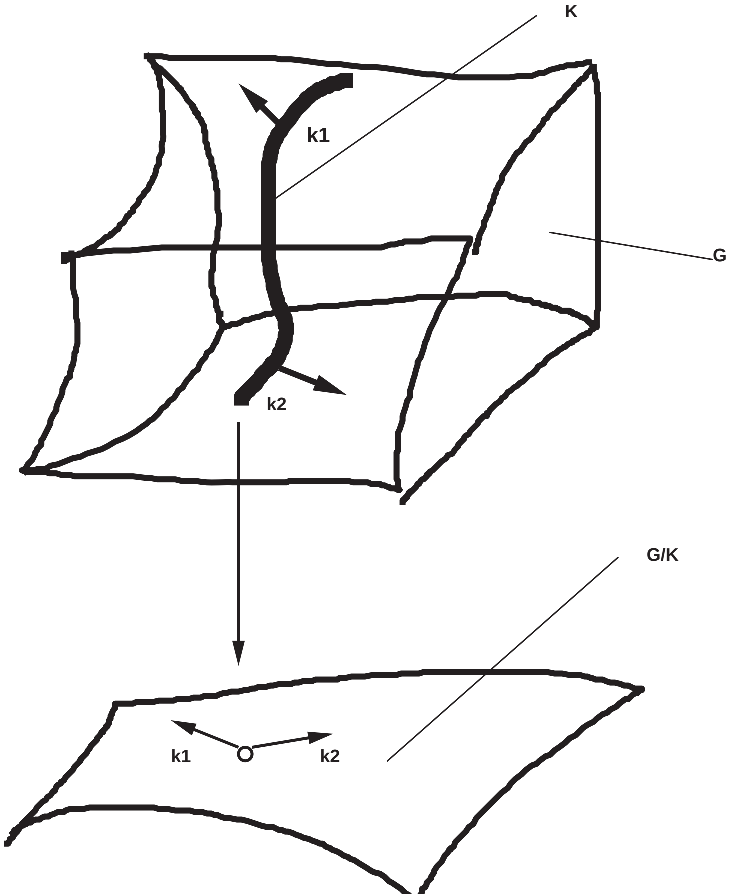
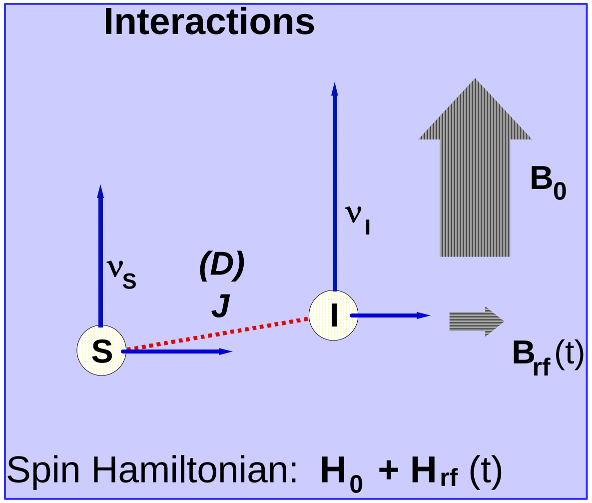
Controllability and Time Optimal Control in Spin Systems

Navin Khaneja, Harvard





KITP Quantum Control, June 10, 2009

Bilinear Control Systems in Quantum Control

$$\frac{d}{dt}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle$$

$$\frac{dU(t)}{dt} = -i[H_d + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

Can the state of a quantum mechanical system be steered between points of interest with available Hamiltonians.

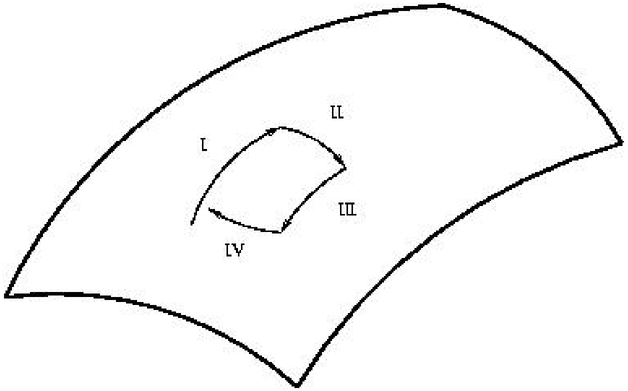
What possible Unitary Transformations can be produced in a given time with available Hamiltonians.

Controllability, Lie Algebras and Chows Theorem

$$\frac{dU}{dt} = -i\,(\sum_j u_j H_j)\,U$$

$$U(\Delta t) = \exp(iH_2\Delta t)\exp(iH_1\Delta t)\exp(-iH_2\Delta t)\exp(-iH_1\Delta t)$$

$$\approx I + (\Delta t)^2 \underbrace{[-iH_1, -iH_2]}_{new\ \ generator}$$



$$\dot{\Theta} = u_1 \begin{pmatrix} & -1 & & & & \\ 1 & & \ddots & & & \\ & \ddots & & -1 & & \\ & & 1 & & -1 & \\ & & & 1 & & 0 \\ & & & & 0 & \end{pmatrix} + u_2 \begin{pmatrix} & 0 & & & & \\ 0 & & \ddots & & & \\ & \ddots & & 0 & & \\ & & 0 & & 0 & \\ & & & 0 & & -1 \\ & & & & 1 & \end{pmatrix} \Theta$$

If the Lie Algebra $\{-iH_j\}_{LA}$ generated by $\{-iH_j\}$ span the Lie algebra of the unitary group, then the system is controllable

If the control amplitude is unbounded then the points that can be reached can be reached in no time

Brockett, Sussman, Jurdjevic

Controllable Linear Systems with unbounded controls can be steered between points in arbitrary small time

$$\frac{dX}{dt} = AX + Bu$$

$$\frac{dX}{dt} = AX + \sum_j u_j b_j$$

$$X(t) = e^{At} X(0) + \int e^{A(t-\tau)} B(\tau) u(\tau) d\tau$$

Even if drift is required, it takes arbitrary small time to steer the system between points of interest, if system is controllable.

Controllability with Drift

$$\frac{dU}{dt} = -i\,[H_0 + \sum_j u_j H_j\,]U$$

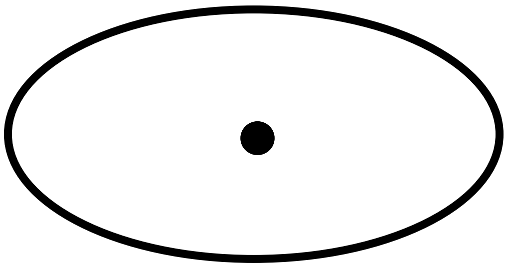
If the Lie Algebra $\{H_{0,} H_j\}_{LA}$ span

