Efficient Control Algorithms for Unitary Transformations: The Cartan Decomposition and Beyond

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Outline

Quantum systems and their transformations

(pure) quantum states (= vectors in $\mathbb{C}^m$, $m < \infty$)

- example: qubit (=quantum bit) is an element of $\mathbb{C}^2$ ($\to$ Bloch sphere)
- combined quantum system: tensor product $\mathbb{C}^{m_1} \otimes \cdots \otimes \mathbb{C}^{m_n}$
  - space of all $\mathbb{Z}$-linear comb. of $v_1 \otimes \cdots \otimes v_n$ ($v_j \in \mathbb{C}^{m_j}$, $\otimes$ bilinear)
  - example: two qubits as given by $\mathbb{C}^2 \otimes \mathbb{C}^2$

quantum operations = unitary transformations $U \in \mathrm{SU}(d)$

- Lie group $\mathrm{SU}(d) = \{ G \in \mathrm{GL}(d,\mathbb{C}) |\, G^{-1} = (G^*)^T,\ \det(G) = 1\}$ (= closed linear matrix group)
- Lie algebra $\mathfrak{su}(d) = \{ g \in \mathfrak{gl}(d,\mathbb{C}) |\, -g = (g^*)^T,\ \mathrm{Tr}(g) = 0\}$
  - tangent space to $\mathrm{SU}(d)$ at the identity
  - vector space with bilinear and skew-symmetric multiplication $[g_1, g_2] := g_1 g_2 - g_2 g_1$ where $[g_1, g_2] \in \mathfrak{su}(d)$ and $[[g_1, g_2], g_3] + [[g_3, g_1], g_2] + [[g_2, g_3], g_1] = 0$ (Jacobi identity)

Quantum computing as a control problem (1/2)

Schrödinger equation as a continuous model for quantum computing

$\frac{d}{dt}\,U(t) = [-iH(t)]\,U(t)$, where $H(t) = H_0 + \sum_{j=1}^{m} v_j(t) H_j$

- unitary transformation $U(t) \in \mathrm{SU}(d)$ (= algorithm)
- system Hamilton operator $H(t)$, where $iH(t) \in \mathfrak{su}(d)$
- control functions $v_j(t)$

(for this talk) **NOT** interested in:

- pure state transformations:
  $\frac{d}{dt}\,|\Psi(t)\rangle = [-iH(t)]\,|\Psi(t)\rangle$, where $|\Psi(t)\rangle$ is a pure state
- numerical computations and decoherence (and similar effects)

- in the last part we briefly consider:
  $\frac{d}{dt}\,\rho = [-iH(t), \rho]$, where ρ is a mixed state

Quantum computing as a control problem (2/2)

Schrödinger equation as a continuous model for quantum computing

$\frac{d}{dt}U(t) = [-iH(t)]\,U(t)$, where $H(t) = H_0 + \sum_{j=1}^{m} v_j(t)H_j$

- unitary transformation $U(t) \in \mathrm{SU}(d)$ (= algorithm)
- system Hamilton operator $H(t)$, where $iH(t) \in \mathfrak{su}(d)$
- control functions $v_j(t)$

- find efficient control algorithms to synthesize unitary transformations (efficient = short evolution time)

controllability (= universality), i.e., all $U \in \mathrm{SU}(d)$ can be obtained

necessary and sufficient condition: $iH_0, iH_1, \ldots, iH_m$ generate $\mathfrak{su}(d)$ (Brockett (1972,1973), Jurdjevic and Sussmann (1972))

Outline

Simulation of unitary transformations

resources (realistic for nuclear spins in nuclear magnetic resonance)

- **instantaneous** operations $U_j \in \mathrm{SU}(2)^{\otimes n} = \mathrm{SU}(2) \otimes \cdots \otimes \mathrm{SU}(2)$
- time-evolution w.r.t. a coupling Hamilton operator H ($-iH \in \mathfrak{su}(2^n)$)

efficient control algorithm for $U \in \mathrm{SU}(2^n)$ with evolution time t

- $U = \left[\prod_{k=1}^{m} \left(U_k \exp(-iHt_k) U_k{}^{-1}\right)\right] U_0$ and $t = \sum_{k=1}^{m} t_k \qquad (t_k \geq 0)$
- Lie group variant: conjugate the orbit $\exp(-iHt_k)$ with instantaneous operations $U_k \in \mathrm{SU}(2)^{\otimes n}$ $\Rightarrow$ piecewise change of the time evolution

Lie algebra variant: simulate $H' = \sum_{k=1}^{m} t_k (U_k H U_k{}^{-1})$

- $iH' \in \mathfrak{su}(2^n)$ and time $t = \sum_{k=1}^{m} t_k$ $(t_k \geq 0)$
- linearized version (first order): $\log(U U_0{}^{-1}) = -i \sum_{k=1}^{m} t_k (U_k H U_k{}^{-1})$
- often easier to solve

Two qubits: Mathematical structure (1/5)

Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$

- condition: $[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}$, $[\mathfrak{k}, \mathfrak{p}] \subset \mathfrak{p}$, $[\mathfrak{p}, \mathfrak{p}] \subset \mathfrak{k}$
- $\mathfrak{k}$ Lie algebra, $\mathfrak{K}$ its Lie group; **but** $\mathfrak{p}$ only a subspace

example: $\mathfrak{G} = \mathrm{SU}(4)$ and $\mathfrak{g} = \mathfrak{su}(4)$

- $\mathfrak{K} = \mathrm{SU}(2) \otimes \mathrm{SU}(2) = \exp(\mathfrak{k})$ where
  $\mathfrak{k} = \mathrm{span}_{\mathbb{R}}\{\mathrm{XI}, \mathrm{YI}, \mathrm{ZI}, \mathrm{IX}, \mathrm{IY}, \mathrm{IZ}\}$
- subspace $\mathfrak{p} = \mathrm{span}_{\mathbb{R}}\{\mathrm{XX}, \mathrm{XY}, \mathrm{XZ}, \mathrm{YX}, \mathrm{YY}, \mathrm{YZ}, \mathrm{ZX}, \mathrm{ZY}, \mathrm{ZZ}\}$

notation: e.g. $\mathrm{XI} = i(\mathrm{X} \otimes \mathrm{I})/2$
where $\mathrm{X} := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\mathrm{Y} := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\mathrm{Z} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\mathrm{I} := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Two qubits: Mathematical structure (2/5)

control algorithms and the Weyl orbit

- $U = \left[\prod_{k=1}^{m} \left(U_k \exp(-iHt_k) U_k{}^{-1}\right)\right] U_0$ and $t = \sum_{k=1}^{m} t_k \qquad (t_k \geq 0)$
- Weyl orbit $\mathcal{W}(p) = \{K p K^{-1}\colon\ K \in \mathfrak{K}\} \cap \mathfrak{a}$ of $p \in \mathfrak{p}$
- max. Abelian subalgebra $\mathfrak{a} \subset \mathfrak{p}$ and $\mathfrak{p} = \bigcup_{K\in\mathfrak{K}} K \mathfrak{a} K^{-1}$

example: $\mathfrak{k} \oplus \mathfrak{p} = \mathfrak{su}(4)$ $\qquad ([\mathfrak{k},\mathfrak{k}] \subset \mathfrak{k},\ [\mathfrak{k},\mathfrak{p}] \subset \mathfrak{p},\ [\mathfrak{p},\mathfrak{p}] \subset \mathfrak{k})$

- $\mathfrak{k} = \mathrm{span}_{\mathbb{R}}\{\mathrm{XI}, \mathrm{YI}, \mathrm{ZI}, \mathrm{IX}, \mathrm{IY}, \mathrm{IZ}\}$
- subspace $\mathfrak{p} = \mathrm{span}_{\mathbb{R}}\{\mathrm{XX}, \mathrm{XY}, \mathrm{XZ}, \mathrm{YX}, \mathrm{YY}, \mathrm{YZ}, \mathrm{ZX}, \mathrm{ZY}, \mathrm{ZZ}\}$
- max. Abelian subalgebra $\mathfrak{a} = \{a_1\mathrm{XX} + a_2\mathrm{YY} + a_3\mathrm{ZZ}\colon\ a_j \in \mathbb{R}\} \subset \mathfrak{p}$
- $\mathcal{W}[b_1\mathrm{XX} + b_2\mathrm{YY} + b_3\mathrm{ZZ}] = \mathcal{W}[(b_1, b_2, b_3)] = \{(b_1, b_2, b_3),$ $(-b_1, -b_2, b_3), (-b_1, b_2, -b_3), (b_1, -b_2, -b_3),$ and all permutations$\}$
- Weyl group $\mathcal{W}$ = symmetric group S_4 $\qquad (|\mathcal{W}| = 24)$

Two qubits: Mathematical structure (3/5)

Weyl orbit $\mathcal{W}(p) = \{KpK^{-1}\colon\ K \in \mathfrak{K}\} \cap \mathfrak{a}$ of $p \in \mathfrak{p}$

- max. Abelian subalgebra $\mathfrak{a} = \{a_1\mathrm{XX} + a_2\mathrm{YY} + a_3\mathrm{ZZ}\colon a_j \in \mathbb{R}\} \subset \mathfrak{p}$
- $\mathcal{W}[b_1\mathrm{XX} + b_2\mathrm{YY} + b_3\mathrm{ZZ}] = \mathcal{W}[(b_1, b_2, b_3)] = \{(b_1, b_2, b_3),$ $(-b_1, -b_2, b_3), (-b_1, b_2, -b_3), (b_1, -b_2, -b_3),$ and all permutations$\}$

Kostant's convexity theorem (1973)

- $\Gamma_{\mathfrak{a}}[\{KpK^{-1}\colon\ K \in \mathfrak{K}\}] =$ convex closure of $\mathcal{W}(p)$
  $\Gamma_{\mathfrak{a}} =$ orthogonal projection to $\mathfrak{a}$ (w.r.t. a natural scalar product on $\mathfrak{g}$)
- idea: What is with $\{KpK^{-1}\colon\ K \in \mathfrak{K}\}$?
  orthogonal projection to $\mathfrak{a}$ = convex closure of the intersection with $\mathfrak{a}$

Two qubits: Mathematical structure (4/5)

Weyl orbit $\mathcal{W}(p) = \{KpK^{-1} \colon K \in \mathfrak{K}\} \cap \mathfrak{a}$ of $p \in \mathfrak{p}$

- max. Abelian subalgebra $\mathfrak{a} = \{a_1 \mathrm{XX} + a_2 \mathrm{YY} + a_3 \mathrm{ZZ} \colon a_j \in \mathbb{R}\} \subset \mathfrak{p}$
- $\mathcal{W}[b_1 \mathrm{XX} + b_2 \mathrm{YY} + b_3 \mathrm{ZZ}] = \mathcal{W}[(b_1, b_2, b_3)] = \{(b_1, b_2, b_3),$ $(-b_1, -b_2, b_3), (-b_1, b_2, -b_3), (b_1, -b_2, -b_3),$ and all permutations$\}$

majorization condition [after Bennett et al. (2002)]

