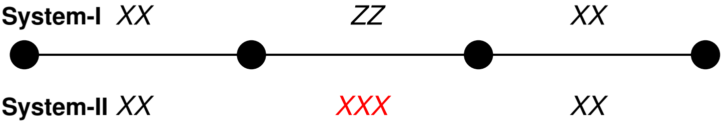
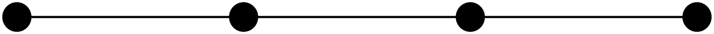


Examples of Quantum Control

3. Decoherence Control: Models with 4 Linearly Coupled Spins

- controls

$(Z \quad -Z) \quad (Z \quad -Z)$



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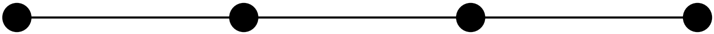
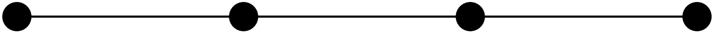
System-I XX ZZ XX



System-II (2 Hz) XX (1 Hz) XXX (2 Hz) XX

- relaxation $(T_2^{-1} : T_1^{-1} = 4.0\ \mathrm{s}^{-1} : 0.024\ \mathrm{s}^{-1} \simeq 170 : 1)$



T_2 : $[ZZ, [ZZ, (\cdot)]]$ $[ZZ, [ZZ, (\cdot)]]$

T_1 : $[A_{2,\bullet}, [A^\dagger_{2,\bullet}, (\cdot)]]$ $[A_{2,\bullet}, [A^\dagger_{2,\bullet}, (\cdot)]]$

- **System-I**: staying within slowly-relaxing subspace
  - drift Hamiltonian D_1 with Ising-ZZ
  - controls $C_{1,2}$

$$\begin{aligned} D_1 &:= J_{xx}\,(xx\mathbb{1}\mathbb{1} + \mathbb{1}\mathbb{1}xx + yy\mathbb{1}\mathbb{1} + \mathbb{1}\mathbb{1}yy) + J_{zz}\,\mathbb{1}zz\mathbb{1} \\ C_1 &:= z\mathbb{1}\mathbb{1}\mathbb{1} - \mathbb{1}z\mathbb{1}\mathbb{1} \\ C_2 &:= \mathbb{1}\mathbb{1}z\mathbb{1} - \mathbb{1}\mathbb{1}\mathbb{1}z\,. \\ &\Rightarrow \langle D_1, C_1, C_2\rangle_{\mathrm{Lie}}\big|_{\mathcal{B}\otimes\mathcal{B}} \overset{\mathrm{rep}}{=} \mathfrak{su}(4) \end{aligned}$$

  - Liouville subspace $\mathcal{B}\otimes\mathcal{B}$
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  - drift: extended to isotropic Heisenberg-XXX

$$\begin{aligned} D_1 + D_2 \;&:=\; J_{xx}\left(xx\mathbb{1}\mathbb{1} + \mathbb{1}\mathbb{1}xx + yy\mathbb{1}\mathbb{1} + \mathbb{1}\mathbb{1}yy\right) \\ &\quad + J_{xyz}\;\left(\mathbb{1}xx\mathbb{1} + \mathbb{1}yy\mathbb{1} + \mathbb{1}zz\mathbb{1}\right) \end{aligned}$$

  - Lie-algebraic closure: in 66-dim. Lie algebra

$$\dim\langle (D_1 + D_2), C_1, C_2\rangle_{\mathrm{Lie}} = 66\;,$$

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  - drift: extended to isotropic Heisenberg-XXX

$$\begin{aligned} D_1 + D_2 \;:=\; & J_{xx}\left(xx\mathbb{1}\mathbb{1} + \mathbb{1}\mathbb{1}xx + yy\mathbb{1}\mathbb{1} + \mathbb{1}\mathbb{1}yy\right) \\ & + J_{xyz}\;\left(\mathbb{1}xx\mathbb{1} + \mathbb{1}yy\mathbb{1} + \mathbb{1}zz\mathbb{1}\right) \end{aligned}$$

  - Lie-algebraic closure: in 66-dim. Lie algebra

$$\dim\langle (D_1 + D_2), C_1, C_2 \rangle_{\mathrm{Lie}} = 66 \;,$$

  - $\mathfrak{su}(4)$ merely subalgebra

System-II:

- full controllability within slowly-relaxing subspace
  - observation

$$e^{-i\pi C_1}(D_1+D_2)e^{i\pi C_1} = D_1 - D_2$$

  - Trotter limit

$$\lim_{n\to\infty}\left(e^{-i(D_1+D_2)/(2n)}e^{-i(D_1-D_2)/(2n)}\right)^n = e^{-iD_1}$$

  - reduction of dynamics

$$\textbf{System-II} \xrightarrow{\text{infinite \# switchings}} \textbf{System-I}$$

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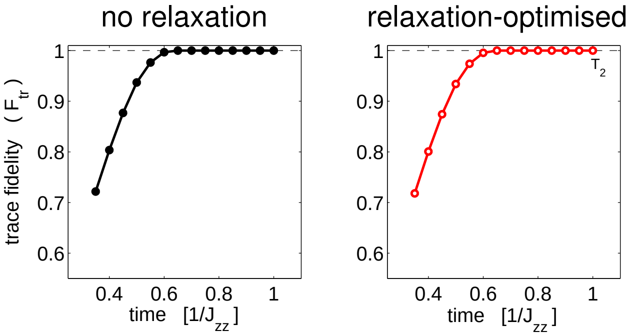
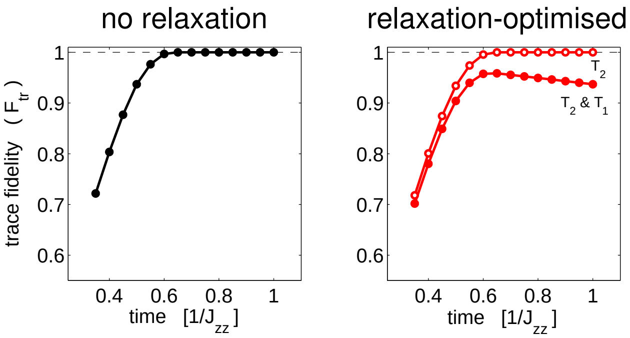
- **System-I**: staying within slowly-relaxing subspace