the Lie algebra of the unitary group, then the system is controllable

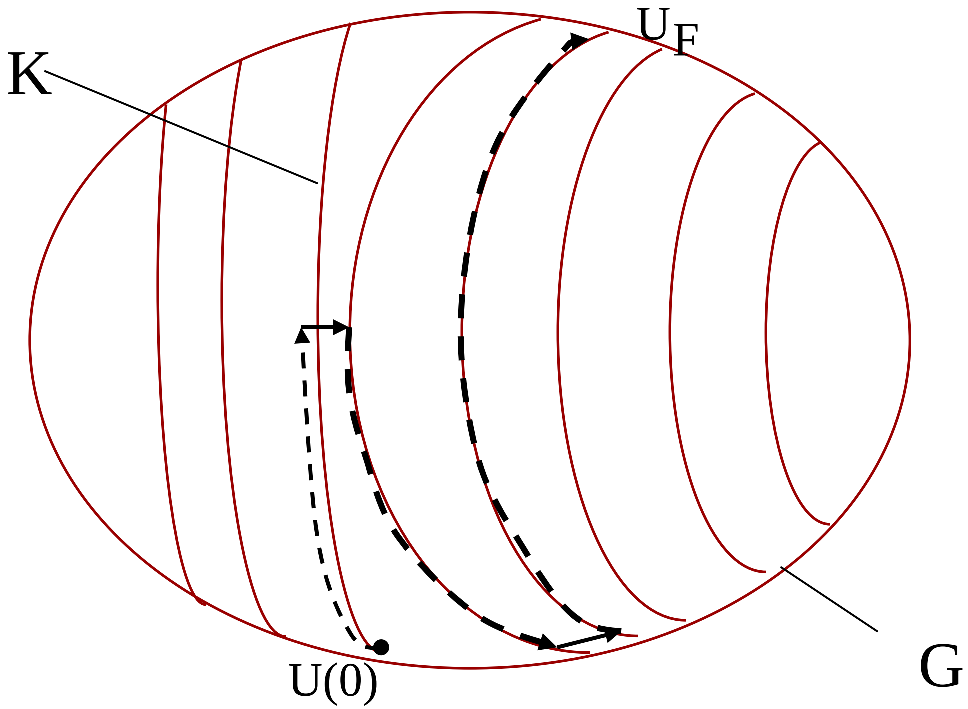
The backward evolution $\exp(iH_0\Delta t)$

is obtained arbitrarily well by waiting long enough on a compact group

Inspite of the Unbounded Controls there is a minimum time to reach anywhere



Time Optimal Control of Quantum Systems



$$k = \{-iH_j\}_{LA}$$

$$K = \exp(k)$$

$$T^*(U) = \inf_t \left\{U \in \bar{R}(t)\right\}$$

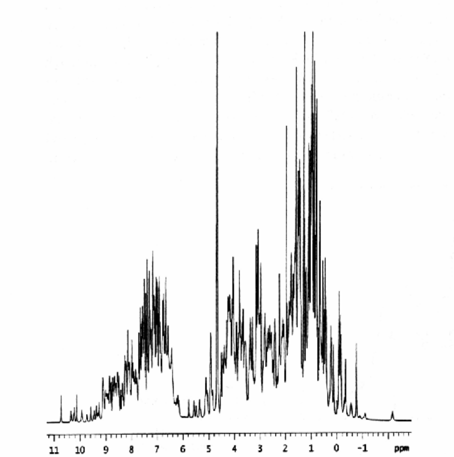
$$T^*(K) = 0$$

$$T^*(K_1 U_1 K_2) = T^*(U_1)$$

$$\frac{dU(t)}{dt} = -i[H_d + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

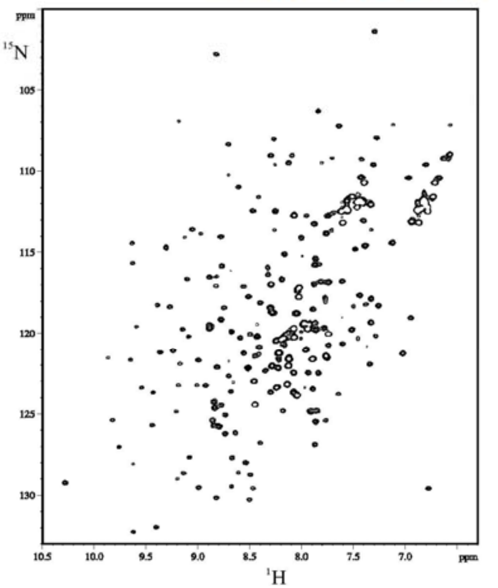
Physical Review A , 63, 032308, 2001

Manipulation of Coupled Spin Dynamics



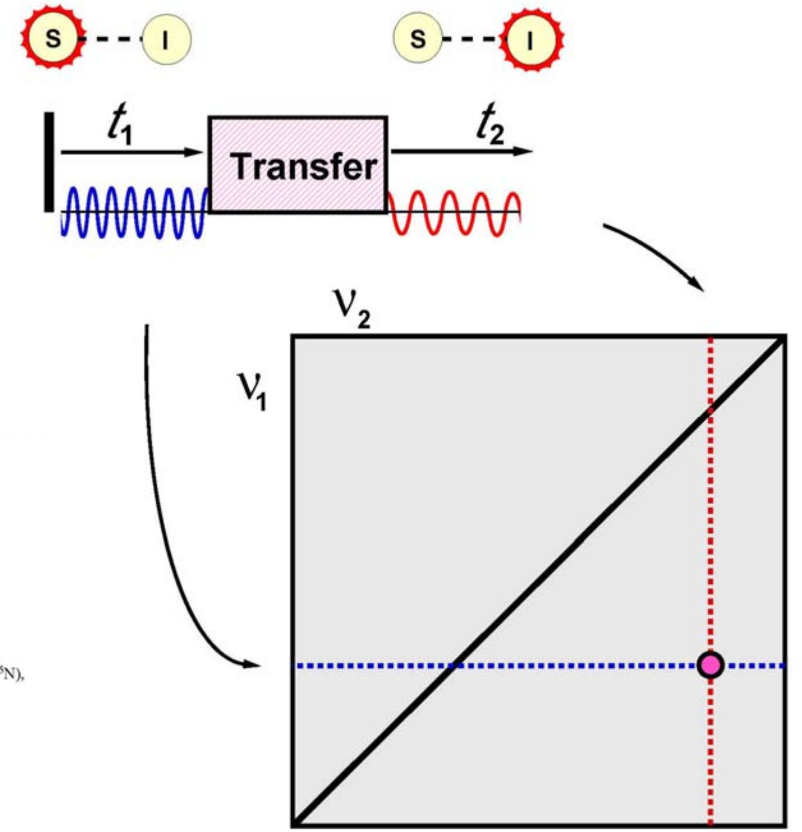
2D NMR

Example: ^{15}N-HSQC of p63



^{15}N labeling:

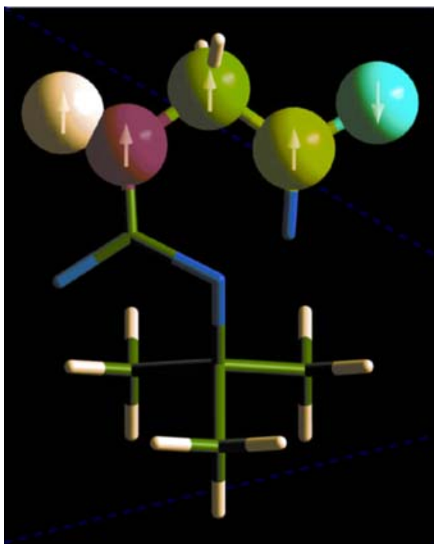
- all N atoms replaced by ^{15}N (ca. 95 % ^{15}N),
- characteristic fingerprint spectrum
- p63: 233 a.a. / 27 kDa
- measured at 750 MHz / 303 K