- assume that $|a_1| \geq |a_2| \geq |a_3|$ and $|b_1| \geq |b_2| \geq |b_3|$
- $\tilde{a}_1 := |a_1|$, $\tilde{a}_2 := |a_2|$, $\tilde{a}_3 := \mathrm{sgn}(a_1 a_2 a_3)|a_3|$
- (a_1, a_2, a_3) is in the convex closure of $\mathcal{W}[(b_1, b_2, b_3)]$ iff $\tilde{a}_1 \leq \tilde{b}_1$, $\tilde{a}_1 + \tilde{a}_2 + \tilde{a}_3 \leq \tilde{b}_1 + \tilde{b}_2 + \tilde{b}_3$, and $\tilde{a}_1 + \tilde{a}_2 - \tilde{a}_3 \leq \tilde{b}_1 + \tilde{b}_2 - \tilde{b}_3$
- Zeier/Grassl/Beth (2004) [see also Yuan/Khaneja (2005 and 2006)] proved the connection to the convex closure of the Weyl orbit

Two qubits: Mathematical structure (5/5)

$\mathfrak{K}\mathfrak{A}\mathfrak{K}$ decomposition ($\mathfrak{A} = \exp(\mathfrak{a})$)

- max. Abelian subalgebra $\mathfrak{a} = \{a_1\mathrm{XX} + a_2\mathrm{YY} + a_3\mathrm{ZZ} \colon a_j \in \mathbb{R}\} \subset \mathfrak{p}$
- $G = K_1 \exp(a_1\mathrm{XX} + a_2\mathrm{YY} + a_3\mathrm{ZZ})K_2 \in \mathfrak{G}$ ($K_j \in \mathfrak{K}$)

remark: $\mathfrak{K}\mathfrak{A}\mathfrak{K}$ decomposition is not unique

- Vidal/Hammerer/Cirac (2002): sufficient to consider all $(a_1, a_2, a_3) + \pi(z_1, z_2, z_3)$ where $z_j \in \mathbb{Z}$
- Vidal/Hammerer/Cirac (2002): $a_j \in [-\pi/2, \pi/2]$ $\Rightarrow$ (to find the optimal control) it is sufficient to consider only $(z_1, z_2, z_3) = (0, 0, 0)$ and $(z_1, z_2, z_3) = (-1, 0, 0)$
- Zeier/Grassl/Beth (2004) [see also Dirr et al. (2006)] proved the connection to the nonuniqueness of the $\mathfrak{K}\mathfrak{A}\mathfrak{K}$ decomposition

Two qubits: results (H = coupling Hamilton operator)

gate simulation [Khaneja/Brockett/Glaser (2001)]

One can simulate U in time t iff $U = K_1 \exp(tW) K_2$ such that $W \in \mathrm{conv}(\mathcal{W}(iH))$, where $K_j \in \mathfrak{K} = \mathrm{SU}(2) \otimes \mathrm{SU}(2)$.

Hamiltonian simulation [Bennett et al. (2002), this formulation by Zeier/Grassl/Beth (2004)]

One can simulate H' in time t iff $K_1(iH'/t){K_1}^{-1} \in \mathrm{conv}\,(\mathcal{W}(iH))$ for some $K_1 \in \mathfrak{K} = \mathrm{SU}(2) \otimes \mathrm{SU}(2)$.

remark [Zeier/Grassl/Beth (2004)]

Bennett et al. (2002) is a special case of Khaneja/Brockett/Glaser (2001)

Two qubits: comments (1/3)

gate simulation [Khaneja/Brockett/Glaser (2001)] (H = Hamiltonian)

One can simulate U in time t iff $U = K_1 \exp(tW) K_2$ such that $W \in \mathrm{conv}(\mathcal{W}(iH))$, where $K_j \in \mathfrak{K} = \mathrm{SU}(2) \otimes \mathrm{SU}(2)$.

comments

- control problem is reduced to convex optimization (via Kostant) which can be solved analytically
- $U_k \exp(-iHt_k) U_k{}^{-1}$ (can be made to) commute with each other in $U = \left[\prod_{k=1}^{m} \left(U_k \exp(-iHt_k) U_k{}^{-1}\right)\right] U_0$ and $t = \sum_{k=1}^{m} t_k \qquad (t_k \geq 0)$
- idea: $\exp(t_1 p_1) \exp(t_2 p_2) = \exp(t_1 p_1 + t_2 p_2 + t_1 t_2 [p_1, p_2]/2 + \cdots)$ remember: $p_1, p_2 \in \mathfrak{p} \Rightarrow [p_1, p_2] \subset \mathfrak{k} \Rightarrow$ new direction lies in fast $\mathfrak{k}$

Two qubits: comments (2/3)

further properties of $\mathfrak{p}$ ($\mathfrak{k} \oplus \mathfrak{p} = \mathfrak{su}(4)$, $[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}$, $[\mathfrak{k}, \mathfrak{p}] \subset \mathfrak{p}$, $[\mathfrak{p}, \mathfrak{p}] \subset \mathfrak{k}$)