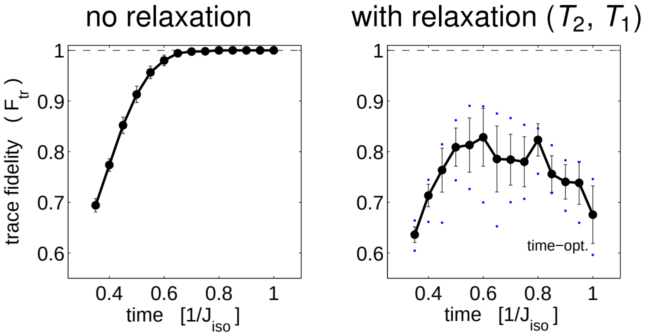
- T_2-relaxation has no effect on quality

- **System-I**: staying within slowly-relaxing subspace



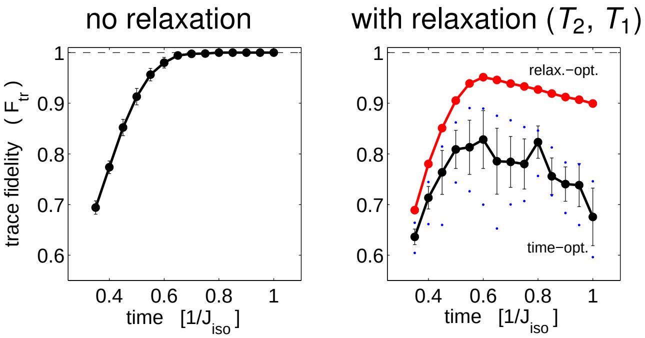
- T_2-relaxation has no effect on quality
- additional T_1-relaxation drops quality

- **System-II**: driving outside slowly-relaxing subspace



- mean of 15 time-optimised pulse sequences
- dissipation affects sequences differently

- **System-II**: driving outside slowly-relaxing subspace

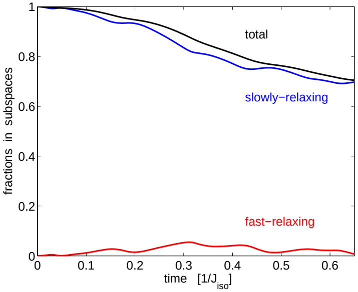


- mean of 15 time-optimised pulse sequences
- dissipation affects sequences differently
- relaxation-optimised: systematic substantial gain

quant-ph/0609037

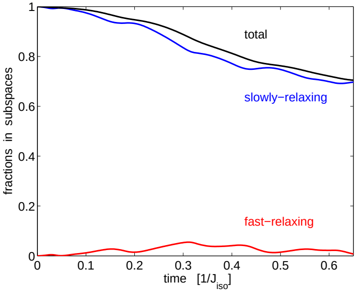
CNOT under **System-II**: Projection into Subspaces

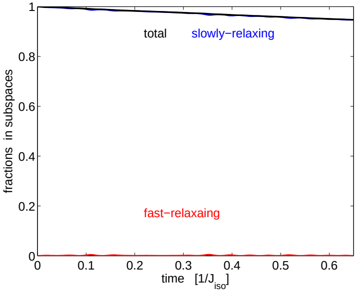
- time-optimised



CNOT under **System-II**: Projection into Subspaces

- time-optimsed
- opt. against decoherence





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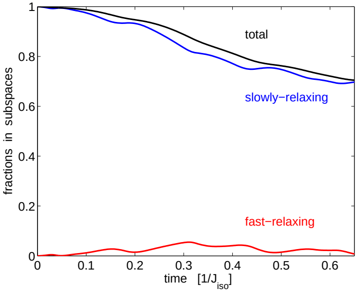
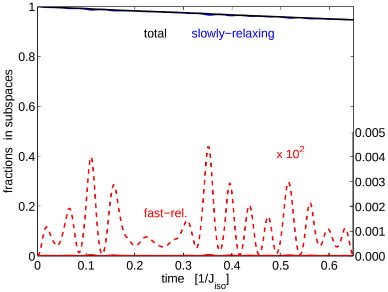


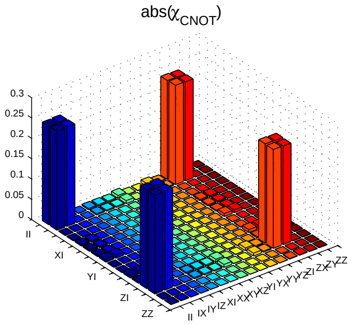


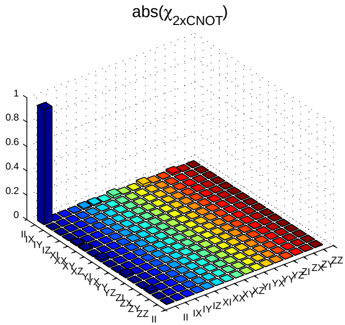
Examples of Quantum Control

3. Realising Quantum Gates with Minimal Relaxation

quant-ph/0609037

- CNOT under **System-II**: Process Tomography of Gate Protected against Dissipation by Optimal Control