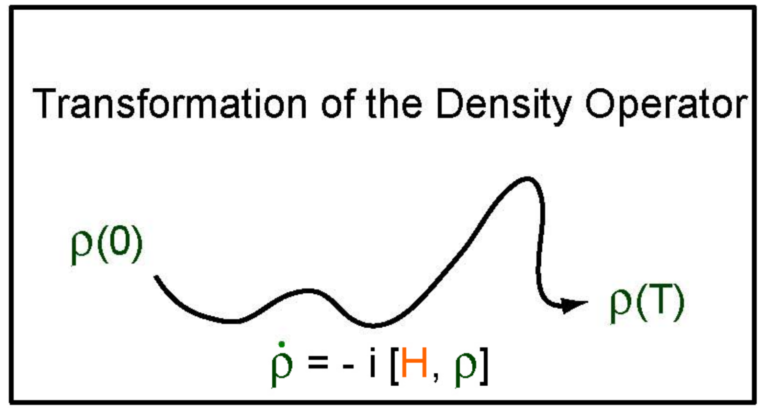


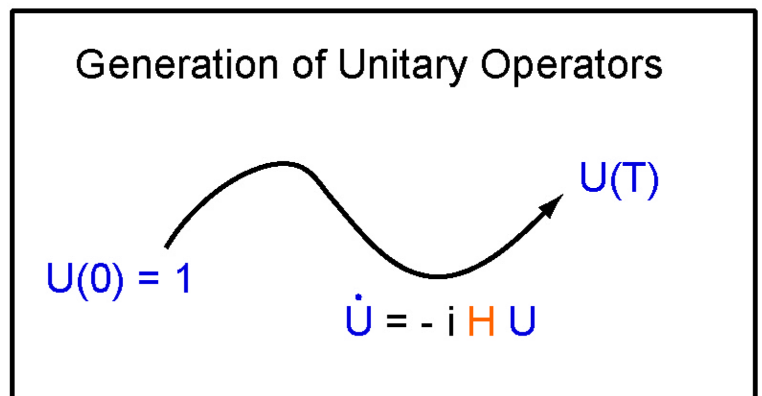
$$s(t_{1,}\, t_2) = \eta \cos(\omega_s t_1) \cos(\omega_I t_2)$$

Time-Optimal Control of Spin Systems

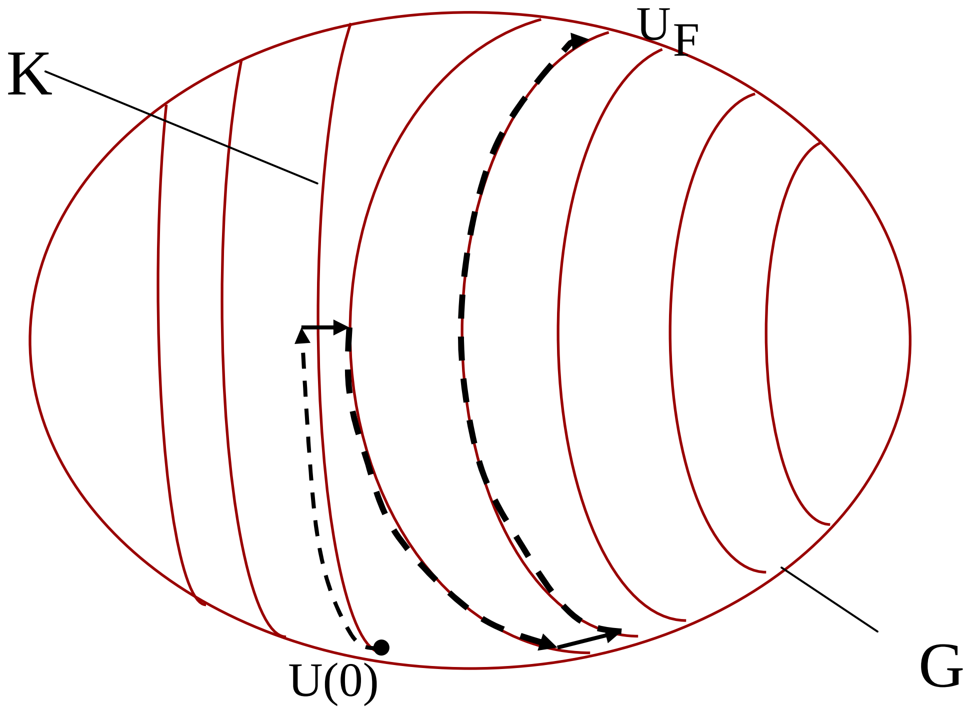
$$H = H_d + \sum u_k H_k$$







Time Optimal Control of Quantum Systems



$$k = \{-iH_j\}_{LA}$$

$$K = \exp(k)$$

$$T^*(U) = \inf_t \left\{U \in \overline{R}(t)\right\}$$

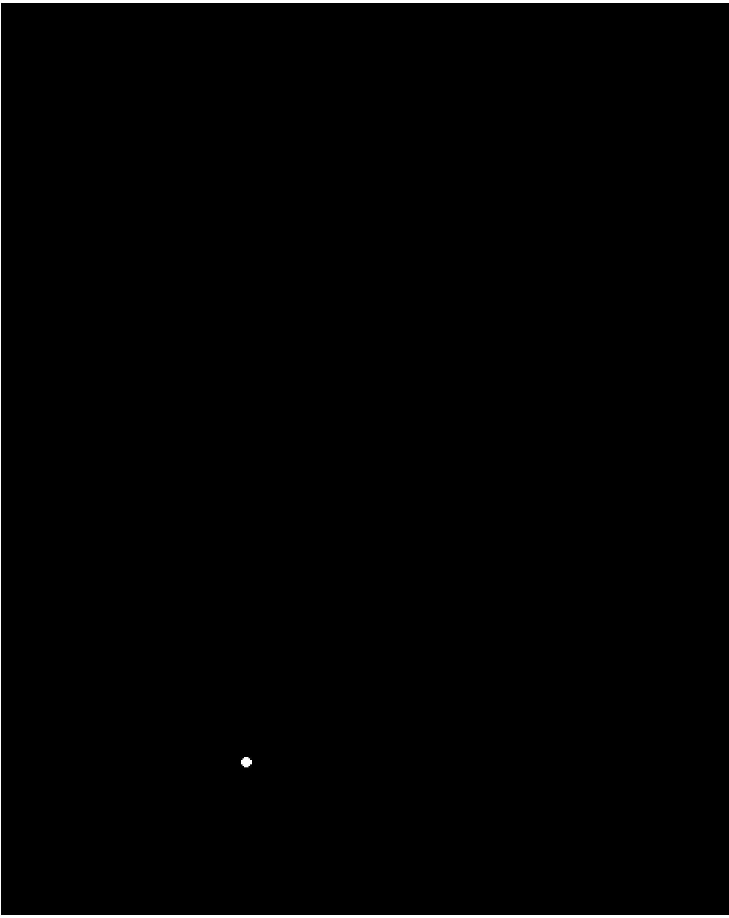
$$T^*(K) = 0$$

$$T^*(K_1 U_1 K_2) = T^*(U_1)$$

$$\frac{dU(t)}{dt} = -i[H_d + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

Physical Review A , 63, 032308, 2001

Cartan Decomposition of Lie Algebra



$$\frac{dU(t)}{dt} = -i[H_d + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

$$g = p \oplus k; \ [p,p] \subseteq k; [k,k] \subseteq k; [p,k] \subseteq p;$$

$$B(X,Y) = tr(ad_X ad_Y); \ p \perp k$$

G/K is a Riemannian Symmetric Space

$$\ldots{}_{+1} \exp(-iH_d t_n) K_n \ldots \exp(-iH_d t_2) K_2 \exp(-iH_d t_1) K_1$$

$$\ldots\exp(-i K^\dagger{}_n H_d K_n \, t_n) \ldots \exp(-i K^\dagger{}_2 H_d K_2 \, t_2) \exp(-i \underbrace{K^\dagger{}_1 H_d K_1}_{Ad_{K_1}(H)} \, t_1)$$

The velocities of the shortest paths in G/K always commute!

Physical Review A , **63**, 032308 (2001)

Cartan Decomposition of Lie algebra and Lie Group.

g be a real semisimple lie algebra

$$g = p \oplus k; \quad p \perp k$$

$$[p,p] \subseteq k; [k,k] \subseteq k; [p,k] \subseteq p;$$

$$Ad_K(p) = p$$

$$\bigcup_K Ad_K(a) = p$$

$$G = \exp(p)K$$

Let $a \subset p$ be the largest Abelian sub-algebra.
Let $A = \exp(a)$.