- $\mathfrak{p}$ is irreducible under the action of $\mathfrak{K}$ by conjugation
- $K\,p\,K^{-1} = \tilde{p} \Leftrightarrow Gp\,G^{-1} = \tilde{p}$ $\quad (p, \tilde{p} \in \mathfrak{p}, G \in \mathfrak{G}, K \in \mathfrak{K})$
  $\Leftrightarrow$ characteristic polynomials of p and $\tilde{p}$ are equal

$\Rightarrow$ three (real) invariants of $p, \tilde{p}$ under conjugation (as $\mathrm{Tr}(p) = \mathrm{Tr}(\tilde{p}) = 0$)

- cp. Makhlin (2002): three (real) invariants for two-qubit operations under local equivalence

- related to Zhang/Vala/Sastry/Whaley (2003): detailed characterization of non-local operations in two-qubit systems

Two qubits: comments (3/3)

gate simulation [Khaneja/Brockett/Glaser (2001)] (H = Hamiltonian)

One can simulate U in time t iff $U = K_1 \exp(tW) K_2$ such that $W \in \mathrm{conv}(\mathcal{W}(iH))$, where $K_j \in \mathfrak{K} = \mathrm{SU}(2) \otimes \mathrm{SU}(2)$.

(incomplete) list of proofs

original proof in Khaneja/Brockett/Glaser (2001),
Vidal/Hammerer/Cirac (2002), more general case in Yuan/Khaneja (2005)

- Childs/Haselgrove/Nielsen (2003): proof of the lower bound relying on majorization conditions on the spectra of $U(Y \otimes Y)U^T(Y \otimes Y)$
- uses Thompson's theorem:
  A, B hermitian than exists A', B' such that $\mathrm{spec}\,(A') = \mathrm{spec}\,(A)$, $\mathrm{spec}\,(B') = \mathrm{spec}\,(B)$, and $\exp(iA)\exp(iB) = \exp(iA' + iB')$

Beyond two qubits

approach for choosing a Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$

- for two qubits: $\mathfrak{k}$ = local part, $\mathfrak{p}$ = non-local part
- n qubits ($n > 2$): local operations $\subsetneq \mathfrak{K}$ (e.g., $\mathrm{SU}(2)^{\otimes n} \subsetneq \mathfrak{K}$)

lower bounds on the evolution time

- assume that all elements of $\mathfrak{K}$ can be applied instantaneously, and not only the elements of $\mathrm{SU}(2)^{\otimes n}$ $\Rightarrow$ we get the evolution time
- $\mathrm{SU}(2)^{\otimes n} \subseteq \mathfrak{K} \Rightarrow$ the evolution time can only be greater

determine suitable $\mathfrak{K}$ [Childs et al. (2003), Zeier/Grassl/Beth (2004)]

- n even: $\mathfrak{K}$ is conjugated to the orthogonal group $\mathrm{O}(2^n)$
- n odd: $\mathfrak{K}$ is conjugated to the (unitary) symplectic group $\mathrm{Sp}(2^{n-1}) = \{U \in \mathrm{U}(2^n) | \, U^T J_{n/2} U = J_{n/2}\}$, where $J_k = \begin{pmatrix} 0_k & I_k \\ -I_k & 0_k \end{pmatrix}$

Algebraic structure analysis for multi-qubit systems

Cartan decomposition $\mathfrak{g} = \mathfrak{l} \oplus \mathfrak{p}$ and symmetric spaces $\mathfrak{G}/\mathfrak{L}$

The Cartan decomposition induces a symmetric space:
n even: $\mathrm{SU}(2^n)/\mathrm{SO}(2^n)$, n odd: $\mathrm{SU}(2^n)/\mathrm{Sp}(2^{n-1})$

general case of $\mathfrak{G}/\mathfrak{L} = \mathrm{SU}(2^n)/\mathrm{SU}(2)^{\otimes n}$ and $\mathfrak{l} =$ Lie algebra$(\mathfrak{L})$

$\mathfrak{g} = \mathfrak{l} \oplus \mathfrak{m}$, where $[\mathfrak{l}, \mathfrak{l}] \subset \mathfrak{l}$ and $[\mathfrak{l}, \mathfrak{m}] \subset \mathfrak{m}$ (but not $[\mathfrak{m}, \mathfrak{m}] \subset \mathfrak{l}$ for $n > 2$)
$\Rightarrow$ no Cartan decomposition

de Rham cohomology of $\mathfrak{G}/\mathfrak{L} = \mathrm{SU}(2^n)/\mathrm{SU}(2)^{\otimes n}$

- antisymmetric invariant
  [in contrast to a symmetric (i.e., polynomial) invariant]
- computed for $n = 2, 3$ [Zeier (2006)]
- potential connections to the structure of entanglement

Outline

Our model: coupled fast and slow qubit system (1/2)

the physical system (high field case, in a double rotating frame)

- free evolution w.r.t. the Hamiltonian $H_0 = J I_z + J(2 S_z I_z)$
- control Hamiltonian on the first qubit (= electron spin): $H_S = \Omega^S(t)[S_x \cos\phi_S(t) + S_y \sin\phi_S(t)]$
- control Hamiltonian on the second qubit (= nuclear spin): $H_I = \Omega^I(t)[I_x \cos\phi_I(t) + I_y \sin\phi_I(t)]$
- time scales $\Omega^I \ll J \ll \Omega^S$ (H_0 faster than some local operations!)
- first qubit = fast qubit and second qubit = slow qubit

notation: $S_\mu = (\sigma_\mu \otimes \mathrm{id}_2)/2$ and $I_\nu = (\mathrm{id}_2 \otimes \sigma_\nu)/2$ $(\mu, \nu \in \{x, y, z\})$
where $\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\mathrm{id}_2 := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Our model: coupled fast and slow qubit system (2/2)

how to synthesize slow transformations (first order approximation)