quant-ph/0609037

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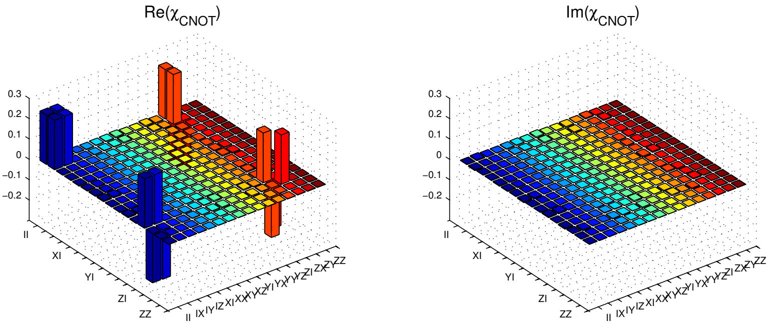
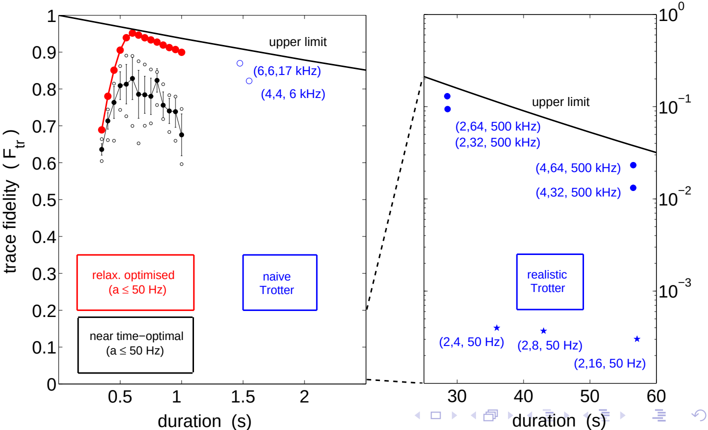


quant-ph/0609037

CNOT under **System-II**: comparison of methods

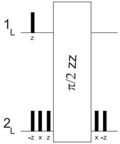
by decoherence control: $>$ 95% fideltity

conventional: $<$ 15% fidelity



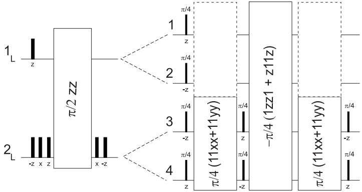
Decoherence-Protected CNOT-Gate via

- logical qubits



Decoherence-Protected CNOT-Gate via

- physical qubits

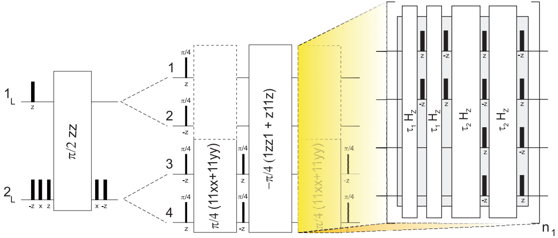


Alternative Decoherence Control

Paper and Pen Approach: TROTTER Expansion

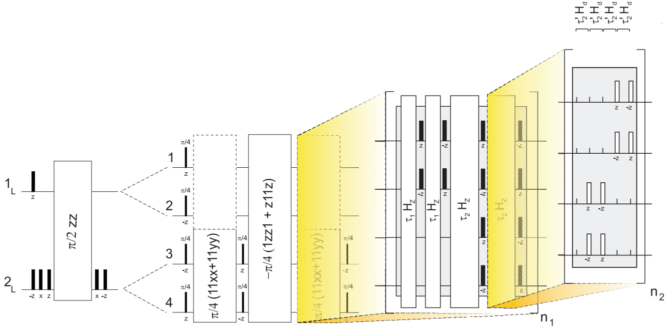
Decoherence-Protected CNOT-Gate via

- realisation by **System-I**



Decoherence-Protected CNOT-Gate via

- realisation by **System-II**



Which Tool in Which Setting?

1. *"anything goes"*: Paul FEYERABEND
   only in ideal case: decoherence-free,
   fully controllable and closed under drift

2. *Timeoptimal Control*:
   whenever slowly-relaxing subsystem controllable and closed under drift

3. *Relaxation-Optimised Control*:
   whenever slowly-relaxing subsystem open, where subsystem
   (i) controllable or
   (ii) to be extended for controllability

Decoherence Control: Take-Home Message

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Expectation value of observables $B = B^\dagger \in \mathcal{B}(\mathcal{H})$:

- pure quantum states:

$$\langle B \rangle := \langle \psi B | \psi \rangle$$

- ensembles:

$$\operatorname{tr}\left(B^\dagger \rho(t)\right) = \operatorname{tr}\left(B^\dagger\, U \rho_0 U^{-1}\right)$$

- C numerical range:
  generalisation to non-Hermitian operators

$$W(C, A) := \{\operatorname{tr}(C^\dagger\, UAU^{-1}) | U \in \mathcal{U}(\mathcal{H})\}$$

Significance of Numerical and C-Numerical Ranges

Generalising Expectation Values

Expectation value of observables $B = B^\dagger \in \mathcal{B}(\mathcal{H})$:

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$$\langle B \rangle := \langle \psi B | \psi \rangle$$

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generalisation to non-Hermitian operators

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Generalise from $B = B^\dagger$ to non-Hermitian operators:

- pure quantum states:

$$\langle B \rangle := \langle \psi B | \psi \rangle \quad \in \quad W(B) := \{\langle \phi B | \phi \rangle, \big| \|\phi\| = 1\}$$

