



# Structure of the space of two-qubit gates, perfect entanglers and quantum control

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# Outline

## **Two-qubit gates as the group $SU(4)$**

- local invariants
- Cartan decomposition and three-torus
- Weyl chamber and local equivalence classes
- local equivalence classes of perfect entanglers

## **Optimal control applications**

## **Two-qubit gates as a metric space**

- metric and invariant volume
- how large are control targets?
- what is the volume of the space of perfect entanglers?

## **Geometric theory and applications:**

Phys. Rev. A **67**, 042313 (2003)

Phys. Rev. Lett. **91**, 027903 (2003)

Phys. Rev. A **69**, 042309 (2004)

Phys. Rev. Lett. **93**, 020502 (2004)

## **Optimal control applications:**

Phys. Rev. A **84**, 042315 (2011)

& a work in progress

## **Metric properties and applications:**

P. Watts et al., submitted (2013)

# I. Introduction and geometric theory



**Jun Zhang**  
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**Shankar Sastry**

**Geometric theory and applications:**  
Phys. Rev. A **67**, 042313 (2003)  
Phys. Rev. Lett. **91**, 027903 (2003)  
Phys. Rev. A **69**, 042309 (2004)  
Phys. Rev. Lett. **93**, 020502 (2004)

## Two-qubit gates

Unitary operators acting on the state of two quantum bits

$$U : \mathcal{H}^4 \rightarrow \mathcal{H}^4$$

form the group of four-by-four unitary matrices  $U(4)$ :

$$U(4) = U(1) \otimes SU(4)$$

where  $U(1)$  is a global phase and  $SU(4)$  is the group of four-by-four unitary matrices with unit determinant.

Examples: in the standard computational basis:  $\mathcal{B} = \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$

$$\begin{aligned}
 U_I &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & U_{H \otimes H} &= \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \\
 U_{CNOT} &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} & U_{CPHASE} &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} & U_Q &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & i & i & 0 \\ 0 & 1 & -1 & 0 \\ i & 0 & 0 & -i \end{pmatrix} \\
 U_{DCNOT} &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} & U_B &= \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} & 0 & 0 & 0 \\ 0 & 1 & 0 & i \\ 0 & i & 0 & 1 \\ 0 & 0 & \sqrt{2} & 0 \end{pmatrix} & U_{\sqrt{SWAP}} &= \frac{e^{-i\pi/8}}{\sqrt{2}} \begin{pmatrix} 1+i & 0 & 0 & 0 \\ 0 & 1 & i & 0 \\ 0 & i & 1 & 0 \\ 0 & 0 & 0 & 1+i \end{pmatrix} & U_{SWAP} &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}
 \end{aligned}$$

## $SU(4)$ group and $su(4)$ algebra

$$SU(4) \text{ group} \quad e^{\sum_{ij} \theta_{ij} T_{ij}} \quad \leftarrow \quad \sum_{ij} \theta_{ij} T_{ij} \quad su(4) \text{ algebra}$$

Generators:

$$T_{ij} = \frac{i}{2} \sigma_i^1 \otimes \sigma_j^2 = \frac{i}{2} \sigma_i^1 \sigma_j^2$$

Example:

$$T_{x0} = \frac{i}{2} \sigma_x^1 \otimes I$$

$[T_{ij}, T_{kl}]$	$T_{x0}$	$T_{y0}$	$T_{z0}$	$T_{0x}$	$T_{0y}$	$T_{0z}$	$T_{xx}$	$T_{xy}$	$T_{xz}$	$T_{yx}$	$T_{yy}$	$T_{yz}$	$T_{zx}$	$T_{zy}$	$T_{zz}$
$T_{x0}$	0	$-T_{z0}$	$T_{y0}$	0	0	0	0	0	0	$-T_{zx}$	$-T_{zy}$	$-T_{zz}$	$T_{yx}$	$T_{yy}$	$T_{yz}$
$T_{y0}$	$T_{z0}$	0	$-T_{x0}$	0	0	0	$T_{zx}$	$T_{zy}$	$T_{zz}$	0	0	0	$-T_{xx}$	$-T_{xy}$	$-T_{xz}$
$T_{z0}$	$-T_{y0}$	$T_{x0}$	0	0	0	0	$-T_{yx}$	$-T_{yy}$	$-T_{yz}$	$T_{xx}$	$T_{xy}$	$T_{xz}$	0	0	0
$T_{0x}$	0	0	0	0	$-T_{0z}$	$T_{0y}$	0	$-T_{xz}$	$T_{xy}$	0	$-T_{yz}$	$T_{yy}$	0	$-T_{zz}$	$T_{zy}$
$T_{0y}$	0	0	0	$T_{0z}$	0	$-T_{0x}$	$T_{xz}$	0	$-T_{xx}$	$T_{yz}$	0	$-T_{yx}$	$T_{zz}$	0	$-T_{zx}$
$T_{0y}$	0	0	0	$-T_{0y}$	$T_{0x}$	0	$-T_{xy}$	$T_{xx}$	0	$-T_{yy}$	$T_{yx}$	0	$-T_{zy}$	$T_{zx}$	0
$T_{xx}$	0	$-T_{zx}$	$T_{yx}$	0	$-T_{xz}$	$T_{xy}$	0	$-T_{0z}$	$T_{0y}$	$-T_{z0}$	0	0	$T_{y0}$	0	0
$T_{xy}$	0	$-T_{zy}$	$T_{yy}$	$T_{xz}$	0	$-T_{xx}$	$T_{0z}$	0	$-T_{0x}$	0	$-T_{z0}$	0	0	$T_{y0}$	0
$T_{xz}$	0	$-T_{zz}$	$T_{yz}$	$-T_{xy}$	$T_{xx}$	0	$-T_{0y}$	$T_{0x}$	0	0	0	$-T_{z0}$	0	0	$T_{y0}$
$T_{yx}$	$T_{zx}$	0	$-T_{xx}$	0	$-T_{yz}$	$T_{yy}$	$T_{z0}$	0	0	0	$-T_{0z}$	$T_{0y}$	$-T_{x0}$	0	0
$T_{yy}$	$T_{zy}$	0	$-T_{xy}$	$T_{yz}$	0	$-T_{yx}$	0	$T_{z0}$	0	$T_{0z}$	0	$-T_{0x}$	0	$-T_{x0}$	0
$T_{yz}$	$T_{zz}$	0	$-T_{xz}$	$-T_{yy}$	$T_{yx}$	0	0	0	$T_{z0}$	$-T_{0y}$	$T_{0x}$	0	0	0	$-T_{x0}$
$T_{zx}$	$-T_{yx}$	$T_{xx}$	0	0	$-T_{zz}$	$T_{zy}$	$-T_{y0}$	0	0	$T_{x0}$	0	0	0	$-T_{0z}$	$T_{0y}$
$T_{zy}$	$-T_{yy}$	$T_{xy}$	0	$T_{zz}$	0	$-T_{zx}$	0	$-T_{y0}$	0	0	$T_{x0}$	0	$T_{0z}$	0	$-T_{0x}$
$T_{zz}$	$-T_{yz}$	$T_{xz}$	0	$-T_{zy}$	$T_{zx}$	0	0	0	$-T_{y0}$	0	$T_{x0}$	$T_{x0}$	$-T_{0y}$	$T_{0x}$	0

## Cartan decomposition of $su(4)$

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

$$[p, k] \subset p$$

$$k = \text{span}\{T_{x0}, T_{y0}, T_{z0}, T_{0x}, T_{0y}, T_{0z}\} \quad [p, p] \subset k$$

$$p = \text{span}\{T_{xx}, T_{xy}, T_{xz}, T_{yx}, T_{yy}, T_{yz}, T_{zx}, T_{zy}, T_{zz}\}$$

$[T_{ij}, T_{kl}]$	$T_{x0}$	$T_{y0}$	$T_{z0}$	$T_{0x}$	$T_{0y}$	$T_{0z}$	$T_{xx}$	$T_{xy}$	$T_{xz}$	$T_{yx}$	$T_{yy}$	$T_{yz}$	$T_{zx}$	$T_{zy}$	$T_{zz}$
$T_{x0}$	0	$-T_{z0}$	$T_{y0}$	0	0	0	0	0	0	$-T_{zx}$	$-T_{zy}$	$-T_{zz}$	$T_{yx}$	$T_{yy}$	$T_{yz}$
$T_{y0}$	$T_{z0}$	0	$-T_{x0}$	0	0	0	$T_{zx}$	$T_{zy}$	$T_{zz}$	0	0	0	$-T_{xx}$	$-T_{xy}$	$-T_{xz}$
$T_{z0}$	$-T_{y0}$	$T_{x0}$	0	0	0	0	$-T_{yx}$	$-T_{yy}$	$-T_{yz}$	$T_{xx}$	$T_{xy}$	$T_{xz}$	0	0	0
$T_{0x}$	0	0	0	0	$-T_{0z}$	$T_{0y}$	0	$-T_{xz}$	$T_{xy}$	0	$-T_{yz}$	$T_{yy}$	0	$-T_{zz}$	$T_{zy}$
$T_{0y}$	0	0	0	$T_{0z}$	0	$-T_{0x}$	$T_{xz}$	0	$-T_{xx}$	$T_{yz}$	0	$-T_{yx}$	$T_{zz}$	0	$-T_{zx}$
$T_{0z}$	0	0	0	$-T_{0y}$	$T_{0x}$	0	$-T_{xy}$	$T_{xx}$	0	$-T_{yy}$	$T_{yx}$	0	$-T_{zy}$	$T_{zx}$	0
$T_{xx}$	0	$-T_{zx}$	$T_{yx}$	0	$-T_{xz}$	$T_{xy}$	0	$-T_{0z}$	$T_{0y}$	$-T_{z0}$	0	0	$T_{y0}$	0	0
$T_{xy}$	0	$-T_{zy}$	$T_{yy}$	$T_{xz}$	0	$-T_{xx}$	$T_{0z}$	0	$-T_{0x}$	0	$-T_{z0}$	0	0	$T_{y0}$	0
$T_{xz}$	0	$-T_{zz}$	$T_{yz}$	$-T_{xy}$	$T_{xx}$	0	$-T_{0y}$	$T_{0x}$	0	0	0	$-T_{z0}$	0	0	$T_{y0}$
$T_{yx}$	$T_{zx}$	0	$-T_{xx}$	0	$-T_{yz}$	$T_{yy}$	$T_{z0}$	0	0	0	$-T_{0z}$	$T_{0y}$	$-T_{x0}$	0	0
$T_{yy}$	$T_{zy}$	0	$-T_{xy}$	$T_{yz}$	0	$-T_{yx}$	0	$T_{z0}$	0	$T_{0z}$	0	$-T_{0x}$	0	$-T_{x0}$	0
$T_{yz}$	$T_{zz}$	0	$-T_{xz}$	$-T_{yy}$	$T_{yx}$	0	0	0	$T_{z0}$	$-T_{0y}$	$T_{0x}$	0	0	0	$-T_{x0}$
$T_{zx}$	$-T_{yx}$	$T_{xx}$	0	0	$-T_{zz}$	$T_{zy}$	$-T_{y0}$	0	0	$T_{x0}$	0	0	0	$-T_{0z}$	$T_{0y}$
$T_{zy}$	$-T_{yy}$	$T_{xy}$	0	$T_{zz}$	0	$-T_{zx}$	0	$-T_{y0}$	0	0	0	0	0	0	$-T_{0x}$
$T_{zz}$	$-T_{yz}$	$T_{xz}$	0	$-T_{zy}$	$T_{zx}$	0	0	0	$-T_{y0}$	0	$T_{x0}$	0	$T_{x0}$	$-T_{0y}$	$T_{0x}$