$H_0 + H_I = 2JS^\beta I_z + \Omega^I(t)(S^\alpha + S^\beta)(I_x \cos\phi_I + I_y \sin\phi_I)$ truncates to

$$H^\alpha(\phi_I) = 2JS^\beta I_z + \Omega^I(t) S^\alpha (I_x \cos\phi_I + I_y \sin\phi_I)$$

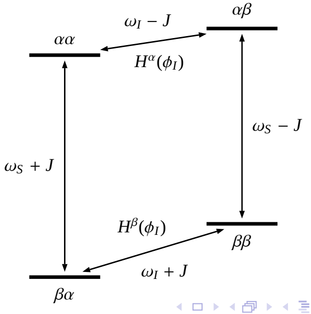
where $S^\beta = (\mathrm{id}_4/2 + S_z) = \begin{pmatrix} \mathrm{id}_2 & 0_2 \\ 0_2 & 0_2 \end{pmatrix}$, $S^\alpha = (\mathrm{id}_4/2 - S_z) = \begin{pmatrix} 0_2 & 0_2 \\ 0_2 & \mathrm{id}_2 \end{pmatrix}$

energy diagram (w.r.t. lab frame)

ω_S, ω_I = natural precession frequency of the first and second qubit

model ⇒ efficiency measure (time):

- count evolution under $H^\alpha(\phi_I)$
- neglect fast operations and H_0



Mathematical structure of our model (1/2)

Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ $\quad (\mathfrak{g} = \mathfrak{su}(4),\ \mathfrak{G} = \mathrm{SU}(4))$

condition: $[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}$, $[\mathfrak{k}, \mathfrak{p}] \subset \mathfrak{p}$, $[\mathfrak{p}, \mathfrak{p}] \subset \mathfrak{k}$ $\quad$ ($\mathfrak{k}$ Lie algebra, $\mathfrak{K}$ its Lie group)

fast operations: $-iS_\mu$ $(\mu \in \{x, y, z\})$ and $-iH_0 \Rightarrow$
$\mathfrak{K} = \exp(\mathfrak{k})$ where $\mathfrak{k} = \mathrm{span}_{\mathbb{R}}\{-iS_\mu, -i2S_\nu I_z, -iI_z \colon\ \mu, \nu \in \{x, y, z\}\}$

$\mathfrak{K} = \mathrm{S}[\mathrm{U}(2) \otimes \mathrm{U}(2)]$ (sometimes called $\mathrm{SU}(2) \times \mathrm{SU}(2) \times \mathrm{U}(1)$)
which is block-diagonal in an appropriately chosen basis

slow operations: e.g., $-iH^\alpha(\phi_I) \Rightarrow$
$\mathfrak{P} = \exp(\mathfrak{p})$ where $\mathfrak{p} = \mathrm{span}_{\mathbb{R}}\{-iI_\gamma, -i2S_\mu I_\gamma \colon\ \gamma \in \{x, y\}, \mu \in \{x, y, z\}\}$

Mathematical structure of our model (2/2)

Weyl orbit $\mathcal{W}(p) = \{KpK^{-1}:\ K \in \mathfrak{K}\} \cap \mathfrak{a}$ of $p \in \mathfrak{p}$

- max. Abelian subalgebra $\mathfrak{a} = \{a_1(-iS^\beta I_x) + a_2(-iS^\alpha I_x) : a_j \in \mathbb{R}\} \subset \mathfrak{p}$
- $\mathcal{W}[b_1(-iS^\beta I_x) + b_2(-iS^\alpha I_x)] = \mathcal{W}[(b_1, b_2)] = \{(b_1, b_2), (b_1, -b_2), (-b_1, b_2), (-b_1, -b_2), (b_2, b_1), (b_2, -b_1), (-b_2, -b_1), (-b_2, b_1)\}$

majorization condition: (a_1, a_2) is in the convex closure of $\mathcal{W}[(b_1, b_2)]$ iff $\max\{|a_1|, |a_2|\} \leq \max\{|b_1|, |b_2|\}$ and $|a_1| + |a_2| \leq |b_1| + |b_2|$

$\mathfrak{K}\mathfrak{A}\mathfrak{K}$ decomposition $(\mathfrak{A} = \exp(\mathfrak{a}))$

- $G = K_1 \exp[a_1(-iS^\beta I_x) + a_2(-iS^\alpha I_x)] K_2 \in \mathfrak{G}$ $(K_j \in \mathfrak{K})$
- is not unique $\Rightarrow$ consider all $(a_1, a_2) + \pi(z_1, z_2)$ where $z_j \in \mathbb{Z}$
- majorization condition simplifies for $a_1, a_2 \in [-\pi, \pi]$
  $\Rightarrow$ sufficient to consider only $(z_1, z_2) = (0, 0)$

Time-optimal control of fast and slow qubit system

Zeier/Yuan/Khaneja (2008)