- ensembles:

$$\operatorname{tr}\left(B^\dagger \rho(t)\right) = \operatorname{tr}\left(B^\dagger \; U \rho_0 U^{-1}\right)$$

- C numerical range:
  generalisation to non-Hermitian operators

$$W(C, A) := \{\operatorname{tr}(C^\dagger \; UAU^{-1}) | U \in \mathcal{U}(\mathcal{H})\}$$

Classical features of $W(A)$ and $W(C, A)$:

- $W(A)$ and $W(C, A)$ are *compact* and *connected*. GOLDBERG & STRAUSS 1977
- $W(A)$ is *convex*. HAUSDORFF 1919, TÖPLITZ 1918
- $W(C, A)$ is *star-shaped*. CHEUNG & TSING '96
- $W(C, A)$ is *convex* if C or A Hermitian. WESTWICK '75
- $W(C, A)$ is a *circular disk centered at the origin* if C or A are unitarily similar to block-shift form LI & TSING '91

Find points on unitary orbit of initial state A that enclose

- minimal Euclidean distance to target state C

$$\min_U \|C - UAU^{-1}\|_2^2 \quad \Leftrightarrow \quad \max_U \operatorname{Re}\operatorname{tr}\{C^\dagger\, UAU^{-1}\}$$

$\Leftrightarrow$ find max. real part of C num. range

- minimal angle to target state C

$$\max_U \cos^2_{A,C}(U) = \max_U \frac{|\operatorname{tr}\{C^\dagger UAU^{-1}\}|^2}{\|A\|_2^2 \cdot \|C\|_2^2}$$

$\Leftrightarrow$ find: C num. radius $r_C(A) = \max_U |\operatorname{tr}\{C^\dagger\, UAU^{-1}\}|$

pro memoria: $\|C - UAU^{-1}\|_2^2 = \|A\|_2^2 + \|C\|_2^2 - 2\operatorname{Re}\operatorname{tr}\{C^\dagger\, UAU^{-1}\}$

Significance of C-Numerical Radius
Geometric Optimisation Problems

Find points on unitary orbit of initial state A that enclose

- minimal Euclidean distance to target state C

$$\min_U ||C - UAU^{-1}||_2^2 \quad \Leftrightarrow \quad \max_U \operatorname{Re}\operatorname{tr}\{C^\dagger \; UAU^{-1}\}$$

$\Leftrightarrow$ find max. real part of C num. range

- minimal angle to target state C

$$\max_U \; \cos^2_{A,C}(U) = \max_U \frac{|\operatorname{tr}\{C^\dagger UAU^{-1}\}|^2}{||A||_2^2 \cdot ||C||_2^2}$$

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pro memoria: $||C - UAU^{-1}||_2^2 = ||A||_2^2 + ||C||_2^2 - 2\operatorname{Re}\operatorname{tr}\{C^\dagger \; UAU^{-1}\}$

Set $f(U) := \operatorname{Re}\operatorname{tr}\{C^\dagger UAU^\dagger\}$; write skew-herm. part: $[\cdot,\cdot]_S$

- calculate Fréchet derivative $Df(U)(\Omega U) = \langle [UAU^\dagger, C^\dagger]_S^\dagger U | \Omega U\rangle$
- identify $Df(U)(\Omega U) = \langle \operatorname{grad} f(U) | \Omega U\rangle$, where
- $\xi \in T_U SU(N)$ reads $\xi = \Omega U$ and $\Omega \in \mathfrak{su}(N)$;
- obtain gradient vector field $\operatorname{grad} f(U) = [UAU^\dagger, C^\dagger]_S^\dagger\, U$
- integrate gradient system $\dot{U} = \operatorname{grad} f(U)$ by
- discretisation scheme $U_{k+1} = e^{-\alpha_k [U_k A U_k^\dagger, C^\dagger]_S}\, U_k$

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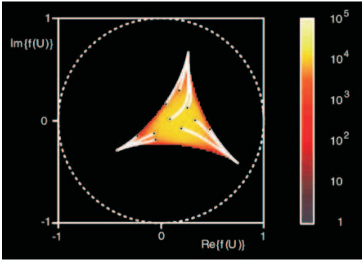
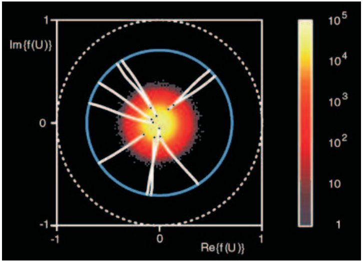
- find $r_C(A)$ by gradient flow on unitary group

$A, C \in \mathrm{Mat}_3(\mathbb{C})$



$A, C \in \mathrm{Mat}_8(\mathbb{C})$



Glaser, T.S.H., Sieveking, Schedletzky, Nielsen, Sørensen, Griesinger, *Science* **280** (1998), 421

Definition (math-ph/0701037 and math-ph/0702005)

The *local C-numerical range* is the set

$$W_{\text{loc}}(C, A) := \{\operatorname{tr}(C^\dagger U A U^\dagger) \mid U \in SU(2)^{\otimes n}\} \subseteq W_C(A),$$

where the unitary orbit is restricted to *local operations* $U =: K \in SU(2) \otimes SU(2) \otimes \cdots \otimes SU(2)$