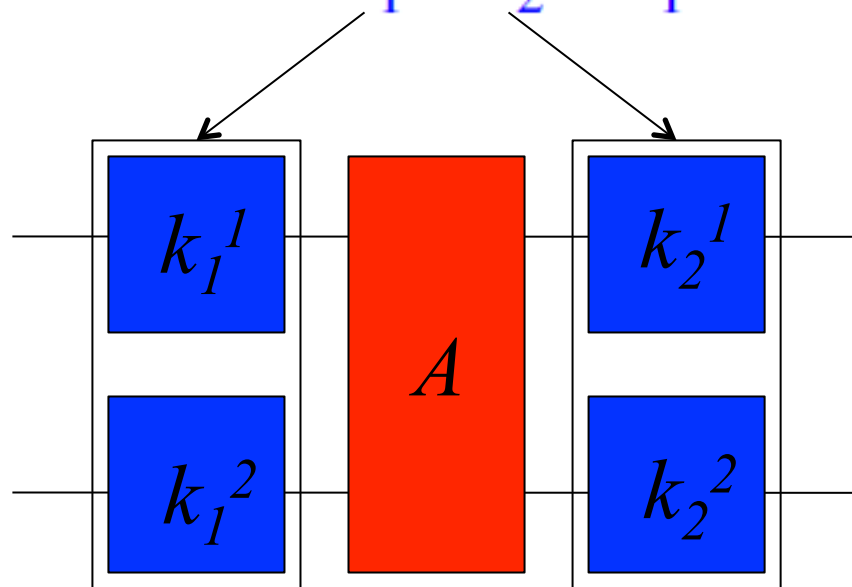
Cartan, maximal Abelian, subalgebra:

$$\mathfrak{a} = \text{span}\{T_{xx}, T_{yy}, T_{zz}\} = \text{span} \frac{i}{2} \{\sigma_x^1 \sigma_x^2, \sigma_y^1 \sigma_y^2, \sigma_z^1 \sigma_z^2\} \subset p$$

## Cartan decomposition of SU(4)

$$U \in SU(4)$$

$$U = k_1 A k_2 = k_1 e^{\frac{i}{2}(c_1 \sigma_x^1 \sigma_x^2 + c_2 \sigma_y^1 \sigma_y^2 + c_3 \sigma_z^1 \sigma_z^2)} k_2$$



$$k_1, k_2 \in SU(2) \otimes SU(2)$$

Parameter counting:

$$6 + 3 + 6 = 15 = 4^2 - 1$$

If two gates have the same  $A$  in the Cartan decomposition, they are locally equivalent:

$$U_1 = k_1 U_2 k_2$$

## Local equivalence and construction of local invariants

Two gates are locally equivalent if they differ only by local operations

$$U_1 = k_1 U_2 k_2 \quad k_1, k_2 \in SU(2) \otimes SU(2)$$

Construction:

1) Cartan decomposition (fix: the standard computational basis)

$$U = k_1 A k_2 = k_1 e^{\frac{i}{2}(c_1 \sigma_x^1 \sigma_x^2 + c_2 \sigma_y^1 \sigma_y^2 + c_3 \sigma_z^1 \sigma_z^2)} k_2$$

2) transformation into the Bell basis

$$Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & i & i & 0 \\ 0 & 1 & -1 & 0 \\ i & 0 & 0 & -i \end{pmatrix} \begin{array}{l} |00\rangle \rightarrow \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ |01\rangle \rightarrow \frac{i}{\sqrt{2}}(|01\rangle + |10\rangle) \\ |10\rangle \rightarrow \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \\ |11\rangle \rightarrow \frac{i}{\sqrt{2}}(|00\rangle - |11\rangle) \end{array}$$

$$U_B = Q^\dagger U Q = Q^\dagger k_1 Q Q^\dagger A Q Q^\dagger k_2 Q = O_1 F O_2$$

$$O_1, O_2 \in SO(4) \quad O_k^T O_k = I$$

$$F = Q^\dagger A Q = \text{diag} \left\{ e^{i \frac{c_1 - c_2 + c_3}{2}}, e^{i \frac{c_1 + c_2 - c_3}{2}}, e^{i \frac{c_1 + c_2 + c_3}{2}}, e^{i \frac{-c_1 + c_2 + c_3}{2}} \right\}$$

$$i/2\{\sigma_x^1 \sigma_x^2, \sigma_y^1 \sigma_y^2, \sigma_z^1 \sigma_z^2\} \rightarrow i/2\{\sigma_z^1, -\sigma_z^2, \sigma_z^1 \sigma_z^2\}$$

J. Makhlin, QIP, 1, 243 (2003)

J. Zhang, J. Vala, S. Sastry, K.B. Whaley  
Phys. Rev. A 67, 042313 (2003)



## Local equivalence and construction of local invariants

$$U_B = Q^\dagger U Q = Q^\dagger k_1 Q Q^\dagger A Q Q^\dagger k_2 Q = O_1 F O_2$$

3) elimination of the local part  $O_1$

$$m = U_B^T U_B = O_2^T F O_1^T O_1 F O_2 = O_2^T F^2 O_2$$

$$O_k^T O_k = I$$

$$F^2 = \text{diag} \{ e^{i(c_1 - c_2 + c_3)}, e^{i(c_1 + c_2 - c_3)}, e^{i(c_1 + c_2 + c_3)}, e^{i(-c_1 + c_2 + c_3)} \}$$

4) characteristic equation of  $m$  and elimination of  $O_2$

$$\lambda^4 - \text{tr}(m)\lambda^3 + \frac{1}{2} [\text{tr}^2(m) - \text{tr}(m^2)] \lambda^2 - \text{tr}^*(m)\lambda + 1 = 0$$

$F^2$  determines the spectrum on the Makhlin matrix  $m$ :  $\text{tr}(m) = \text{tr}(F^2)$

## Local invariants

$$g_1 = \text{Re} \left\{ \frac{\text{tr}^2(m)}{16} \right\}, g_2 = \text{Im} \left\{ \frac{\text{tr}^2(m)}{16} \right\}, g_3 = \frac{\text{tr}^2(m) - \text{tr}(m^2)}{4}$$

## Local equivalence classes

Local invariants:

$$g_1 = \operatorname{Re} \left\{ \frac{\operatorname{tr}^2(m)}{16} \right\}, \quad g_2 = \operatorname{Im} \left\{ \frac{\operatorname{tr}^2(m)}{16} \right\}, \quad g_3 = \frac{\operatorname{tr}^2(m) - \operatorname{tr}(m^2)}{4}$$

Uniquely characterize a class of gates that are equivalent up to local, single qubit, transformations; they define **local equivalence classes [U]**.

Relation between the Cartan decomposition and local invariants:

$$\sigma(\mathbf{F}^2) = \left\{ e^{i(c_1 - c_2 + c_3)}, e^{i(c_1 + c_2 - c_3)}, e^{-i(c_1 + c_2 + c_3)}, e^{i(-c_1 + c_2 + c_3)} \right\}$$

$$g_1 = \frac{1}{4} [\cos(2c_1) + \cos(2c_2) + \cos(2c_3) + \cos(2c_1) \cos(2c_2) \cos(2c_3)]$$

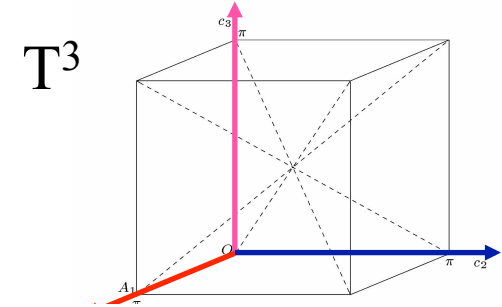
$$g_2 = \frac{1}{4} \sin(2c_1) \sin(2c_2) \sin(2c_3)$$

$$g_3 = \cos(2c_1) + \cos(2c_2) + \cos(2c_3)$$

# Weyl chamber

Non-local factor  $A$  of the Cartan decomposition has the structure of three-torus

$$A = e^{\frac{i}{2} (c_1 \sigma_x^1 \sigma_x^2 + c_2 \sigma_y^1 \sigma_y^2 + c_3 \sigma_z^1 \sigma_z^2)}$$



Local invariants

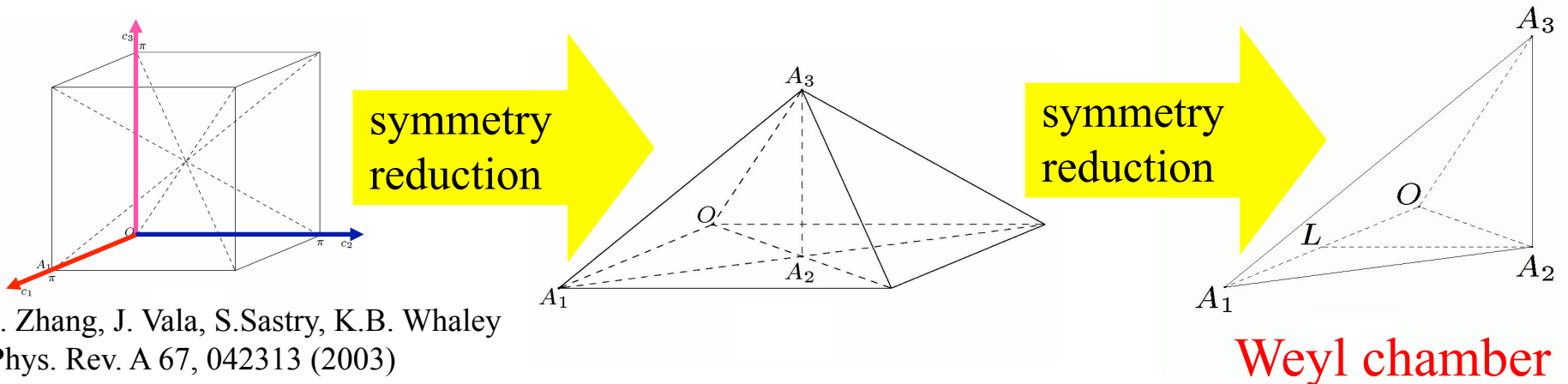
$$g_1 = \frac{1}{4} [\cos(2c_1) + \cos(2c_2) + \cos(2c_3) + \cos(2c_1)\cos(2c_2)\cos(2c_3)]$$

$$g_2 = \frac{1}{4} \sin(2c_1)\sin(2c_2)\sin(2c_3)$$

$$g_3 = \cos(2c_1) + \cos(2c_2) + \cos(2c_3)$$

- $\{X \in \mathfrak{a} : c_1 - c_2 = 0\}, \quad \{X \in \mathfrak{a} : c_1 + c_2 = \pi\}$
- $\{X \in \mathfrak{a} : c_1 - c_3 = 0\}, \quad \{X \in \mathfrak{a} : c_1 + c_3 = \pi\}$
- $\{X \in \mathfrak{a} : c_2 - c_3 = 0\}, \quad \{X \in \mathfrak{a} : c_2 + c_3 = \pi\}$