G = KAK

$g = su(n)$ $k = so(n)$ $p = -iS$ S traceless Symmetric

$$h = -i\begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix} \in a$$

$$G = K_1 \exp(-i\begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix})K_2$$

$$a^+ = \{\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots \geq \lambda_n\}$$

K = SO(n)

Cartan Decomposition

$$g = p \oplus k;$$

$$[p,p] \subseteq k; [k,k] \subseteq k; [p,k] \subseteq p;$$

$$g = su(m+n)$$

$$k = su(m) \times su(n) \times u(1)$$

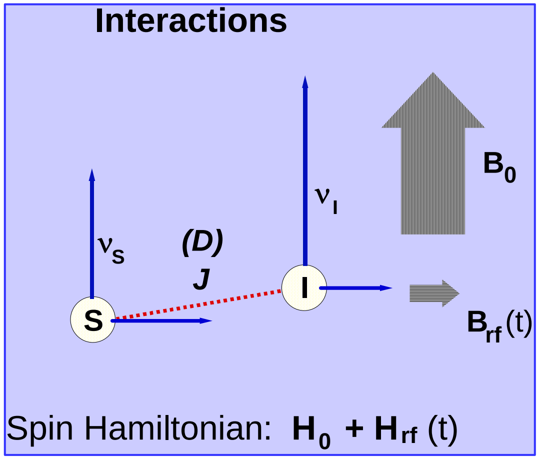
$$p = -i \underbrace{\begin{bmatrix} 0 & c \\ c^{\dagger} & 0 \end{bmatrix}}$$

$$K = \exp(-i \underbrace{\begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}}_{k}) = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix}$$

$$a^{+} = \begin{bmatrix} 0 & D & 0 \\ D & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$D = diag\{\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots \geq \lambda_m \geq 0\}$$

Cartan Decompositions in Two-Spin Systems and Canonical Decomposition of SU(4)



$$\frac{dU}{dt} = -i[\sum_{\alpha,\beta} J_{\alpha\beta} I_\alpha S_\beta + u_1 I_x + u_2 I_y + u_3 S_x + u_4 S_y]U$$

$$k = \{-i\ I_\alpha, -iS_\beta\}\ ;\quad p = \{-iI_\alpha S_\beta\}$$

$$G = SU(4);\quad K = SU(2) \otimes SU(2)$$

$$I_\alpha = \sigma_\alpha \otimes I\,;$$

$$S_\alpha = I \otimes \sigma_\alpha\,;$$

$$I_\alpha S_\beta = \sigma_\alpha \otimes \sigma_\beta\,;$$

$$a = \{-iI_x S_x, -iI_y S_y, -iI_z S_z\}$$

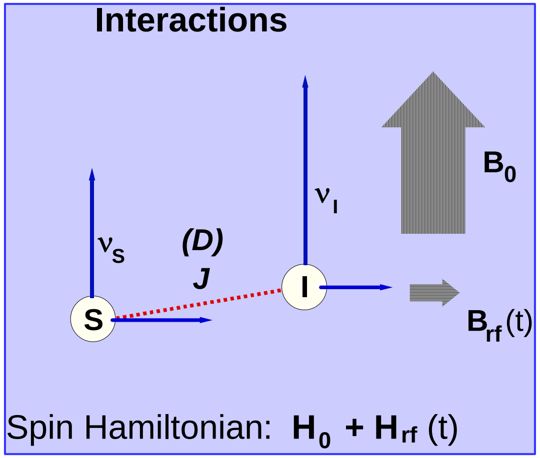
$$G = K\ \exp(-i(\alpha_x I_x S_x + \alpha_y I_y S_y + \alpha_z I_z S_z\ ))\ K$$

$$(\alpha_x, \alpha_y, \alpha_z) \qquad \alpha_x \geq \alpha_y \geq |\,\alpha_z\,|$$

Khaneja, Brockett, Glaser, Physical Review A , 63, 032308, 2001

Another Canonical Decomposition of SU(4): Electron Nuclear Spin Dynamics

$$H_c = J I_z S_z \quad ; \quad \Omega_S \;\square\; J \;\square\; \Omega_I$$



$$k = -i\left\{S_\alpha, S_\beta I_z, \; I_z\right\}$$

$$K = \exp(-i\underbrace{\begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}}_{k}) = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix}$$

$$a = -i\left\{S_z I_{x,} \;\; I_x\right\} \qquad -i\begin{bmatrix} 0 & 0 & \lambda_1 & 0 \\ 0 & 0 & 0 & \lambda_2 \\ \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \end{bmatrix}$$

Zeier, Yuan, Khaneja, PRA (2008)

$$\{\lambda_1 \geq \lambda_2 \geq 0\}$$

$$G = SU(4); \quad K = SU(2) \times SU(2) \times U(1)$$

$$K_1 \exp(-i\,\lambda_1 \sigma_x \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \lambda_2 \sigma_x \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}) K_2$$

Controllability and Cartan Decomposition

G = KAK

$$k = so(n)$$

$$K = \exp(k) = SO(n)$$

$$\frac{dU(t)}{dt} = -i[H_d + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

$$H_d = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$$

$$K_{n+1}\exp(-iH_d t_n)K_n \ldots \exp(-iH_d t_2)K_2 \exp(-iH_d$$

$$K_b \exp(-i P^{\dagger}{}_n H_d P_n\, t_n)\ldots\exp(-i P^{\dagger}{}_2 H_d P_2\, t_2)\exp(-i \underbrace{P^{\dagger}{}_1 H_d P_1}_{Ad_{P_1}(H_d)}\, t_1)K_a$$

$$= K_b \exp(-i\begin{pmatrix} \mu_1 & & & \\ & \mu_2 & & \\ & & \ddots & \\ & & & \mu_n \end{pmatrix})K_a$$

Reachable Set

G = KAK

$$\frac{dU(t)}{dt} = -i[H_d + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

$$K = \exp(k) = SO(n)$$

$$H_d = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$$

$$A(t) = K^{\dagger}{}_1(t)U(t)K_2{}^{\dagger}(t)$$

$$K_1(t)A(t)K_2(t) = U(t)$$

$$\frac{dA(t)}{dt} = diag(Ad_K(-iH_d))A(t)$$

Schur Convexity

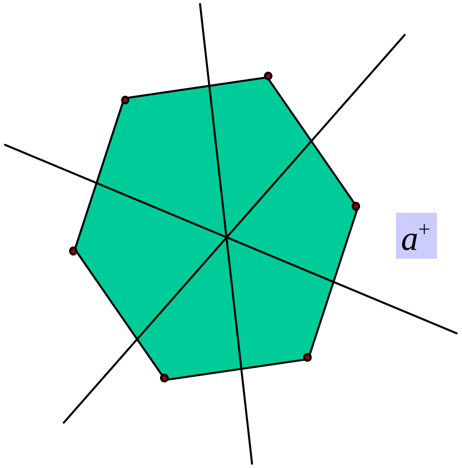
$$diag\begin{pmatrix}\cos\theta & -\sin\theta \\ \sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}\lambda_1 & 0 \\ 0 & \lambda_2\end{pmatrix}\begin{pmatrix}\cos\theta & \sin\theta \\ -\sin\theta & \cos\theta\end{pmatrix}$$

$$=\cos^2\theta\begin{pmatrix}\lambda_1 \\ \lambda_2\end{pmatrix}+\sin^2\theta\begin{pmatrix}\lambda_2 \\ \lambda_1\end{pmatrix}$$

$$K\begin{bmatrix}\lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n\end{bmatrix}K^\dagger=\begin{bmatrix}a_{11} & \ddots & & \ddots \\ \ddots & a_{22} & \ddots & \\ & \ddots & \ddots & \ddots \\ \ddots & & \ddots & a_{nn}\end{bmatrix}$$

$$\underbrace{\begin{bmatrix}a_{11} \\ a_{22} \\ \vdots \\ a_{nn}\end{bmatrix}}_{a}\prec\underbrace{\begin{bmatrix}\lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n\end{bmatrix}}_{\lambda} \quad ; \quad a=\sum_j \alpha_j P_j(\lambda)$$