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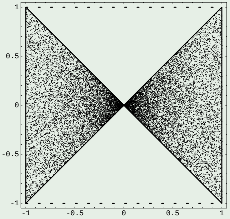
Example (I non convex)

$$A := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1+i & 0 \\ 0 & 1-i \end{pmatrix}$$

$$C := \mathrm{diag}\,(1,0,0,0)$$



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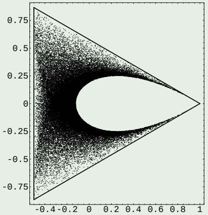
Example (II neither star-shaped nor simply connected)

$$A := \begin{pmatrix} 1 & 0 \\ 0 & e^{2i\pi/3} \end{pmatrix}^{\otimes 3}$$

$$C := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}^{\otimes 3}$$



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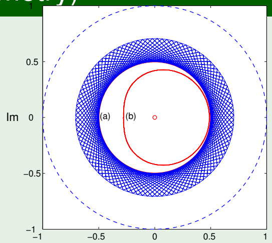
Example (III distinct circular symmetry)

$$A := \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$



Time-Reversal by Local Operations

Statement of the Problem

Question:

Which quantum evolutions are reversible by local unitary operations ?

- Problem: given a Hamiltonian H and a time $t > 0$, ? $\exists\, \{K_1, K_2\} \subset SU(2)^{\otimes n}$: $K_1\, e^{-itH}\, K_2 = e^{+itH}$
- Cases:
  1. $K_2 = K_1^{-1}$: local inversion for all $t \in \mathbb{R}$
  2. $K_2 \neq K_1^{-1}$: local inversion pointwise at some $\tau \in \mathbb{R}$
- Applications:
  - local refocussing quantum evolutions: Hahn's echo
  - Hamiltonian simulation

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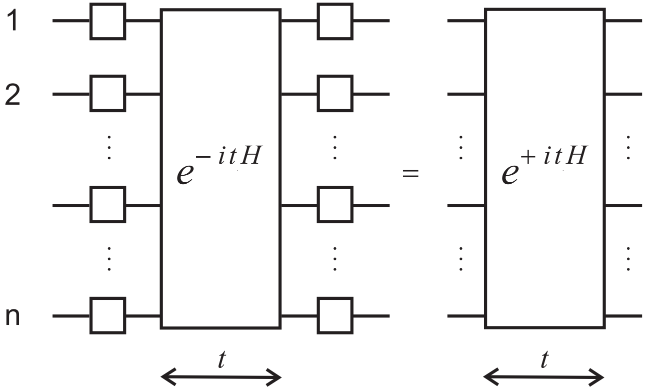

$$\text{Type-I}: \quad K \cdot U(t) \cdot K^{-1} = U(-t) = U(t)^{-1}$$

$$\text{Type-II}: \quad K_1 \cdot U(\tau) \cdot K_2 = U(-\tau) = U(\tau)^{-1}$$

- minimise $f(K) := \operatorname{tr}\{KHK^\dagger H\}$ over $K \in \mathbf{SU}(2)^{\otimes n}$
- gradient flow on *local* unitaries

$$\dot{K} = \operatorname{grad} f(K) = P_{\mathfrak{k}}([(KHK^{-1}), H])\, K$$
$$= -P_{\mathfrak{k}}\big(\operatorname{ad}_H \circ \operatorname{Ad}_K(H)\big)\, K\,,$$

$$K_{r+1} = e^{-\alpha_r P_{\mathfrak{k}}([(KHK^{-1}),H])} K_r$$

$P_{\mathfrak{k}}$: projection onto subalgebra $\mathfrak{k}$ of generators of local unitaries $\mathbf{K} = \mathbf{SU}(2)^{\otimes n}$.

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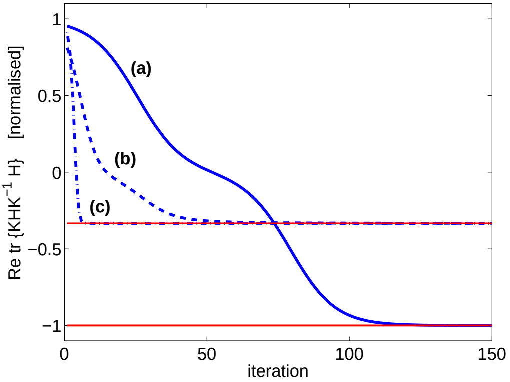
- Examples

  (a) ISING ZZ-interaction on cyclic graph C_4 (bipartite)

  (b) ISING ZZ-interaction on cyclic graph C_3 (not bipartite)

  (c) HEISENBERG XXX interaction (isotropic coupling)



Corollary (Relations I: Local C-Numerical Range)

For $H = H^\dagger$ with $\|H\|_2 = 1$ the following are equivalent:

1. *the Hamiltonian H is locally sign-reversible;*
2. *for its local C-numerical range $-1 \in W_{\text{loc}}(H, H)$;*
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$$W_{\text{loc}}(H, H) = [-1\,;\,+1];$$

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Corollary (Relations II: Lie algebras)

For $H = H^\dagger$ with $\|H\|_2 = 1$ the following are equivalent:

1. *the Hamiltonian H is locally sign-reversible;*
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3. *H is locally unitarily similar to a $\bar{H}$ with $\mathrm{Ad}_{K_z}(\bar{H}) = -\bar{H}$;*
4. *let $\mathfrak{g} = \mathfrak{g}_0 \oplus \bigoplus_{i \neq j} \mathbb{C}\, E_{ij}$ be the root-space decomposition of $\mathfrak{sl}(N, \mathbb{C})$; H is locally unitarily similar to a linear combination of root-space elements to non-zero roots $\bar{H} := \sum_{\lambda=1}^{m} c_\lambda E_{ij}^{(\lambda)}$ satisfying a system of linear equations $\sum_\ell p_{\lambda,\ell} \cdot \phi_\ell = \pi (\mathrm{mod}\, 2\pi)$*