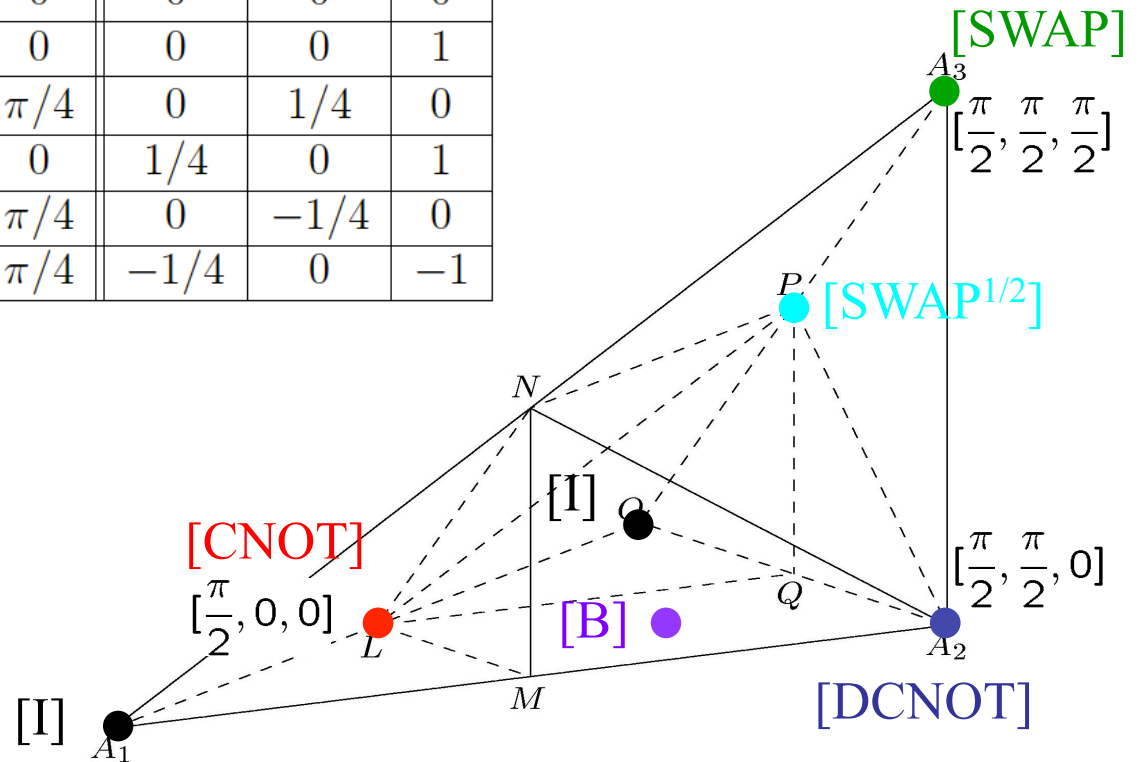
are invariant with interchanges of  $c_1, c_2,$  and  $c_3$  with & without sign flips:



## Examples

Each point inside of the Weyl chamber corresponds to one local equivalence class. This is unique with except of the base of the Weyl chamber.

point (gate)	$c_1$	$c_2$	$c_3$	$g_1$	$g_2$	$g_3$
$O, A_1$ ([I])	$0, \pi$	0	0	1	0	3
$A_2$ ([DCNOT])	$\pi/2$	$\pi/2$	0	0	0	-1
$A_3$ ([SWAP])	$\pi/2$	$\pi/2$	$\pi/2$	-1	0	-3
$B$ ([B-Gate])	$\pi/2$	$\pi/4$	0	0	0	0
$L$ ([CNOT])	$\pi/2$	0	0	0	0	1
$P$ ([ $\sqrt{\text{SWAP}}$ ])	$\pi/4$	$\pi/4$	$\pi/4$	0	$1/4$	0
$Q, M$	$\pi/4, 3\pi/4$	$\pi/4$	0	$1/4$	0	1
$N$	$3\pi/4$	$\pi/4$	$\pi/4$	0	$-1/4$	0
$R$	$\pi/2$	$\pi/4$	$\pi/4$	$-1/4$	0	-1



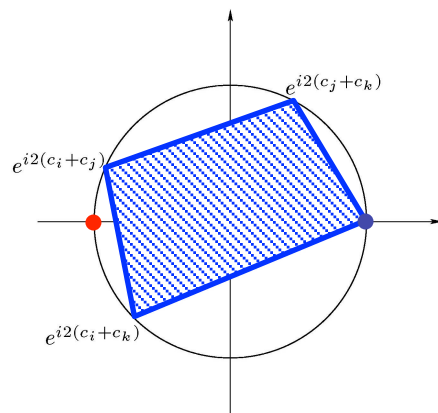
# Perfect entanglers

## *Definition*

A two qubit gate is called a **perfect entangler** if it can produce a maximally entangled state from a product state.

## *Theorem*

A two qubit gate  $U$  is a perfect entangler if and only if **the convex hull** of the eigenvalues of the Makhlin matrix  $m(U)$  contains zero.



## *Examples*

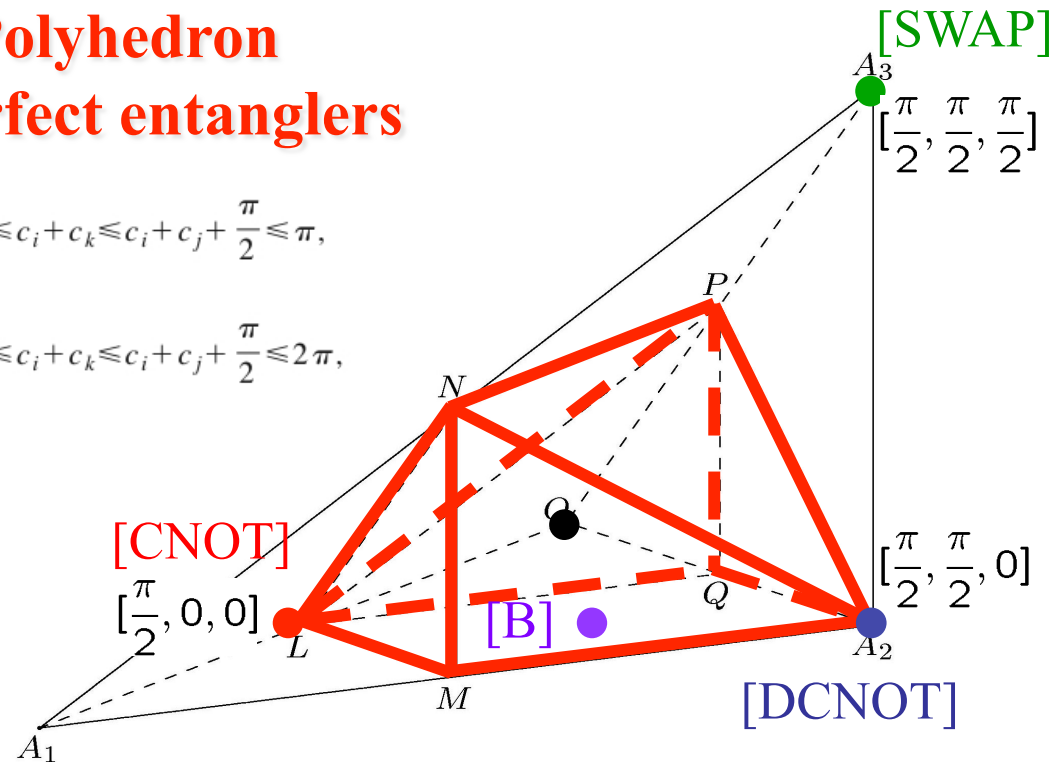
**CNOT**

$$\sigma[m(\text{CNOT})] = \{1, 1, -1, -1\}$$

## Polyhedron of perfect entanglers

$$\frac{\pi}{2} \leq c_i + c_k \leq c_i + c_j + \frac{\pi}{2} \leq \pi,$$

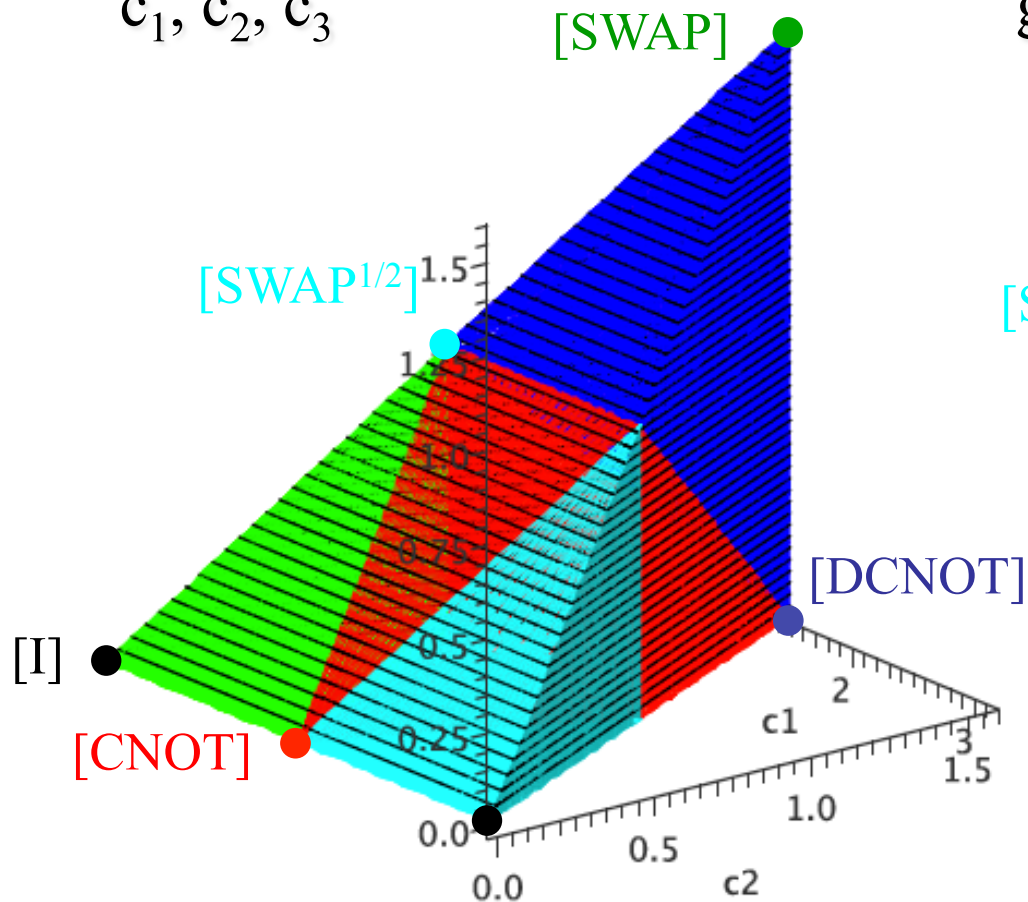
$$\frac{3\pi}{2} \leq c_i + c_k \leq c_i + c_j + \frac{\pi}{2} \leq 2\pi,$$