The minimal time to synthesize $G \in \mathrm{SU}(4)$ is $\min\{(|t_1| + |t_2|)/\Omega^I\}$ such that $G = K_1 \exp[t_1(-iS^{\beta} I_x) + t_2(-iS^{\alpha} I_x)]K_2$

remarks

- slow operations: $-iH^{\alpha}(0)$, we use the Weyl orbit of $-iS^{\alpha} I_x$: $b_1 = 0$ and $b_2 = 1 \Rightarrow \mathcal{W}[(b_1, b_2)] = \{(-1, 0), (1, 0), (0, -1), (0, 1)\}$
- Yuan/Zeier/Khaneja/Lloyd (2009): applied similar techniques in a tunable coupling scheme of super-conducting qubits

Examples of time-optimal controls

minimum time $t_{\min}$ for CNOT[2, 1], CNOT[1, 2], and SWAP

1. $e^{i\pi/4}\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&0&1&0\\0&1&0&0\end{pmatrix} = \exp[\pi(-i2S_x I_z + iS_x + iI_z)/2] \Rightarrow t_{\min} = 0$
   (as it is contained in $\mathfrak{K}$ = fast operations)
2. $e^{i\pi/4}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} = \exp[\pi(-i2S_z I_x + iS_z + iI_x)/2] =$
   $\exp(i\pi S_z/2)\exp(-it' H_0/J)\exp\left[-i\pi H^{\alpha}(\pi)/\Omega^I\right]$
   (where $t' = -\pi J/\Omega^I \mod 2\pi \geq 0$)
   $\Rightarrow t_{\min} = \pi/\Omega^I$
3. $e^{i\pi/4}\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{pmatrix} = \exp[\pi(i2S_x I_x + i2S_y I_y + i2S_z I_z)/2] =$
   $e^{i\pi S_z/2}e^{-i\pi S_x/2}e^{-i3\pi H_0/(2J)}e^{i\pi S_y/2}e^{-it' H_0/J}\exp\left[-i\pi H^{\alpha}(\pi)/\Omega^I\right]$
   $\times e^{-i\pi S_x/2}e^{-i\pi H_0/(2J)}e^{-i\pi S_y/2}$
   $\Rightarrow t_{\min} = \pi/\Omega^I$

Outline

Control algorithms and density matrices

efficient control algorithms for $U \in \mathrm{SU}(2^n)$ with execution time t

- $U = \left[\prod_{k=1}^{m} \left(U_k \exp(-iHt_k) U_k{}^{-1}\right)\right] U_0$ and $t = \sum_{k=1}^{m} t_k \qquad (t_k \geq 0)$
- time-evolution w.r.t. a given Hamilton operator H $(-iH \in \mathfrak{su}(2^n))$
- conjugate the orbit $\exp(-iHt_k)$ with **instantaneous** operations $U_k \in \mathrm{SU}(2)^{\otimes n} = \mathrm{SU}(2) \otimes \cdots \otimes \mathrm{SU}(2)$

local equivalence of density matrices ρ and $\tilde{\rho}$

- local equivalent if $U \rho U^{-1} = \tilde{\rho}$ for some $U \in \mathrm{SU}(2)^{\otimes n} = \mathrm{SU}(2) \otimes \cdots \otimes \mathrm{SU}(2)$
- related to mixed state transformations: $\frac{d}{dt}\rho = [-iH(t), \rho]$, where ρ is a mixed state
- recall: ρ can be written as $c \cdot \mathrm{Id} + H$ where $-iH \in \mathfrak{su}(2^n)$ and $c \in \mathbb{R}$

Adjoint representation and adjoint orbits

adjoint representation

- Lie group $\mathfrak{G}$ [i.e. $\mathrm{SU}(2^n)$] and its Lie algebra $\mathfrak{g}$ [i.e. $\mathfrak{su}(2^n)$]
- adjoint representation $\mathrm{Ad}(G)(\tilde{g}) := G\tilde{g}G^{-1}$ $\qquad (G \in \mathfrak{G}, \tilde{g} \in \mathfrak{g})$
- infinitesimal version $\mathrm{ad}(g)(\tilde{g}) := [g, \tilde{g}]$ $\qquad (g, \tilde{g} \in \mathfrak{g})$

adjoint orbit of $\tilde{g} \in \mathfrak{g}$ w.r.t. $\mathfrak{K} \subset \mathfrak{G}$

- $\mathrm{Ad}(\mathfrak{K})(\tilde{g}) := \{\mathrm{Ad}(K)(\tilde{g})\colon K \in \mathfrak{K}\} = \{K\tilde{g}K^{-1}\colon K \in \mathfrak{K}\}$
- especially important if $\mathfrak{K} = \mathrm{SU}(2)^{\otimes n} = \mathrm{SU}(2) \otimes \cdots \otimes \mathrm{SU}(2)$

example: $\mathrm{Ad}(\mathfrak{K})$-orbit of $\mathrm{ZZI} + \mathrm{IZZ}$ (analyzed by hand)

- support in $\mathfrak{su}(2) \otimes \mathfrak{su}(2) \otimes \mathrm{Id}$ and $\mathrm{Id} \otimes \mathfrak{su}(2) \otimes \mathfrak{su}(2)$
- orbit is not linearly closed $\Leftrightarrow$ What is the dimension of the orbit?
- orbit contains (e.g.) $\mathrm{XXI} \pm \mathrm{IXY}$ but not $\mathrm{XXI} \pm \mathrm{IYY}$