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Theorem

Let $\mathbf{K}$ *be a compact connected subgroup of* $U(N)$ *with Lie algebra* $\mathfrak{k}$, *and let* $\mathfrak{t}$ *be a torus algebra of* $\mathfrak{k}$. *Then the relative* C*-numerical range* $W_{\mathbf{K}}(C, A_+)$ *of a matrix* $A_+ \in \text{Mat}_N(\mathbb{C})$ *is a circular disc centered at the origin of the complex plane for all* $C \in \text{Mat}_N(\mathbb{C})$ *if and only if there exists a* $K \in \mathbf{K}$ *and a* $\Delta \in \mathfrak{t}$ *such that* $KA_+K^\dagger$ *is an eigenoperator to* ad_Δ *with a non-zero eigenvalue*

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If $KA_+K^\dagger$ *is an eigenoperator of* ad_Δ *to eigenvalue* $+ip$ *and* $A_- := A_+^\dagger$, *then* $KA_-K^\dagger$ *shows the eigenvalue* $-ip$. A_+ *and* A_- *share the same relative* C*-numerical range of circular symmetry,* $W_{\mathbf{K}}(C, A_+) = W_{\mathbf{K}}(C, A_-)$.

Corollary

Let $\mathbf{K} = SU_{\text{loc}}(2^n)$ with A_+ and $A_- := A_+^\dagger$ sharing same circular-disc shaped $W_{\text{loc}}(C, A_\pm)$ for all C. Then

(1) *any $A_\lambda := A_+ + \lambda A_-$ with $\lambda \in \mathbb{C}$, e.g., $H := A_+ + A_-$ is locally sign reversible;*

(2) *the converse does not hold: there are locally reversible Hermitian H with no decomposition into a single pair $\{H_+, H_-\}$ sharing the same rotationally symmetric $W_{\text{loc}}(C, H_\pm)$;*

(3) *any locally sign reversible Hermitian $H \in \mathrm{Mat}_{2^n}(\mathbb{C})$ can be decomposed into at most $\binom{2^n}{2}$ pairs $(H_+^{(1)}, H_-^{(1)}), (H_+^{(2)}, H_-^{(2)}), \dots$ each with same rotationally symmetric $W_{\text{loc}}(C, H_\pm^{(\ell)})$.*

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Definition

The *constrained C-numerical range of A* is defined by

$$W(C,A)\big|_{\text{constraint}} := \{\operatorname{tr}(UAU^\dagger C^\dagger) \mid \text{constraint}\} \subseteq W(C,A)\,.$$

Example (I. Invariance)

Maximise transfer from A to C leaving E invariant:

$$\max_U |\operatorname{tr}\{UAU^\dagger C^\dagger\}| \quad \text{subject to} \quad UEU^\dagger = E$$

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Example (II. Orthogonality)

Maximise transfer A to C while suppressing A to D:

$$\max_U |\operatorname{tr}\{UAU^\dagger C^\dagger\}| \quad \text{subject to} \quad \operatorname{tr}\{UAU^\dagger D^\dagger\} = m_0$$

with $m_0 \in W(D,A)$ unique point in $W(D,A)$ closest to 0.
Perfect match: $0 \in W(D,A) \Leftrightarrow \mathcal{O}_u(A) \cap \mathcal{H}_{D^\perp} \neq \{\}$

Corollary

The constrained C-numerical range is a connected set in the complex plane, if the constraint can be fulfilled by restricting the full unitary group $U(N)$ to a compact and connected subgroup $\mathbf{K} \subseteq U(N)$. Then

1. *constrained and relative C-numerical range coincide*

$$W(C, A)|_{\text{constraint}} = W_{\mathbf{K}}(C, A)$$

2. *optimisation problem solved within $W_{\mathbf{K}}(C, A)$, e.g. by relative C-numerical radius $r_{\mathbf{K}}(C, A)$*

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is straightforward: the stabiliser group

$$\mathbf{K}_E := \{K \in U(N) \,|\, KEK^\dagger = E\}$$

is generated by

$$\mathfrak{k}_E := \{k \in \mathfrak{u}(N) \,|\, \operatorname{ad}_k(E) \equiv [k, E] = 0\} \quad .$$

Lemma (Example I: Invariance)

1. *The set $\mathfrak{k}_E$ is closed under the Lie bracket, hence it is a subalgebra to $\mathfrak{u}(N)$ thus generating the stabiliser group $\mathbf{K}_E \subseteq U(N)$.*
2. *$\mathfrak{k}_E$ satisfies a homogeneous linear system:*

$$\mathfrak{k}_E = \ker \mathrm{ad}_E \cap \mathfrak{su}(N)$$
$$= \{k \in \mathfrak{su}(N) | (\mathbb{1} \otimes E - E^t \otimes \mathbb{1}) \operatorname{vec}(k) = 0\}.$$

3. *Constrained and relative C numerical range coincide: $W(C, A)\big|_{\mathrm{Ad}_U(E)=E} = W_{\mathbf{K}_E}(C, A)$.*
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Algorithm: Gradient Flow with Lagrange Constraint

1. Define Lagrange function (with $f_C(U) : \mathrm{tr}\{C^\dagger UAU^\dagger\}$):

$$L(U) := |f_C(U)|^2 - \lambda \left(\mathrm{tr}\{UEU^\dagger E^\dagger\} - ||E||_2^2\right)$$

2. Fréchet derivative (with $(\cdot)_S$ as skew-Hermitian part):

$$D\left\{|f_C(U)|^2 - \lambda f_E(U) + \lambda \, \|E\|_2^2\right\}(iHU)$$

$$= \mathrm{tr}\left\{ \left(2\left(f_C^*(U)[UAU^\dagger, C^\dagger]\right)_S - \lambda[UEU^\dagger, E^\dagger]\right) iH\right\}$$