# Weyl chamber and local equivalence classes

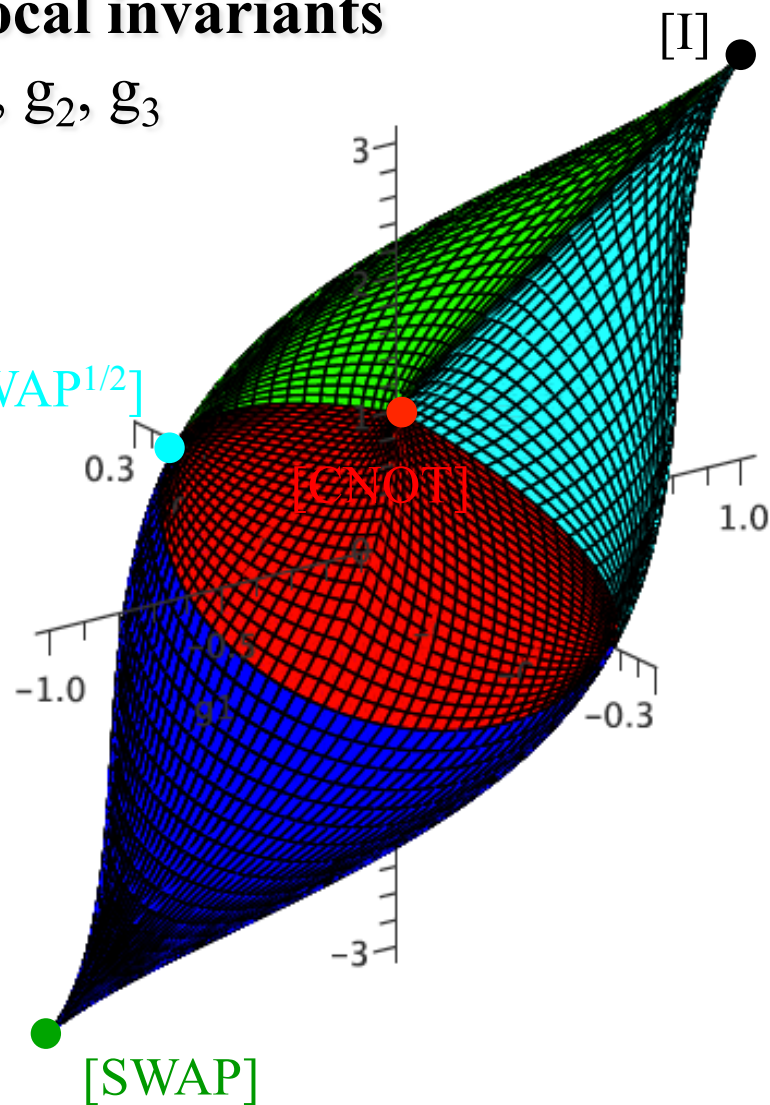
## Weyl chamber coordinates

$c_1, c_2, c_3$



## Local invariants

$g_1, g_2, g_3$



# Generation of non-local gates: example

Josephson junction charge-coupled qubits

$$H = -(\alpha E_L/2) (\sigma_x^1 + \sigma_x^2) + \alpha^2 E_L \sigma_y^1 \sigma_y^2$$

curvature

translation

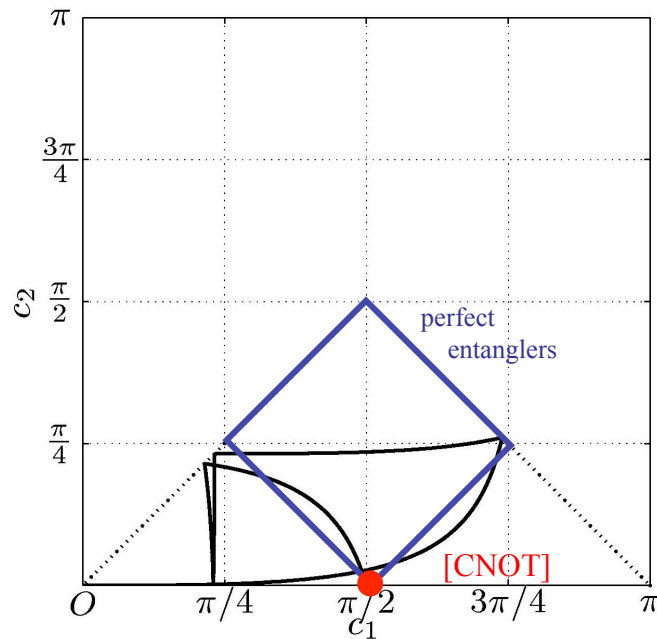
Weyl chamber trajectory:

$$c_1(t) = \alpha^2 E_L t - \omega(\alpha, t),$$

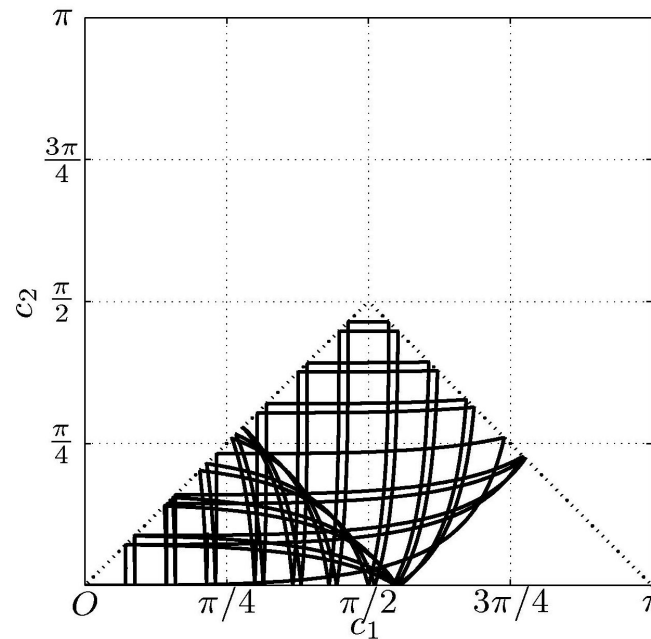
$$c_2(t) = \alpha^2 E_L t + \omega(\alpha, t),$$

$$c_3(t) = 0.$$

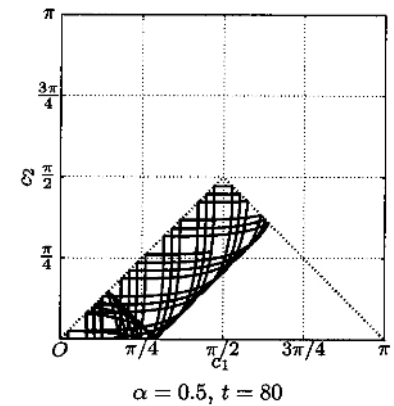
$$\omega(\alpha, t) = \tan^{-1}\left(\frac{\alpha^2 + 1}{2}\right)$$



$$\alpha = 1.1991, t = 2.7309$$



$$\alpha = 1.1991, t = 20$$



$$\alpha = 0.5, t = 80$$





**Optimal control applications:**  
Phys. Rev. A **84**, 042315 (2011)  
&  
a work in progress

## II. Optimal control applications



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**Jiri Vala**  
**Paul Watts**

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**V E R S I T Ä T**

**Christianne Koch**  
**Daniel Reich**

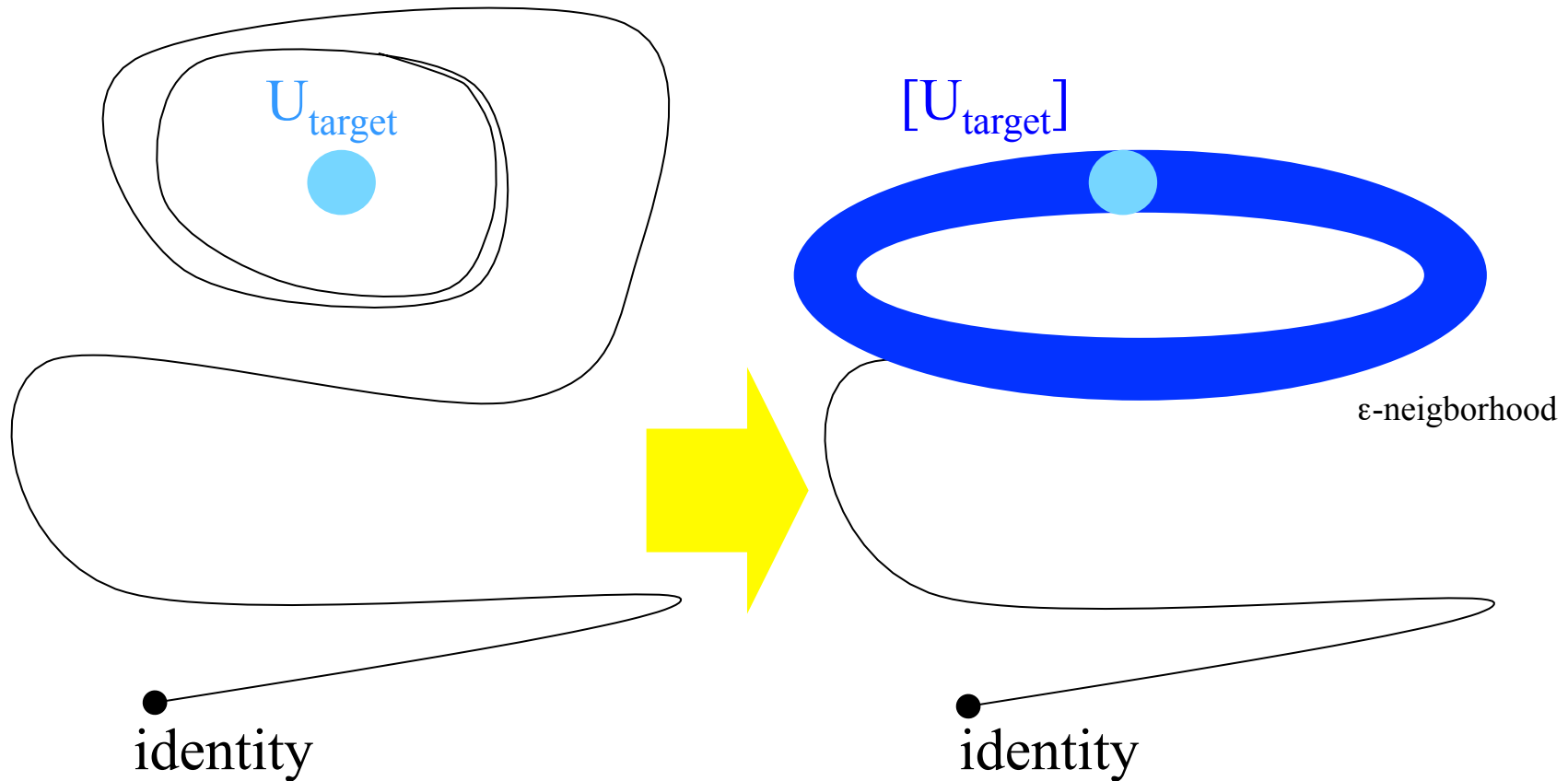


**Haidong Yuan**



# Optimal control

Optimization target is defined not as a specific target gate  $U_{target}$  but rather its local equivalence class  $[U_{target}]$ , i.e.  $SU(2) \times SU(2)$  orbit of  $U_{target}$ .