Diagonal of a Symmetric Matrix is Majorized (lies in the convex hull) of its eigenvalues



Reachable Set

G = KAK

$$\frac{dU(t)}{dt} = -i[H_d + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

$$k = so(n)$$

$$K_1(t)A(t)K_2(t) = U(t)$$

$$\frac{dA(t)}{dt} = diag(Ad_K(-iH_d))A(t)$$

$$diag(Ad_K(-iH_d)) = -i\sum_j \alpha_j P_j(\lambda)$$

$$diag(A(T)) = \exp(-i\sum_j \underbrace{\int_0^T \alpha_j(t) P_j(\lambda)\, dt}_{\mu})$$

Reachable Set

$$\frac{dU(t)}{dt} = -i[H_d + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

$$H_d = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$$

$$\begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{bmatrix} \prec \lambda T$$

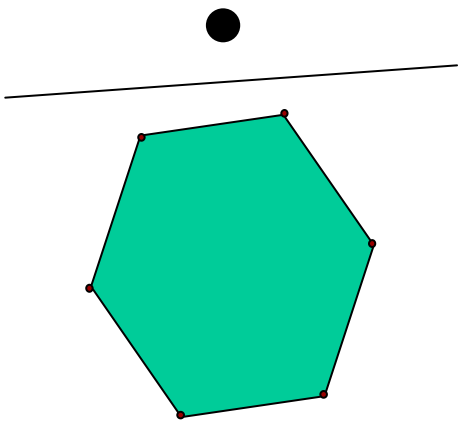
$$\overline{R}(T) = K_1 \exp(-i \begin{bmatrix} \mu_1 & & & \\ & \mu_2 & & \\ & & \ddots & \\ & & & \mu_n \end{bmatrix}) K_2$$

Schur Convexity

$$tr\left(Z\,K\begin{bmatrix}\lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n\end{bmatrix}K^\dagger\right) \qquad K\begin{bmatrix}\lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n\end{bmatrix}K^\dagger = \begin{bmatrix}a_{11} & \ddots & & \ddots \\ \ddots & a_{22} & \ddots & \\ & \ddots & \ddots & \ddots \\ \ddots & & \ddots & a_{nn}\end{bmatrix}$$

$$Z = \begin{pmatrix}\mu_1 & & & \\ & \mu_2 & & \\ & & \ddots & \\ & & & \mu_n\end{pmatrix}$$

$$\begin{bmatrix}a_{11} \\ a_{22} \\ \vdots \\ a_{nn}\end{bmatrix} \prec \begin{bmatrix}\lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n\end{bmatrix}$$



$$tr([Z, Ad_K(H_d)]k)$$

$$[p, p] \in k$$

$$K \to \exp(k)K$$

Kostant Convexity

$$g = su(p+q) \quad k = su(p)\times su(q)\times u(1)$$

$$g = p \oplus k;\ [p,p] \subseteq k;[k,k] \subseteq k;[p,k] \subseteq p;$$

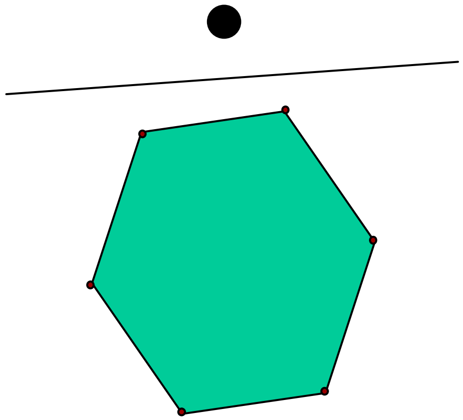
$$B(X,Y) = tr(ad_X ad_Y);\ \ p \perp k$$

$$a \subseteq p, \quad \text{maximal abelian subalgebra}$$

$$\Delta(X) = Ad_K(X) \cap a; \quad c(\Delta(X))\ \textit{is the convex hull of}\ \Delta_X$$

$$T : p \rightarrow a \quad \textit{orthogonal projection}$$

$$T : Ad_K(X) = c(\Delta(X))$$



$$A = \Gamma(Ad_K(X))\ A$$

$$U(t) = K_1(t)A(t)K_2(t)$$

$$A(t) = \exp(T\sum_j \alpha_j Ad_{k_j}(X))$$

$$\sum_j \alpha_j \leq 1$$

Time Optimal Tori Theorem

$$\frac{dU(t)}{dt} = -i[H_d + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

$$g = p + k; \quad p \perp k$$

$$[p,p] \subseteq k; [k,k] \subseteq k; [p,k] \subseteq p;$$

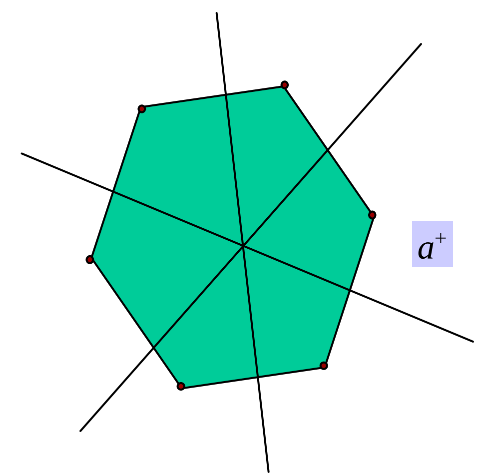
$$a \subseteq p, \quad \max imal\ abelian\ suba\lg ebra$$

$$\Delta(X) = Ad_K(X) \cap a; \quad c(\Delta(X))\ is\ the\ convex\ hull\ of\ \Delta(X)$$

$$X = -iH_d$$

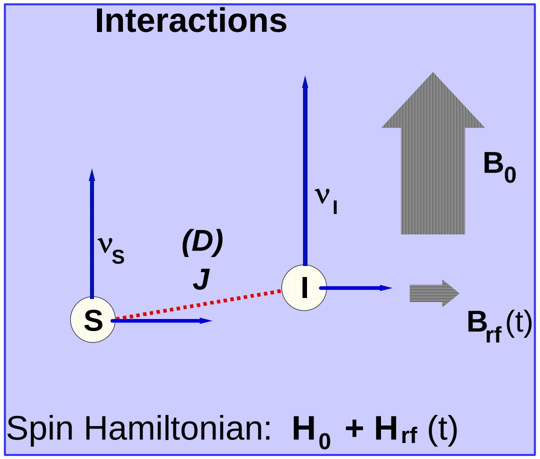
$$K_1 \exp(c(\Delta(X))\, t)\, K_2\, ;$$

$$K_1 \exp(t \sum_i \alpha_i Ad_{K_i}(X))\, K_2\, ;$$



Physical Review A, **63**, 032308 (2001)