Restricting representations and orbits

philosophy

- start some representation [e.g., the adjoint representation $\mathrm{Ad}(\mathfrak{G})$] or an adjoint orbit $\mathrm{Ad}(\mathfrak{G})(\tilde{g})$ where $\tilde{g} \in \mathfrak{g}$
- restrict $\mathfrak{G}$ to a subgroup $\mathfrak{K}$
- we consider $\mathfrak{G} = \mathrm{SU}(2^n)$ and $\mathfrak{K} = \mathrm{SU}(2)^{\otimes n} = \mathrm{SU}(2) \otimes \cdots \otimes \mathrm{SU}(2)$

restricting Ad from $\mathrm{SU}(2^n)$ to $\mathrm{SU}(2)^{\otimes n}$

- the irreducible representation $\mathrm{Ad}[\mathrm{SU}(2^n)]$ decomposes if we restrict
- $\mathfrak{su}(2^n) \Rightarrow [\mathrm{Id} \oplus \mathfrak{su}(2)]^{\otimes n} = \mathrm{Id}^{\otimes n} \oplus \cdots \oplus \mathfrak{su}(2)^{\otimes n}$; $\quad [\mathrm{Id}^{\otimes n} \notin \mathfrak{su}(2^n)]$

Decomposing the adjoint representation Ad

two qubits: $\mathfrak{G} = \mathrm{SU}(4)$, $\mathfrak{K} = \mathrm{SU}(2) \otimes \mathrm{SU}(2)$

- $[\mathrm{Id} \oplus \mathfrak{su}(2)]^{\otimes 2} = \mathrm{Id}^{\otimes 2} \oplus [\mathfrak{su}(2) \otimes \mathrm{Id}] \oplus [\mathrm{Id} \otimes \mathfrak{su}(2)] \oplus [\mathfrak{su}(2) \otimes \mathfrak{su}(2)]$
- $\Rightarrow$ vector space decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p} =$ local $\oplus$ nonlocal
  - $\mathfrak{k} = [\mathfrak{su}(2) \otimes \mathrm{Id}] \oplus [\mathrm{Id} \otimes \mathfrak{su}(2)]$ is a subalgebra of dimension $3 + 3 = 6$
  - $\mathfrak{p} = \mathfrak{su}(2) \otimes \mathfrak{su}(2)$ is an irreducible subspace of dimension 9

three qubits: $\mathfrak{G} = \mathrm{SU}(2^3)$, $\mathfrak{K} = \mathrm{SU}(2) \otimes \mathrm{SU}(2) \otimes \mathrm{SU}(2)$

- $[\mathrm{Id} \oplus \mathfrak{su}(2)]^{\otimes 3} = \mathrm{Id}^{\otimes 3} \oplus \mathfrak{k} \oplus \mathfrak{m}_1 \oplus \mathfrak{m}_2 \oplus \mathfrak{m}_3 \oplus \mathfrak{m}_4$, where
  - $\mathfrak{k} = [\mathfrak{su}(2) \otimes \mathrm{Id} \otimes \mathrm{Id}] \oplus [\mathrm{Id} \otimes \mathfrak{su}(2) \otimes \mathrm{Id}] \oplus [\mathrm{Id} \otimes \mathrm{Id} \otimes \mathfrak{su}(2)]$
  - $\mathfrak{m}_1 = \mathfrak{su}(2) \otimes \mathfrak{su}(2) \otimes \mathrm{Id}$, where $\dim(\mathfrak{m}_1) = 9$
  - $\mathfrak{m}_2 = \mathfrak{su}(2) \otimes \mathrm{Id} \otimes \mathfrak{su}(2)$, where $\dim(\mathfrak{m}_2) = 9$
  - $\mathfrak{m}_3 = \mathrm{Id} \otimes \mathfrak{su}(2) \otimes \mathfrak{su}(2)$, where $\dim(\mathfrak{m}_3) = 9$
  - $\mathfrak{m}_4 = \mathfrak{su}(2) \otimes \mathfrak{su}(2) \otimes \mathfrak{su}(2)$, where $\dim(\mathfrak{m}_4) = 27$
- $\mathfrak{k}$ is a subalgebra of dimension $3 + 3 + 3 = 9$
- $\mathfrak{m}_1 \oplus \mathfrak{m}_2 \oplus \mathfrak{m}_3 \oplus \mathfrak{m}_4$ is a subspace of dimension 54 (NOT irreducible)

Kostant's convexity theorem (revisited) $(\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p})$

Kostant's convexity theorem (1973):

- orth. projection of $\{KpK^{-1}\colon\ K \in \mathfrak{K}\}$ to $\mathfrak{a}$
  $=$ convex closure of $\{KpK^{-1}\colon\ K \in \mathfrak{K}\} \cap \mathfrak{a}$
- $\mathfrak{a}$ = max. commutative subalgebra in $\mathfrak{p}$ and $p \in \mathfrak{p}$

versions of Kostant's convexity theorem

version A: project to a max. commutative subalgebra $\mathfrak{a}$ of $\mathfrak{p}$

version B: project to a max. commutative subalgebra $\mathfrak{t}_{\mathfrak{g}}$ of $\mathfrak{g}$
(usually generalizations consider only version B)

Generalizations of Kostant's convexity theorem (1/2)

dualism between irred. representations and (integral) adjoint orbits

both corresp. to integral points in $\mathfrak{t}_\mathfrak{g}$ (= max. Abelian subalgebra in $\mathfrak{g}$)

restrict the group $\mathfrak{G}$ to a subgroup $\mathfrak{K}$

problem 1: find all $t' \in \mathfrak{t}_\mathfrak{k}$ corresp. to restricted adjoint orbits of $t \in \mathfrak{t}_\mathfrak{g}$

problem 2: (asymptotic decomp.) find all rational $(t', t) \in (\mathfrak{t}_\mathfrak{k}, \mathfrak{t}_\mathfrak{g})$ s.t.