# Optimal control

M.M. Muller et al.,  
Phys. Rev. A 84, 042315 (2011).

## Direct optimization functional

$$J_T^D = 1 - \frac{1}{N} \text{Re}[\text{Tr}\{\hat{\mathcal{O}}^+ \hat{\mathcal{P}}_N \hat{\mathcal{U}}(T, 0; \varepsilon) \hat{\mathcal{P}}_N\}]$$

with possible additional terms

$$J = J_T^D + g_a + g_b$$

finite pulse fluence

$$g_a = \lambda_a \int_0^T [\varepsilon(t) - \varepsilon_{\text{ref}}(t)]^2 / S(t) dt$$

loss of population

$$g_b = \frac{\lambda_b}{NT} \int_0^T \sum_{m=1}^N \langle \varphi_m(t) | \hat{\mathcal{P}}_{\text{avoid}} | \varphi_m(t) \rangle dt$$

## Optimization functional based on local invariants

$$J_T^{LI} = \Delta g_1^2 + \Delta g_2^2 + \Delta g_3^2 + 1 - \frac{1}{N} \text{Tr}\{\hat{\mathcal{U}}_{T,N} \hat{\mathcal{U}}_{T,N}^+\}$$

Krotov iteration

$$\varepsilon^{(i+1)}(t) = \varepsilon^{(i)}(t) + \frac{S(t)}{\lambda_a} \text{Im} \left\{ \sum_{k=1}^N \langle \chi_k^{(i)}(t) | \frac{\partial \hat{\mathcal{H}}^{(i+1)}}{\partial \varepsilon} | \varphi_k^{(i+1)}(t) \rangle + \frac{1}{2} \sigma(t) \sum_{k=1}^N \langle \Delta \varphi_k^{(i+1)}(t) | \frac{\partial \hat{\mathcal{H}}^{(i+1)}}{\partial \varepsilon} | \varphi_k^{(i+1)}(t) \rangle \right\}$$

## Case I: Effective spin model

Trapped polar molecules with  $^2\Sigma_{1/2}$  electronic ground state subject to a near resonant microwave driving inducing strong dipole-dipole coupling:

$$\hat{H}_{\text{eff}}(t) = \frac{\hbar|\Omega(t)|}{8} \sum_{i,j=1}^4 \hat{\sigma}_i A_{ij}(x_0,t) \hat{\sigma}_j$$

SrF molecules in optical lattice with  $a=300$  nm and 15GHz microwave fields with different polarizations

$$\hat{H}(t) = \hat{H}_0 + S(t)\hat{H}_1$$

M.M. Muller et al.,  
Phys. Rev. A 84, 042315 (2011).

drift

$$\hat{H}_0 = \begin{pmatrix} 5.711 & 0.324 & 0.324 & 0 \\ 0.324 & -1.840 & 1.054 & 0 \\ 0.324 & 1.054 & 1.840 & 0 \\ 0 & 0 & 0 & -2.030 \end{pmatrix}$$

control

$$\hat{H}_1 = S(t) \begin{pmatrix} -153.65 & 0 & 0 & 3.906 \\ 0 & 153.65 & 16.085 & 0 \\ 0 & 16.085 & 153.65 & 0 \\ 3.906 & 0 & 0 & -153.65 \end{pmatrix}$$

↓  
envelope function

cw field:

CNOT:  $\delta = 1.2$  kHz and  $\Omega = 590$  kHz

B-gate:  $\delta = 1.2$  kHz and  $\Omega = 4.74$  MHz

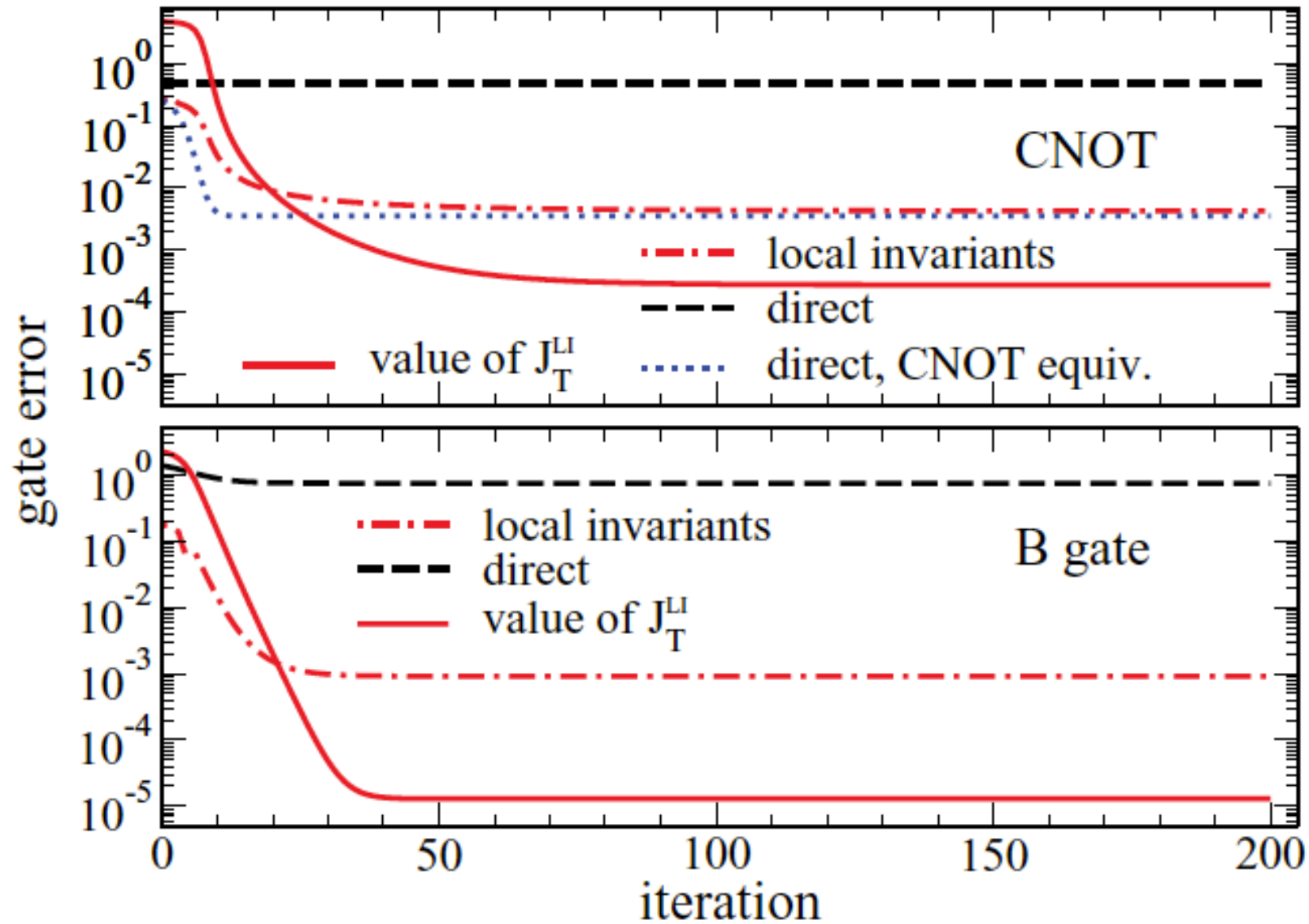
pulsed field:

CNOT:  $\delta = 50$  kHz and  $\Omega_0 = 1.81$  MHz

B-gate:  $\delta = 84$  kHz and  $\Omega_0 = 1.81$  MHz

# Case I: Results

M.M. Muller et al.,  
Phys. Rev. A 84, 042315 (2011).



## Case II: Rydberg gate with trapped neutral atoms

Atoms of  $^{87}\text{Rb}$  trapped by optical tweezers with a non-local gate implemented by simultaneous near resonant two-photon transition to Rydberg states

$$\begin{aligned} |0\rangle &= |5s_{1/2}, F = 2, M_F = 2\rangle & |i\rangle &= |5p_{1/2}, F = 2, M_F = 2\rangle \\ |1\rangle &= |5s_{1/2}, F = 1, M_F = 1\rangle & |r\rangle &= |5d_{3/2}, F = 3, M_F = 3\rangle \end{aligned}$$

The Hamiltonian for a single trapped atom in RWA

M.M. Muller et al.,  
Phys. Rev. A 84, 042315 (2011).

$$\begin{aligned} \hat{H}_j^{(1)}(t) &= |0\rangle\langle 0| \otimes (\hat{T} + V_{\text{trap}}(\hat{\mathbf{x}}_j)) + |1\rangle\langle 1| \otimes (\hat{T} + V_{\text{trap}}(\hat{\mathbf{x}}_j)) \\ &+ |i\rangle\langle i| \otimes \left( \hat{T} + \frac{\delta_R}{2} \right) + |r\rangle\langle r| \otimes \left( \hat{T} + \frac{\delta_B}{2} \right) \\ &+ \frac{\Omega_R(t)}{2} (|0\rangle\langle i| + |i\rangle\langle 0|) \otimes \mathbb{1}_{\hat{\mathbf{x}}_j} \\ &+ \frac{\Omega_B(t)}{2} (|i\rangle\langle r| + |r\rangle\langle i|) \otimes \mathbb{1}_{\hat{\mathbf{x}}_j} \end{aligned}$$

$$\begin{aligned} \omega_R &= 795 \text{ nm} \\ \omega_B &= 474 \text{ nm} \\ \delta_R &= 2\pi \cdot 600 \text{ MHz} \\ \delta_B &= 0 \\ \Omega_{R,0} &= \Omega_{B,0} = 2\pi \cdot 260 \text{ MHz} \end{aligned}$$