3. Recursive scheme:

$$U_{k+1} = e^{-\alpha\left(2\left(f_C^*(U_k)[U_kAU_k^\dagger, C^\dagger]\right)_S - \lambda[U_kEU_k^\dagger, E^\dagger]\right)} U_k$$

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Maximising transfer from A to C while suppressing A to D

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is more complicated: the constrained set

$$\tilde{K}_D := \{K \subseteq SU(N) \,|\, \operatorname{tr}\{KAK^\dagger D^\dagger\} = m_0\}$$

is in general no subgroup $\mathbf{K}_D$.
Thus the generic constrained C-numerical range

$$W(C,A)\big|_{\mathrm{Ad}_U \perp D} = m_0 \subseteq W(C,A)$$

will not be connected.

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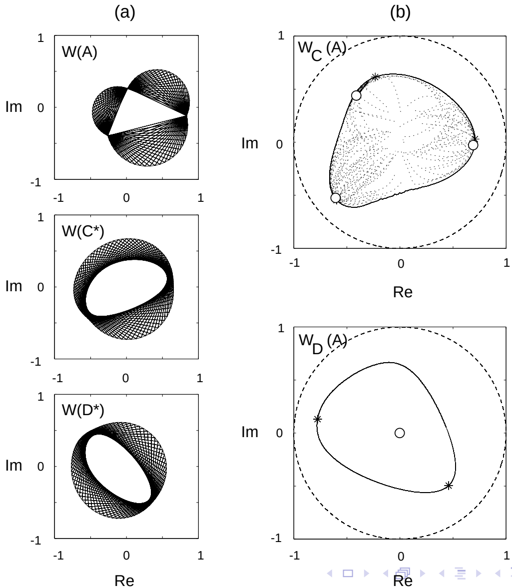
Example (II. Orthogonality)

Maximise transfer from A to C and suppress A to D for

$$A = \begin{pmatrix} 0.8359-0.1152i & 0 & 0 \\ 0 & -0.2593-0.3906i & 0 \\ 0 & 0 & 0.0151+0.2609i \end{pmatrix}$$

$$C = \begin{pmatrix} -0.0318+0.0690i & -0.3522-0.3185i & 0.2351-0.3050i \\ -0.0404+0.0656i & 0.0844-0.2880i & 0.2135+0.3234i \\ 0.3086+0.1076i & 0.1742-0.2291i & -0.2368+0.3585i \end{pmatrix}$$

$$D = \begin{pmatrix} -0.2910-0.3480i & -0.2395+0.0274i & -0.2428+0.0656i \\ 0.0836-0.2790i & -0.1836-0.0203i & -0.2427+0.2396i \\ -0.3906-0.1387i & 0.1989-0.2725i & -0.0442+0.3871i \end{pmatrix}$$



(a)
(b)
W(A)
W(C*)
W(D*)
W
C
(A)
W
D
(A)
Im
Re
1
0
-1

- Maximising real part in $W_{\rm loc}(C,A)$ minimises distance from C to *local unitary orbit* of A

$$\max_{K \in SU(2)^{\otimes n}} \operatorname{Re} \operatorname{tr}\{C^\dagger KAK^{-1}\} \Leftrightarrow \min_{K \in SU(2)^{\otimes n}} ||KAK^{-1} - C||_2$$

- Application to Quantum Information Theory: let A be a given rank-1 state of the form $A = |\psi\rangle\langle\psi|$ and $C = \operatorname{diag}(1,0)^{\otimes n}$ [thus $W_{\rm loc}(C,A) \to W_{\rm loc}(A)$]

Corollary (Interpretation)

The minimial Euclidean distance is a measure of (pure-state) entanglement; i.e. it quantifies how far A is from the local equivalence class of the tensor-product state C.

- Maximising real part in $W_{\text{loc}}(C, A)$ minimises distance from C to *local unitary orbit* of A

$$\max_{K \in SU(2)^{\otimes n}} \operatorname{Re} \operatorname{tr}\{C^\dagger KAK^{-1}\} \Leftrightarrow \min_{K \in SU(2)^{\otimes n}} \|KAK^{-1} - C\|_2$$

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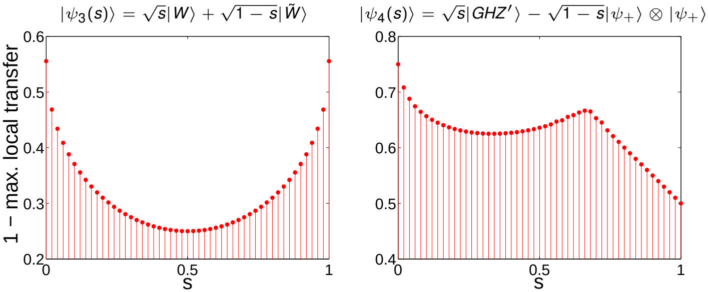
- Examples:
  pure-state entanglement parameterised by s



- CPU times: local gradient flows *very fast* as compared to global techniques
- Example 1: distance to 3-qubit W-type states
- Example 2: distance to 4-qubit GHZ-type states

qubits	semidefinite prog. cpu-time [sec][1]	by gradient flow cpu-time [sec][2]	speed-up
3	10.92	0.30	36.4
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[1] Eisert *et al.* (processor with 2.2 GHz, 1 GB RAM)
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Relation to SVD