Two-Spin Systems and Canonical Decomposition of SU(4)



$$g = p + k; \quad p \perp k$$

$$[p,p] \subseteq k; [k,k] \subseteq k; [p,k] \subseteq p;$$

$$g = su(4)$$

$$k = \{-i \ I_\alpha, -iS_\beta\} \ ; \quad p = \{-iI_\alpha S_\beta\}$$

$$G = SU(4); \quad K = SU(2) \otimes SU(2)$$

$$I_\alpha = \sigma_\alpha \otimes I \, ;$$

$$S_\alpha = I \otimes \sigma_\alpha \, ;$$

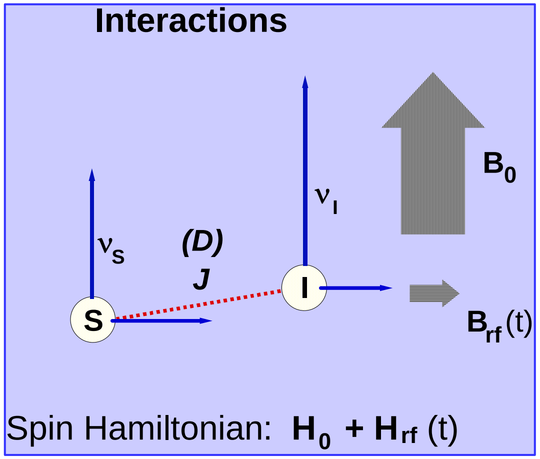
$$I_\alpha S_\beta = \sigma_\alpha \otimes \sigma_\beta \, ;$$

$$a = \{-iI_xS_x, -iI_yS_y, -iI_zS_z\}$$

$$G = K \ \exp(-i(\alpha_x I_x S_x + \alpha_y I_y S_y + \alpha_z I_z S_z \ )) \ K$$

$$\alpha_x \geq \alpha_y \geq |\alpha_z|$$

Cartan Decompositions , Two-Spin Systems and Canonical Decomposition of SU(4)



$$U_l\left(\sum_{\alpha\beta} J_{\alpha\beta} I_\alpha S_\beta\right) U_l^\dagger \rightarrow \underbrace{\alpha_x I_x S_x + \alpha_y I_y S_y + \alpha_z I_z S_z}_{H_1}$$

$$[J_{\alpha\beta}]_{3X3}$$

$$(\alpha_x, \alpha_y, \alpha_z) \qquad \alpha_x \geq \alpha_y \geq |\alpha_z|$$

$$U_2 \exp(-iH_4 t_4) \exp(-iH_3 t_3) \exp(-iH_2 t_2) \exp(-iH_1 t_1) U_1$$

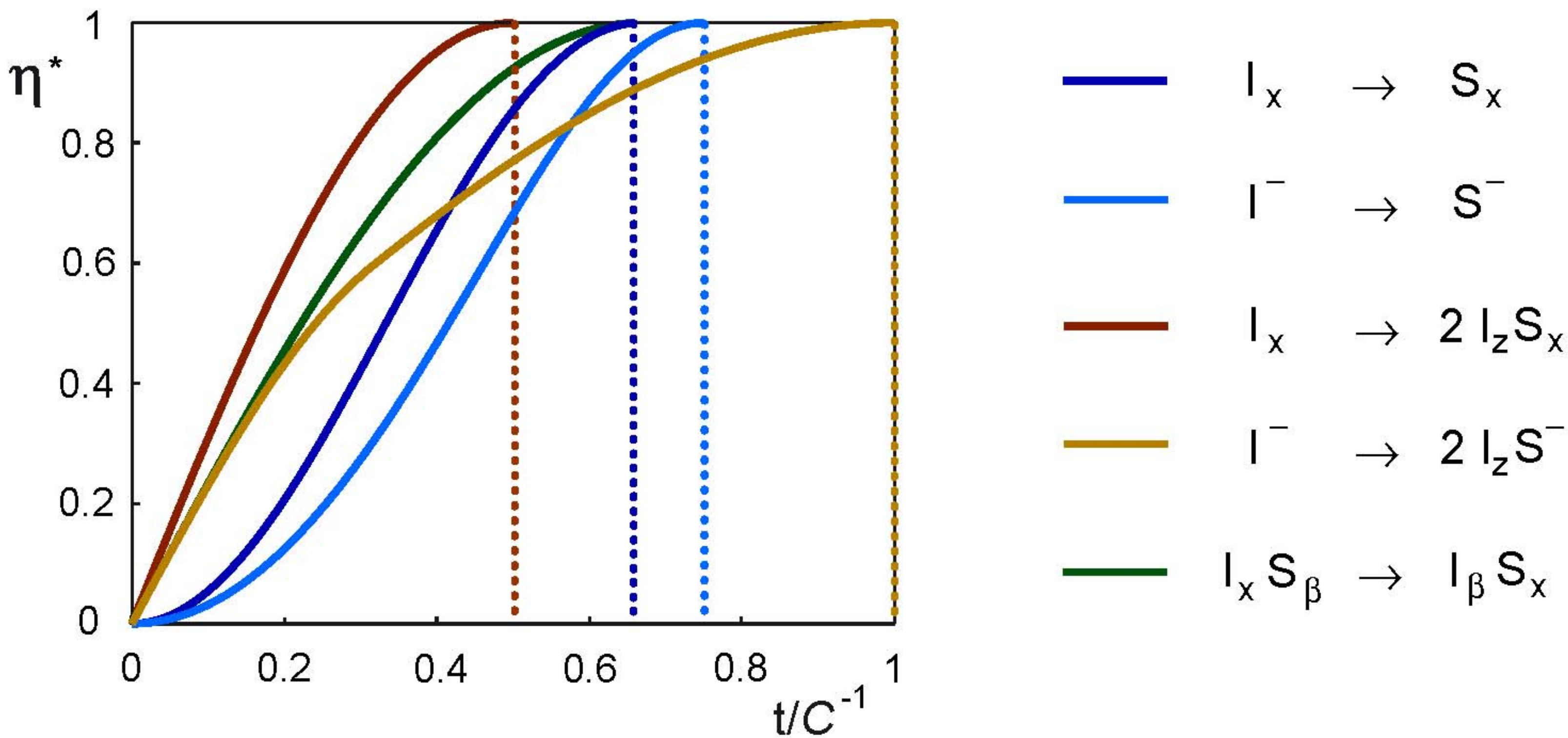
$$c(\Delta(X)) =$$

$$\{q_x \leq \alpha_x; \quad q_x + q_y \pm |q_z| \leq \alpha_x + \alpha_y \pm |\alpha_z|\}$$

$$K_1 \exp(-i\, c(\Delta(X))\, t)\, K_2\, ;$$

TOP (time-optimal pulse) curves for dipolar coupling

$(\mu_1, \mu_2, \mu_3) = (-1/2, -1/2, 1)$



Khaneja, Kramer, Glaser (2004)

Computations

$$|1\rangle = (|01\rangle + |10\rangle)\frac{-i}{\sqrt{2}};$$

$$|3\rangle = (|00\rangle - |11\rangle)\frac{-i}{\sqrt{2}};$$

$$|2\rangle = (|00\rangle + |11\rangle)\frac{1}{\sqrt{2}};$$

$$|4\rangle = (|01\rangle - |10\rangle)\frac{1}{\sqrt{2}};$$

$$U_1 A U_2 \rightarrow \Theta_1 D \Theta_2$$

$$\Theta_1 D^2 \Theta_1^T = UU^T$$

Eigenvalue Problem

$$P = \exp(-i\pi I_x S_y)\exp(-i\pi I_y S_y)$$

$$U = PVP^\dagger$$

Reachable set under time varying drift

$$\frac{dU(t)}{dt} = -i[H_d(t) + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

$$k = \{-iH_j\}_{LA}$$

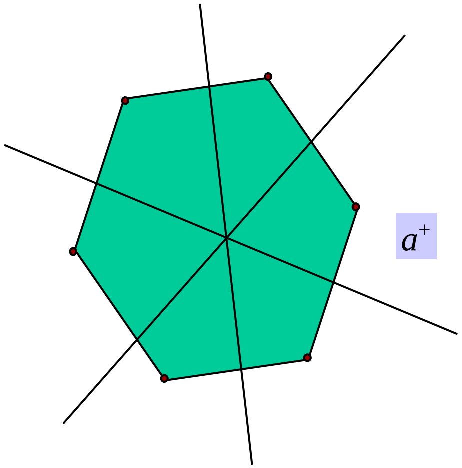
$$K = \exp(k)$$

$$g = p + k; \quad p \perp k$$

$$-iH_d(t) \in p$$

$$X^+(t) = Ad_K(-iH_d(t)) \cap a^+$$

$$Y = \int_0^T X^+(\tau)d\tau$$



$$K_1 \exp(c(\Delta(Y))t)K_2$$

H. Yuan and N. Khaneja
System and Control Letters (2006)

Reachable Set

$$\frac{dU(t)}{dt} = -i[H_d(t) + \sum_{j=1}^{m} u_j H_j]U(t); \quad U(0) = I$$

$$k = so(n)$$

$$H_d(t) = \begin{bmatrix} \lambda_1(t) & & & \\ & \lambda_2(t) & & \\ & & \ddots & \\ & & & \lambda_n(t) \end{bmatrix}$$

$$K = \exp(k) = SO(n)$$

$$Y = \int_0^T \lambda^{\downarrow}(\tau)d\tau$$

$$\begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{bmatrix} \prec Y$$

$$K_1 \exp(-i\begin{bmatrix} \mu_1 & & & \\ & \mu_2 & & \\ & & \ddots & \\ & & & \mu_n \end{bmatrix})K_2$$