The total two-atom Hamiltonian

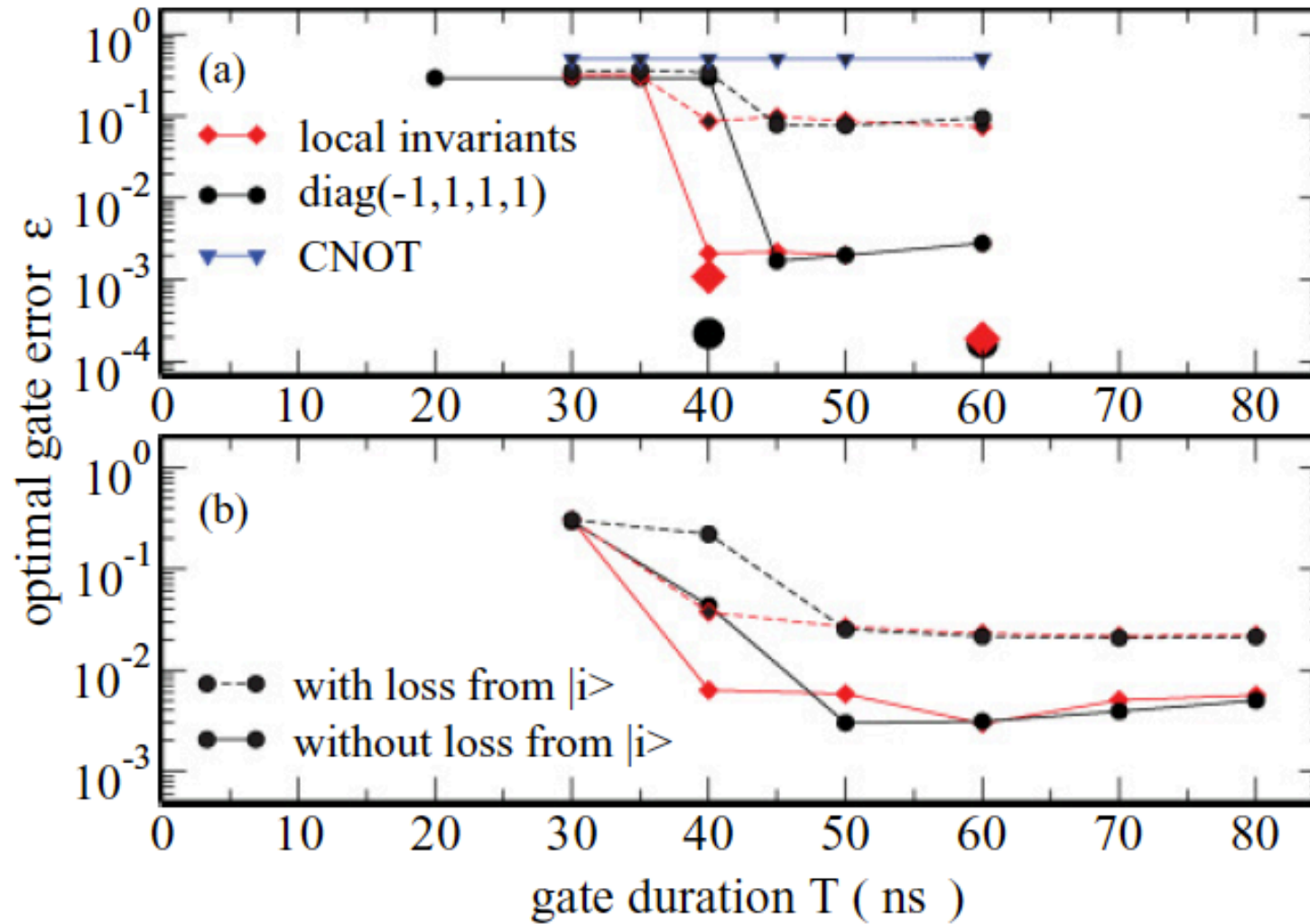
$$\hat{H}^{(2)}(t) = \hat{H}_1^{(1)}(t) \otimes \mathbb{1}_{4,2} \otimes \mathbb{1}_{\hat{\mathbf{x}}_2} + \mathbb{1}_{4,1} \otimes \hat{H}_2^{(1)}(t) \otimes \mathbb{1}_{\hat{\mathbf{x}}_1} + \boxed{|rr\rangle\langle rr| \otimes \frac{u_0}{\hat{r}^3}}$$

Rydberg-Rydberg interaction

50MHz at  $r_0 = 4\mu\text{m}$ , i.e. 10 ns in  $|rr\rangle$  to pick the phase  $\pi$

## Case II: Results

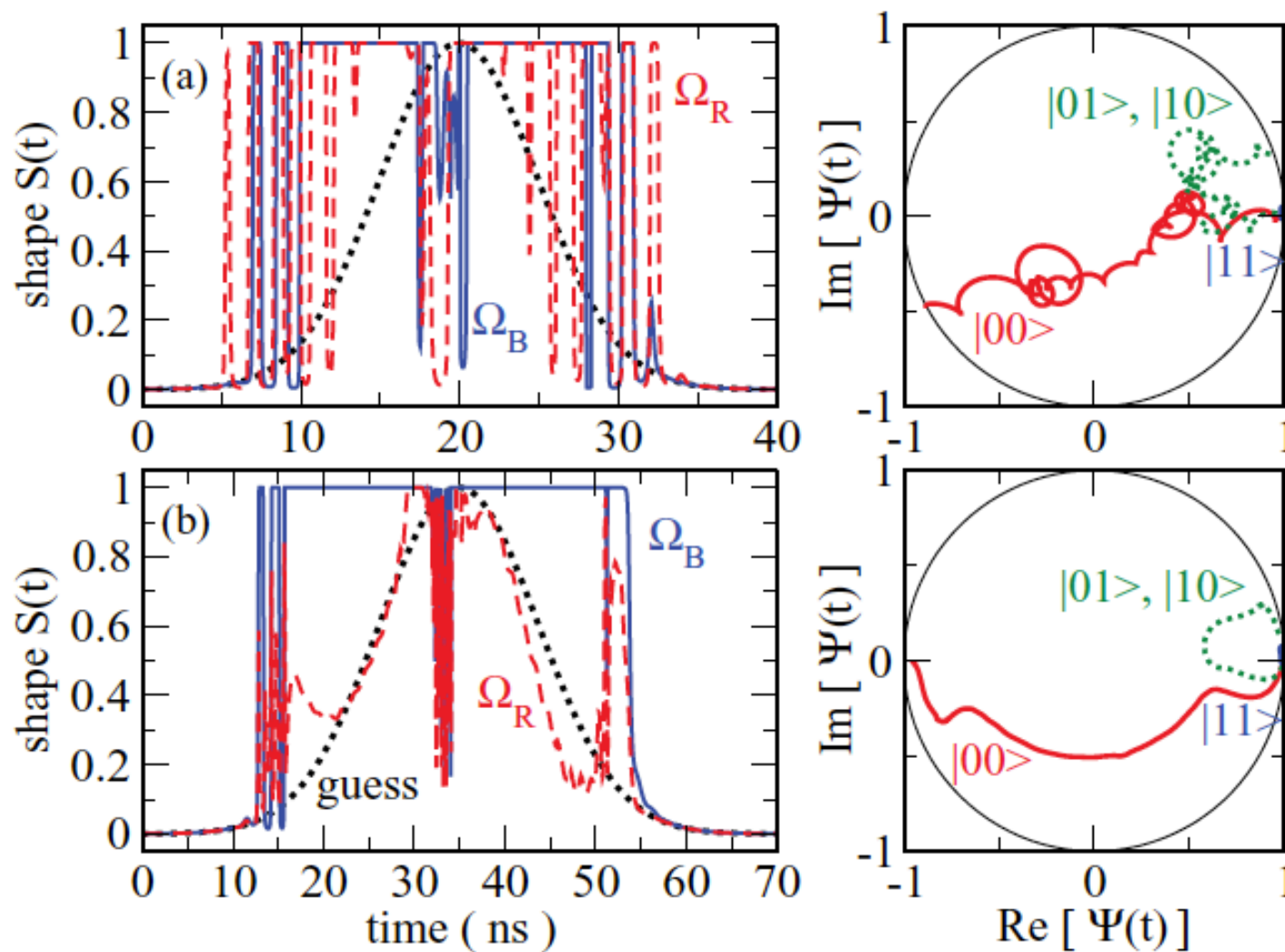
M.M. Muller et al.,  
Phys. Rev. A 84, 042315 (2011)



## Case II: Effect of spontaneous emission

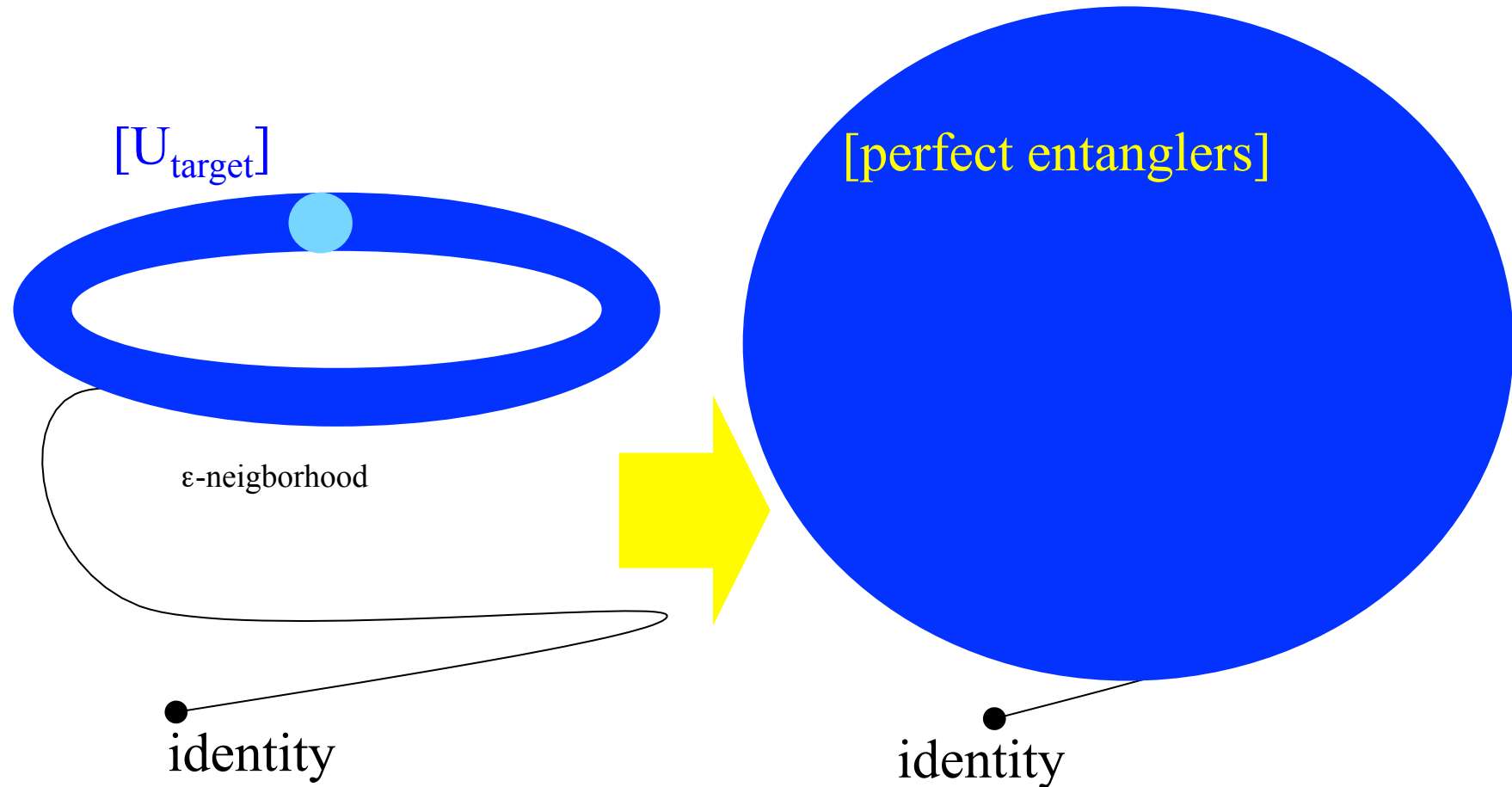
M.M. Muller et al.,  
Phys. Rev. A 84, 042315 (2011)

spontaneous  
emission



## Perfect entanglers

Optimization target is defined not as a specific local equivalence class  $[U_{target}]$ , i.e.  $SU(2) \times SU(2)$  orbit of  $U_{target}$ , but **the full set of perfect entanglers**