a) $\exists n \in \mathbb{N}$ s.t. (nt', nt) is integral and

b) decomposition of the representation nt contains nt'

remark: if t index of the representation $V \Rightarrow$
nt index of the representation (inner tensor product) $V^{\otimes n}$

Generalizations of Kostant's convexity theorem (2/2)

restrict the group $\mathfrak{G}$ to a subgroup $\mathfrak{K}$

problem 1: find all $t' \in \mathfrak{t}_{\mathfrak{k}}$ corresp. to restricted adjoint orbits of $t \in \mathfrak{t}_{\mathfrak{g}}$

problem 2: (asymptotic decomp.) find all rational $(t', t) \in (\mathfrak{t}_{\mathfrak{k}}, \mathfrak{t}_{\mathfrak{g}})$ s.t.

a) $\exists n \in \mathbb{N}$ s.t. (nt', nt) is integral and
b) decomposition of the representation nt contains nt'

- Heckman (1980,1982): problems 1 and 2 are equivalent
- Kirwan (1984): restriction of a compact Lie group to a Lie subgroup (for convexity one has to restrict to a certain convex cone of $\mathfrak{t}_{\mathfrak{k}}$)
- Kirwan's result gives no practical method for explicit computations!
- Berenstein/Sjamaar (2000):
  computational methods relying on integral cohomology groups

Spectra and current status

spectra of reduced density matrices

- density matrices: ρ_{AB}, ρ_A, and ρ_B [and more tensor components]
- consider: $\operatorname{spec}\rho_{AB}$, $\operatorname{spec}\rho_A$, and $\operatorname{spec}\rho_B$
- problem: What combinations of spectra are possible?
- equivalent to the discussed restrictions of representations

$\longrightarrow$ Keyl/Werner (2001), Klyachko (2004), Christandl/Mitchison (2005), ...

decomposition of an adjoint orbit $\mathrm{Ad}(\mathfrak{G})g$ ($g \in \mathfrak{g}$, g integral)

- dream: decompose $\mathrm{Ad}(\mathfrak{G})g$ into $\mathrm{Ad}(\mathfrak{K})$-orbits using the equivalent asymptotic decompositions of representations
- status: preliminary computations

Commutator relations for two and three qubits

important for the analysis of products of adjoint orbits

two qubits $[\mathfrak{G} = \mathrm{SU}(2^2), \mathfrak{K} = \mathrm{SU}(2)^{\otimes 2}]$

- $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ where $\mathfrak{k} = [\mathfrak{su}(2) \otimes \mathrm{Id}] \oplus [\mathrm{Id} \otimes \mathfrak{su}(2)]$ and $\mathfrak{p} = \mathfrak{su}(2) \otimes \mathfrak{su}(2)$
- $[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}$ and $[\mathfrak{k}, \mathfrak{p}] \subset \mathfrak{p}$, $[\mathfrak{p}, \mathfrak{p}] \subset \mathfrak{k}$

three qubits $[\mathfrak{G} = \mathrm{SU}(2^3), \mathfrak{K} = \mathrm{SU}(2)^{\otimes 3}]$

- $[\mathrm{Id} \oplus \mathfrak{su}(2)]^{\otimes 3} = \mathrm{Id}^{\otimes 3} \oplus \mathfrak{k} \oplus \mathfrak{m}_1 \oplus \mathfrak{m}_2 \oplus \mathfrak{m}_3 \oplus \mathfrak{m}_4$, where
    - $\mathfrak{k} = [\mathfrak{su}(2) \otimes \mathrm{Id} \otimes \mathrm{Id}] \oplus [\mathrm{Id} \otimes \mathfrak{su}(2) \otimes \mathrm{Id}] \oplus [\mathrm{Id} \otimes \mathrm{Id} \otimes \mathfrak{su}(2)]$
    - $\mathfrak{m}_1 = \mathfrak{su}(2) \otimes \mathfrak{su}(2) \otimes \mathrm{Id}$, $\mathfrak{m}_2 = \mathfrak{su}(2) \otimes \mathrm{Id} \otimes \mathfrak{su}(2)$, $\mathfrak{m}_3 = \mathrm{Id} \otimes \mathfrak{su}(2) \otimes \mathfrak{su}(2)$, and $\mathfrak{m}_4 = \mathfrak{su}(2) \otimes \mathfrak{su}(2) \otimes \mathfrak{su}(2)$
- $[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}$, $[\mathfrak{k}, \mathfrak{m}_i] \subset \mathfrak{m}_i$, $[\mathfrak{m}_j, \mathfrak{m}_j] \subset \mathfrak{k}$, $[\mathfrak{m}_4, \mathfrak{m}_4] \subset \mathfrak{k} \oplus \mathfrak{m}_4$, and (e.g.) $[\mathfrak{m}_1, \mathfrak{m}_2] \subset \mathfrak{m}_4$ $(i \in \{1,2,3,4\}, j \in \{1,2,3\})$

Summary

summary

- control algorithms for two coupled qubits with fast local control
- lower bounds for coupled multi-qubit systems with fast local control
- control algorithms for a coupled electron-nuclear spin system
- representation theory might help to understand multi-qubit systems

http://www.org.chemie.tu-muenchen.de/people/zeier/

Thank you for your attention!