Another K+P Problem

$$\dot{X} = UX \; ; U \in p$$

$$\eta = \int_0^1 U^T U \, dt$$

$$U(t) = \exp(-M_0 t) \; M_1 \; \exp(M_0 t)$$

$$M_0 \in k \; ; M_1 \in p$$

$$\dot{\Theta} = \begin{bmatrix} 0 & -u & -v \\ u & 0 & 0 \\ v & 0 & 0 \end{bmatrix} \Theta \quad ; \exp(\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix})$$

$$u = A\cos(\omega t + \theta); v = A\sin(\omega t + \theta)$$

Dynamics of n-coupled Spins

The dynamics of coupled spin ½ particles is described by an element of $SU(2^n)$

A basis of Lie algebra of $su(2^n)$ can be expressed as tensor product of pauli spin matrices

$$I_{k\alpha} = I_2 \otimes \ldots \sigma_\alpha \ldots \otimes I_2, \quad \alpha \in \{x, y, z\}$$

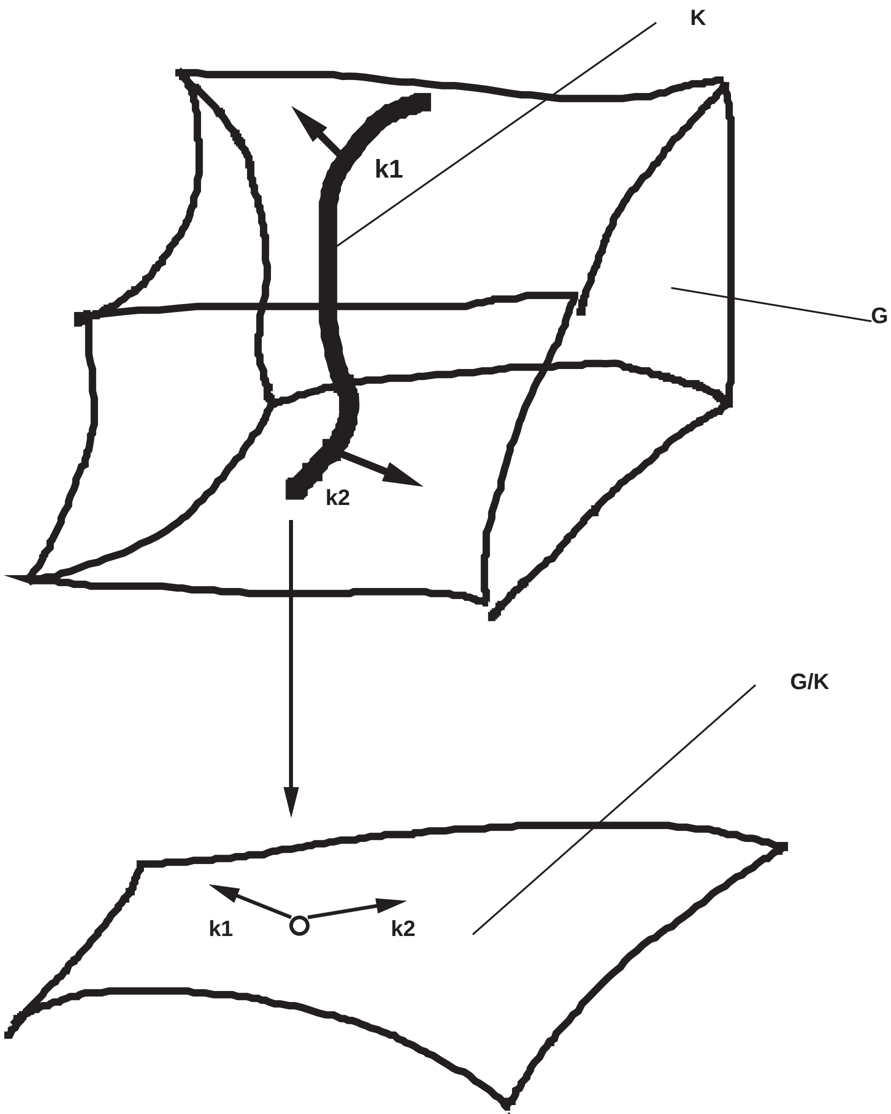
$$su(2^n) = -i\{I_{k_1\alpha}, 2I_{k_1\alpha}I_{k_2\beta}, 4I_{k_1\alpha}I_{k_2\beta}I_{k_3\gamma}, \ldots\}$$

$$H_o = \sum_k \omega_k I_{kz}, \quad H_c = \sum_{kj} J_{kj} \; 2I_{kz}I_{jz}$$

$$\dot{U} = -i[H_o + Hc + \sum_k u_k^1 I_{kx} + u_k^2 I_{ky}]U$$

Control Subgroup $SU(2) \otimes SU(2) \otimes \ldots \otimes SU(2)$

$$[p, p] \notin k$$

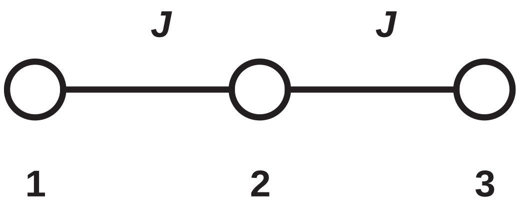


$$H_1 = I_{1z}I_{2x} + I_{2x}I_{3z}$$

$$H_2 = I_{1z}I_{2y} + I_{2y}I_{3z}$$

$$H_3 = 2I_{1z}I_{2z}I_{3z} + I_{2z}/2$$

Time Optimal Quantum Information Processing

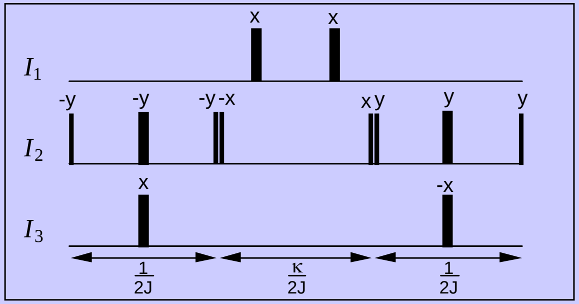


$$U = \exp\left(-iH_{eff}\right)$$

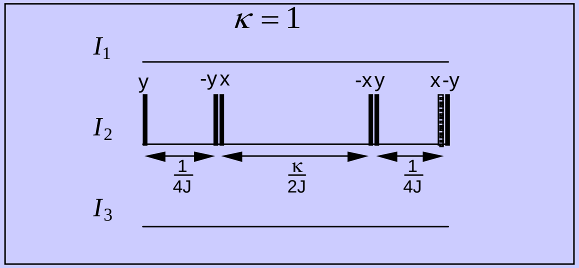
$$H_{eff} = 2\pi\kappa\left(I_{1\alpha} I_{2\beta} I_{3\gamma}\right)$$

$$\tau^* = \frac{\sqrt{\kappa(4-\kappa)}}{2J}$$

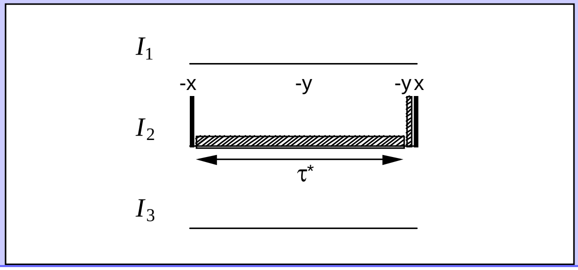
conventional experiment (with decoupling)



improved experiment (without decoupling)