## Optimal control: perfect entanglers

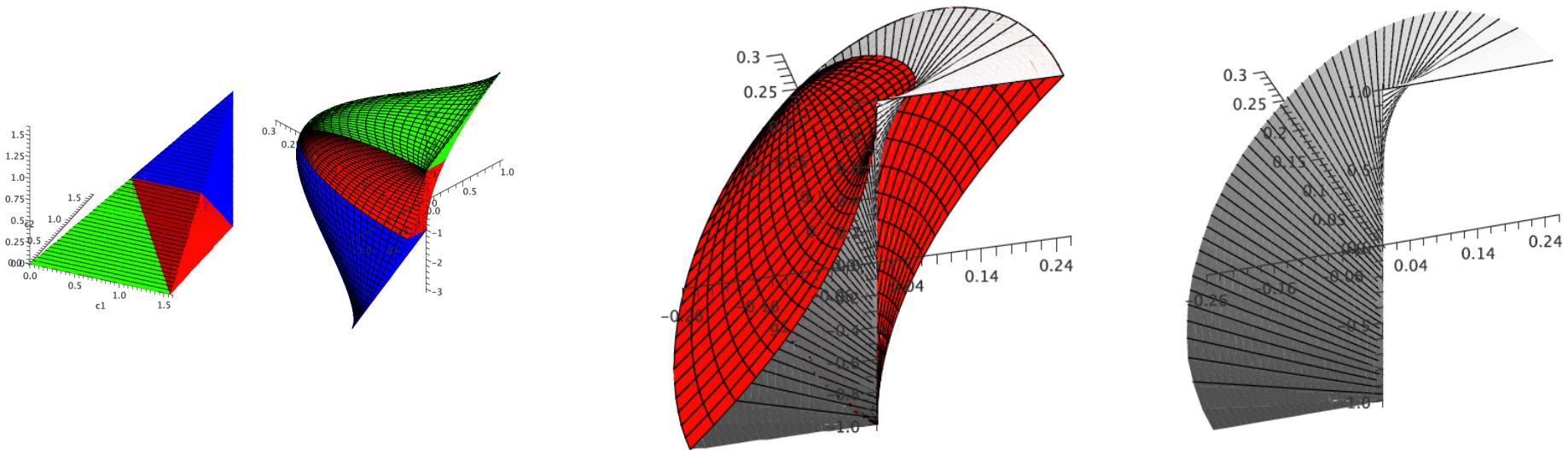
**Direct optimization functional**

$$J_T^D = 1 - \frac{1}{N} \text{Re}[\text{Tr}\{\hat{O}^+ \hat{P}_N \hat{U}(T, 0; \varepsilon) \hat{P}_N\}]$$

**is to be based on the function**

$$\mathcal{D}(U) = g_3 \sqrt{g_1^2 + g_2^2} - g_1$$

**which goes to zero when the evolution operator reaches perfect entanglers**



**Numerical experiment:** Tommaso Calarco (first results),  
Christiane Koch (in progress)

## III. Two-qubit gates as a metric space



**Jiri Vala**  
**Paul Watts**  
**Maurice O'Connor**

**Metric properties and applications:**  
P. Watts et al., submitted (2013)

## Decomposition and parametrisation of $SU(4)$

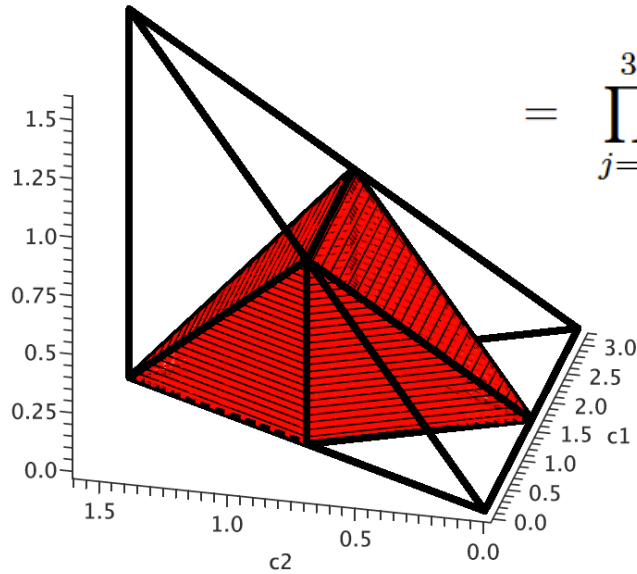
$$U = k_1 A k_2$$

1) Local part

$$\begin{aligned} k(\vec{\alpha}, \vec{\beta}) &= \exp\left(-\frac{i}{2}\vec{\alpha} \cdot \vec{\sigma}\right) \otimes \exp\left(-\frac{i}{2}\vec{\beta} \cdot \vec{\sigma}\right) \\ &= \left[ I \cos\left(\frac{\alpha}{2}\right) - i\hat{\alpha} \cdot \vec{\sigma} \sin\left(\frac{\alpha}{2}\right) \right] \otimes \left[ I \cos\left(\frac{\beta}{2}\right) - i\hat{\beta} \cdot \vec{\sigma} \sin\left(\frac{\beta}{2}\right) \right] \end{aligned}$$

2) Non-local part

$$\begin{aligned} A(c_1, c_2, c_3) &= \exp\left(-\frac{i}{2} \sum_{j=1}^3 c_j \sigma_j \otimes \sigma_j\right) \\ &= \prod_{j=1}^3 \left[ I \otimes I \cos\left(\frac{c_j}{2}\right) - i\sigma_j \otimes \sigma_j \sin\left(\frac{c_j}{2}\right) \right] \end{aligned}$$



Restriction to the Weyl chamber:

$$\begin{aligned} 0 \leq c_3 \leq c_2 \leq c_1 \leq \frac{\pi}{2} \quad & \& \\ \frac{\pi}{2} < c_1 < \pi, \quad & 0 \leq c_3 \leq c_2 < \pi - c_1 \end{aligned}$$

Parameters:

$$x = (x^1, \dots, x^{15}) = (\alpha_1, \theta_1, \phi_1, \beta_1, \lambda_1, \xi_1, \alpha_2, \theta_2, \phi_2, \beta_2, \lambda_2, \xi_2, c_1, c_2, c_3)$$

## Invariant measure

Calculation of the Haar measure for SU(4) and its Cartan subalgebra:

We start with the Maurer-Cartan form

$$\Theta := U^{-1}dU$$

which can be rewritten in terms of Lie algebra generators and coordinate 1-forms

$$\Theta = -iE^A{}_{\mu}(x) T_A dx^{\mu}$$

where  $\Theta$  is an  $N \times N$  matrix whose determinant gives us the Haar measure

$$d\mu = \frac{|\det E(x)| d^N x}{\int_M |\det E(x')| d^N x'}$$

The results for SU(2):

$$\begin{aligned}\Theta_{SU(2)} &= e^{i\vec{\alpha}\cdot\vec{\sigma}/2} de^{-i\vec{\alpha}\cdot\vec{\sigma}/2} = -\frac{i}{2} \sum_i \zeta^i(\vec{\alpha}) \sigma_i \\ d\mu_{SU(2)}(\alpha, \theta, \phi) &= \frac{1}{8\pi^2} \sin^2\left(\frac{\alpha}{2}\right) \sin\theta d\alpha \wedge d\theta \wedge d\phi\end{aligned}$$

## Haar measure for SU(4)

$$d\mu = d\mu_{SU(2)}(\vec{\alpha}_1) \wedge d\mu_{SU(2)}(\vec{\beta}_1) \wedge d\mu_{SU(2)}(\vec{\alpha}_2) \wedge d\mu_{SU(2)}(\vec{\beta}_2) \wedge d\mu_{\mathcal{A}}(c_1, c_2, c_3)$$

Local parts:

$$d\mu_{SU(2)}(\alpha, \theta, \phi) = \frac{1}{8\pi^2} \sin^2\left(\frac{\alpha}{2}\right) \sin\theta \, d\alpha \wedge d\theta \wedge d\phi$$

Non-local part:

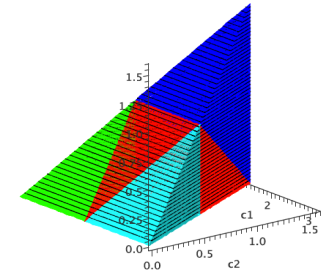
$$\begin{aligned} d\mu_{\mathcal{A}}(c_1, c_2, c_3) &= \frac{48}{\pi} |\sin(c_1 + c_2) \sin(c_1 - c_2) \sin(c_1 + c_3) \sin(c_1 - c_3) \\ &\quad \times \sin(c_2 + c_3) \sin(c_2 - c_3)| \, dc_1 \wedge dc_2 \wedge dc_3, \\ &= M_{\mathcal{A}}(c_1, c_2, c_3) \, dc_1 \wedge dc_2 \wedge dc_3 \end{aligned}$$

The full SU(4):

$$\begin{aligned} d\mu &= \frac{3}{256\pi^9} \prod_{i=1}^2 \left[ \sin^2\left(\frac{\alpha_i}{2}\right) \sin\theta_i \sin^2\left(\frac{\beta_i}{2}\right) \sin\lambda_i \right] \\ &\quad \times \prod_{1 \leq j < k \leq 3} [\sin(c_j + c_k) \sin(c_j - c_k)] \, d^{15}x. \end{aligned}$$

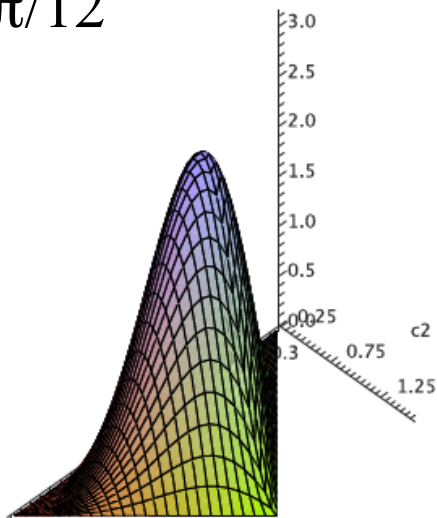
# What is the size of control targets?

Control targets in the Weyl chamber can be defined as a small neighborhood of the local equivalence class, e.g. a cube of the volume  $V_{Wc} = a^3$ .