- observe: singular-value decomposition (SVD) for $X, Y \in \mathbb{C}^{N_1 \times N_2}$: $V_{X,Y} \in U(N_1)$, $W_{X,Y} \in U(N_2)$

$$\begin{aligned}
\Sigma_X &= V_X X W_X \\
\operatorname{vec} \Sigma_X &= (W_X^t \otimes V_X) \operatorname{vec} X \\
|\Sigma_X\rangle &= (W_X^t \otimes V_X)|x\rangle \\
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- maximisation

$$\max_{V,W} \operatorname{tr}\{|Y\rangle\langle Y|(W^t \otimes V)|X\rangle\langle X|(W^* \otimes V^\dagger)\}$$
$$= \operatorname{tr}\{|\Sigma_X\rangle\langle\Sigma_X| \cdot |\Sigma_Y\rangle\langle\Sigma_Y|\} = |\langle\Sigma_X|\Sigma_Y\rangle|^2$$

- this proves the following Theorem:

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Theorem

For $X, Y \in \mathbb{C}^{N_1 \times N_2}$ let $X = V_X^\dagger \Sigma_X W_X^\dagger$, $Y = V_Y^\dagger \Sigma_Y W_Y^\dagger$ be their singular value decompositions with $V_X, V_Y \in U(N_1)$, $W_X, W_Y \in U(N_2)$ and Σ_X, Σ_Y sorted by magnitude. Moreover, set $|x\rangle := \operatorname{vec} X$ and $|y\rangle := \operatorname{vec} Y$. Then the maximum local transfer between $|x\rangle\langle x|$ and $|y\rangle\langle y|$ is

$$\max_{U \in SU(N_2) \otimes SU(N_1)} \operatorname{tr}\{|x\rangle\langle x| U |y\rangle\langle y| U^\dagger)\} = \left(\operatorname{tr}\{\Sigma_X^\dagger \Sigma_Y\}\right)^2.$$

Equality is actually achieved with $V_X, V_Y \in SU(N_1)$ and $W_X, W_Y \in SU(N_2)$ in $U := (W_X^* \otimes V_X^\dagger) \cdot (W_Y^t \otimes V_Y)$.

Corollary (Bipartite Pure-State Entanglement)

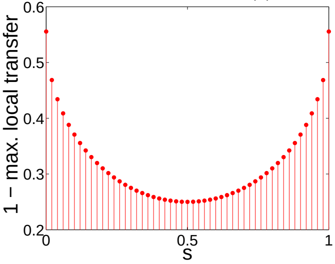
The minimum Euclidean distance of an arbitrary bipartite pure state $|x\rangle\langle x|$ *to the local unitary orbit of* $|y\rangle\langle y| = \operatorname{diag}(1, 0, 0, \ldots, 0)$, *i.e. the nearest separable pure state, is determined by the largest singular value in* $\Sigma_X = VXW$ *with* $|x\rangle := \operatorname{vec} X$.

Corollary (Multipartite Pure-State Entanglement)

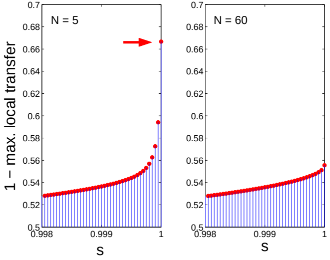
The minimum Euclidean distance of an arbitrary multipartite pure state $\sum_k \lambda_k (x_1 x_2 \circ x_n)$ to the nearest separable pure state $y_1 y_2 \circ y_n$ is determined by the largest singular value in Σ_X derived from the best rank-1 approximation to $\sum_k \lambda_k (x_1 x_2 \circ x_n)$ seen as higher-order tensor.

- **3-Qubit Example:**
  $|\psi_3(s)\rangle = \sqrt{s}|W\rangle + \sqrt{1-s}|\tilde{W}\rangle$

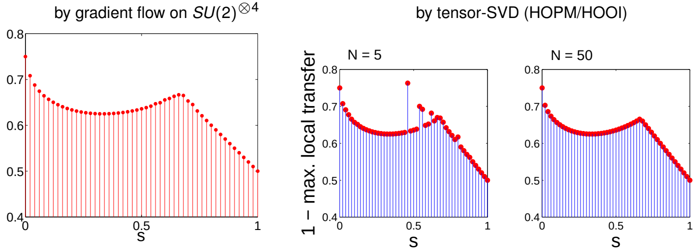
by gradient flow on $SU(2)^{\otimes 3}$



by tensor-SVD (HOPM/HOOI)



- 4-Qubit Example:
$$|\psi_4(s)\rangle = \sqrt{s}|GHZ'\rangle - \sqrt{1-s}|\psi_+\rangle \otimes |\psi_+\rangle$$



Applications: Grad. Flows vs Tensor SVD

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- Example 2: distance to 4-qubit GHZ-type states

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qubits	tensor-SVD (HOPM) cpu-time [sec][2]	tensor-SVD (HOOI) cpu-time [sec][2]	speed-ups
3	2.39	5.37	4.6 (2.0)
4	3.93	7.03	26.5 (14.8)

1 Eisert *et al.* (processor with 2.2 GHz, 1 GB RAM)
2 average of 50 runs, Athlon XP1800+ (1.1 GHz, 512 MB RAM)

Conclusions

1. Gradient Flows on Riem. Manifolds & Lie Groups
   - powerful tool for optimisation and control
2. Quantum Control: key in future technology
   - offers also rewarding theoretical challenges
3. Quantum CISC Compiler: use of parallel cluster
   - extend modules beyond 1 and 2-qubit interactions
4. Optimal Control of Open Quantum Systems
   - dressed to physical hardware
   - generalises decoherence-free subspace
5. Constrained Optimisation
   - local time reversal
   - tensor SVD for pure-state entanglement
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