OPTIMAL experiment (without decoupling)



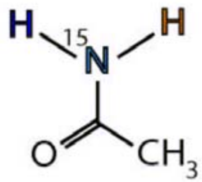
$$\frac{SU(8)}{SU(2)\otimes SU(2)\otimes SU(2)}$$

$$H_1 = I_{1z} I_{2x} + I_{2x} I_{3z}$$
$$H_2 = I_{1z} I_{2y} + I_{2y} I_{3z}$$
$$H_3 = 2 I_{1z} I_{2z} I_{3z} + I_{2z}/2$$

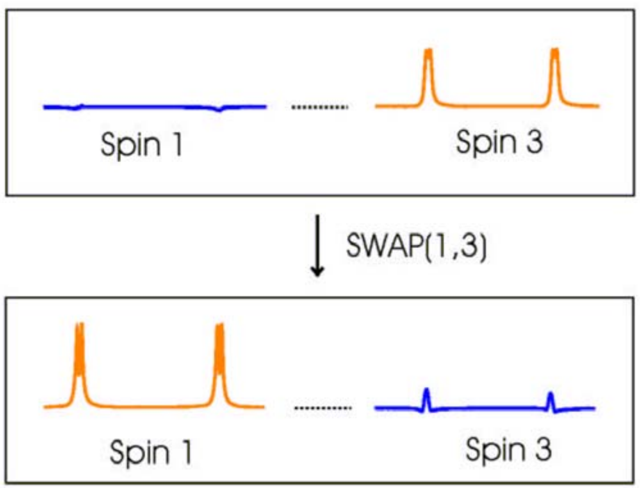
Khaneja, Glaser, Brockett

Physical Review A, **65**, 032301 (2002)

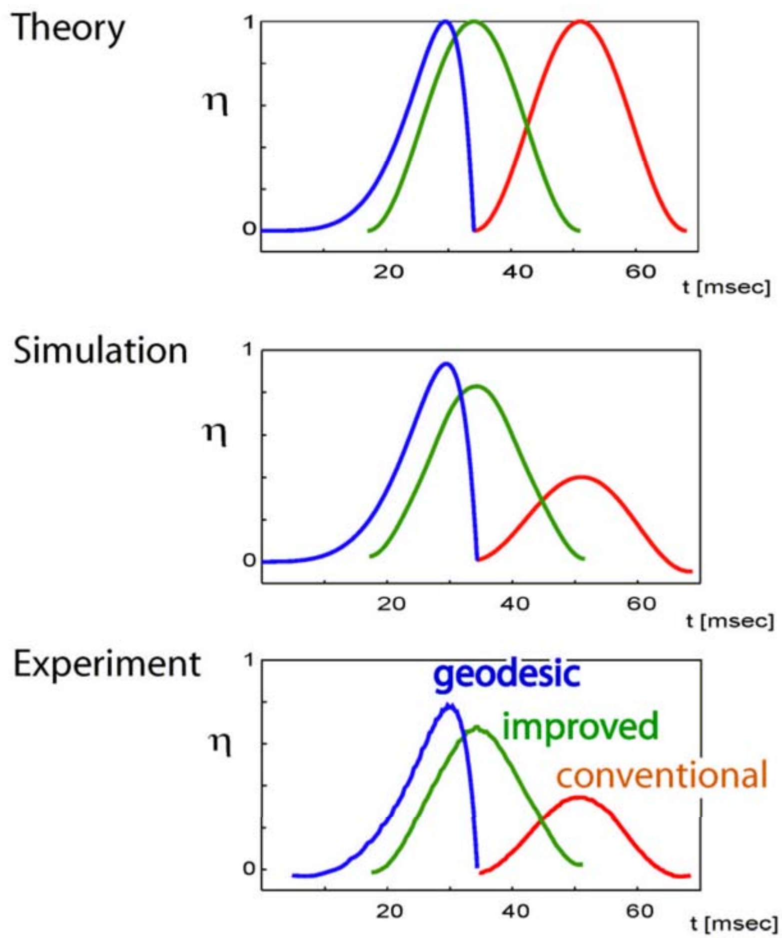
Indirect SWAP Operation



[^{15}N]-Acetamide



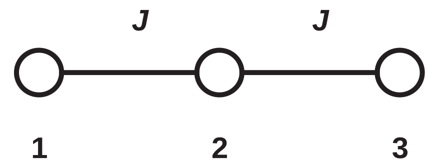
Efficiency η of indirect SWAP sequences



Reiss, Khaneja, Glaser
J. Mag. Reson. 165 (2003)

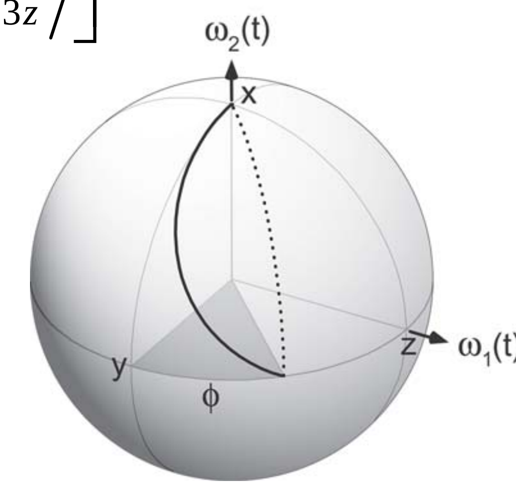
Geometry, Control and NMR

$$\frac{d}{dt}\begin{bmatrix} \langle I_{1x} \rangle \\ \langle 2I_{1y}I_{2z} \rangle \\ \langle 2I_{1y}I_{2x} \rangle \\ \langle 4I_{1y}I_{2y}I_{3z} \rangle \end{bmatrix} = \begin{bmatrix} 0 & -1 & & \\ 1 & 0 & -u & \\ & u & 0 & -1 \\ & & 1 & 0 \end{bmatrix} \begin{bmatrix} \langle I_{1x} \rangle \\ \langle 2I_{1y}I_{2z} \rangle \\ \langle 2I_{1y}I_{2x} \rangle \\ \langle 4I_{1y}I_{2y}I_{3z} \rangle \end{bmatrix}$$



$$\tan\theta = \frac{x_3}{x_2}$$

$$\frac{d}{dt}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 & -\cos\theta & 0 \\ \cos\theta & 0 & -\sin\theta \\ 0 & \sin\theta & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$



$$\theta = \omega t$$

$$\exp(-i2\pi\kappa I_{1z}I_{2z}I_{3z}), \quad \frac{\sqrt{\kappa(4-\kappa)}}{2J}$$

$$\frac{(dx)^2 + (dz)^2}{y^2}$$

Khaneja, et.al PRA 2007

Ensemble Controllability

The problem of manipulating quantum systems with uncertainities or inhomogeneities in parameters govering the system dynamics is ubiquitous in coherent spectroscopy and quantum information processing.

Typical settings include
a) Resonance offsets
b) Inhomogeneities in the strength of excitation field (systematic errors)
c) Time dependent noise (nonsystematic errors)
d) Addressing errors or cross talk

Widespread use of composite pulse sequences and pulse shaping first to correct for errors or compensate for inhomogeneties

a) Understanding controllability of quantum dynamics with inhomogeneities.
b) Understanding what aspect of system dynamics makes compensation possible.
c) What kind of inhomogeneities or errors can or cannot be corrected.