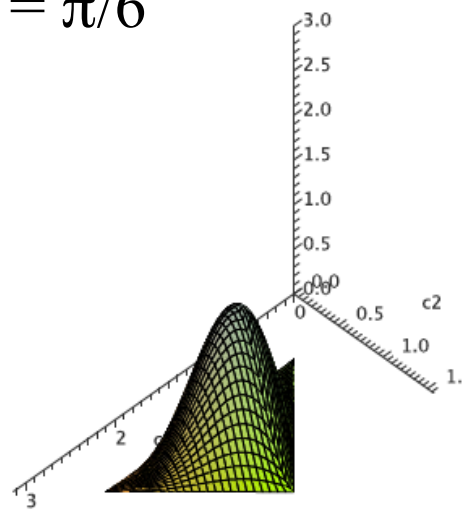


**The corresponding invariant volume in the full  $SU(4)$  depends on the location in the Weyl chamber**

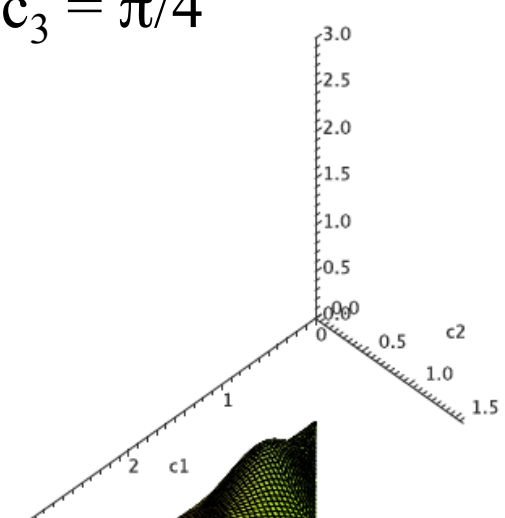
$$c_3 = \pi/12$$



$$c_3 = \pi/6$$



$$c_3 = \pi/4$$



## Examples

$$V(\mathcal{U}) = \int_{(SU(2) \otimes SU(2)) \times (SU(2) \otimes SU(2)) \times \mathcal{U}} d\mu = \int_{\mathcal{U}} d\mu_{\mathcal{A}}$$

[1] at  $(0, 0, 0)$

$$a^9/40\pi + O(a^{11})$$

[SWAP] at  $(\pi/2, \pi/2, \pi/2)$

$$a^9/40\pi + O(a^{11})$$

$[\sqrt{\text{SWAP}}]$  at  $(\pi/4, \pi/4, \pi/4)$

$$8a^6/5\pi + O(a^8)$$

[B-gate] at  $(\pi/2, \pi/4, 0)$

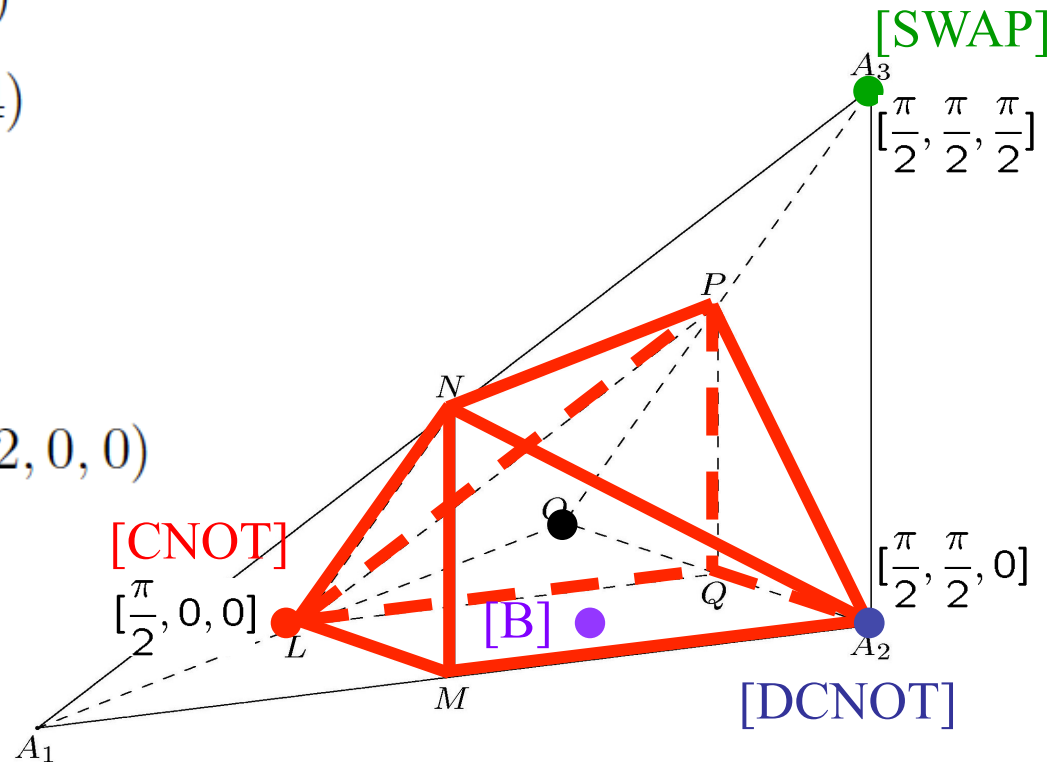
$$12a^3/\pi + O(a^5)$$

[CNOT]/[CPHASE] at  $(\pi/2, 0, 0)$

$$4a^5/\pi + O(a^7)$$

[DCNOT] at  $(\pi/2, \pi/2, 0)$

$$4a^5/\pi + O(a^7)$$

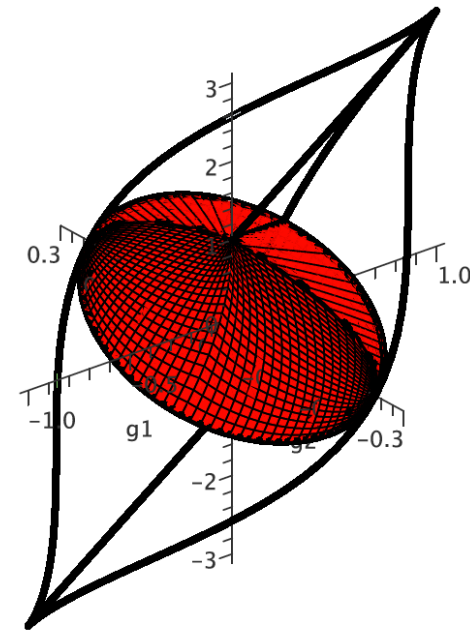
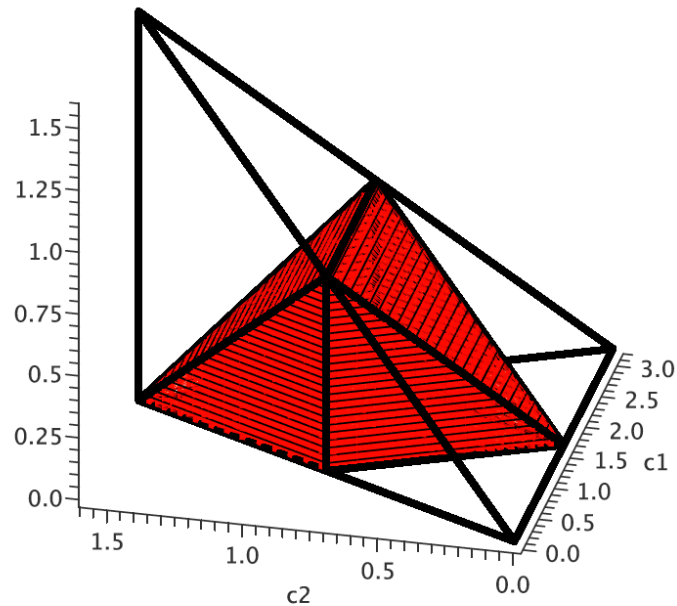


## Invariant volume of perfect entanglers

The perfect entanglers occupy a half of the volume of the Weyl chamber but the invariant volume of the perfect entanglers in the full  $SU(4)$  is the integral

$$V(\mathcal{U}) = \int_{(SU(2) \otimes SU(2)) \times (SU(2) \otimes SU(2)) \times \mathcal{U}} d\mu = \int_{\mathcal{U}} d\mu_{\mathcal{A}}$$

over the perfect entanglers in the Weyl chamber



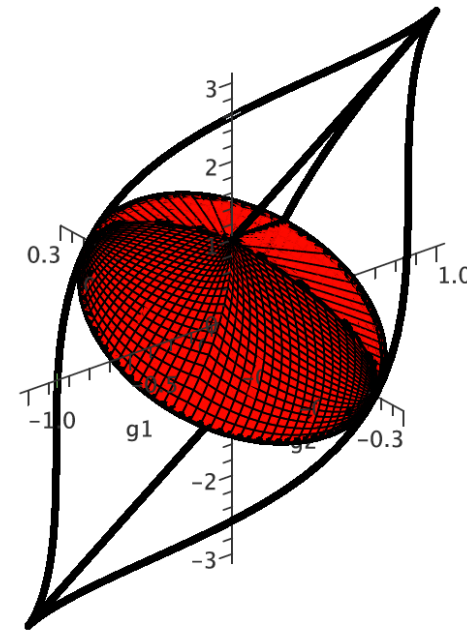
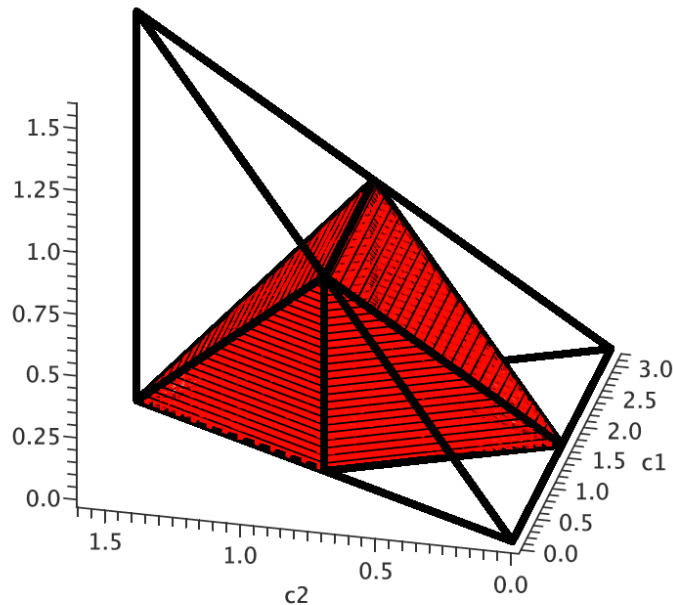


## Invariant volume of perfect entanglers

The perfect entanglers occupy a half of the volume of the Weyl chamber but the invariant volume of the perfect entanglers in the full  $SU(4)$  is the integral

$$V(\mathcal{U}) = \int_{(SU(2) \otimes SU(2)) \times (SU(2) \otimes SU(2)) \times \mathcal{U}} d\mu = \int_{\mathcal{U}} d\mu_{\mathcal{A}}$$

over the perfect entanglers in the Weyl chamber



Perfect entanglers occupy **over 84%** of the total volume of  $SU(4)$

Targeting perfect entanglers as clay pigeon shooting



## Conclusions

### **Geometric theory of two-qubit gates**

- provides powerful representation of two-qubit local equivalence classes;
- allows insights into structure and properties of perfect entanglers;
- gives intuitive picture of two-qubit quantum evolution;
- enables analytical construction of two-qubit quantum circuits;
- leads to new gates (B – gate) and implementations.

### **Optimal control applications**

- relaxing constraints on the optimization target relaxes constraints on physical interactions, optimization process and implementation;
- optimization to a given local equivalence class converges faster and more reliably;
- optimization to the set of perfect entanglers promises to maximize entanglement generation, preliminary results are quite encouraging

### **Metric properties**

- derived expressions for the invariant length element and volume in the representation particularly suitable for quantum information processing;
- true size of optimization targets; the largest in the center of the Weyl chamber;
- perfect entanglers are (almost) everywhere!



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Jun Zhang**

**Jiri Vala  
Paul Watts  
Maurice O'Connor**



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Ollscoil na hÉireann Mú Nuid



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**Haidong Yuan**

