how to get the best two-qubit gate for a real physical system

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joint work with
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Birgitta Whaley, Tommaso Calarco

arXiv:1104.2337

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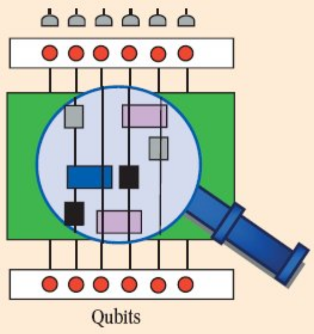
what is needed to build a quantum computer ?



DiVincenzo criteria

DiVincenzo, Fortschr. Physik 48, 771 (2000)

1. scalable system of well-characterized qubits
2. long decoherence times
3. initialize qubits
4. universal set of quantum gates
5. read-out of qubits

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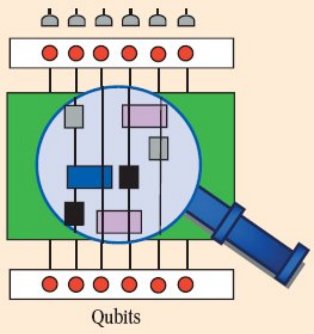

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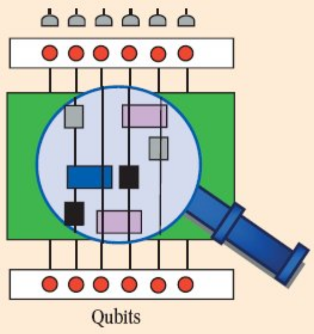
→ **trapped neutral atoms or molecules**

optimal control & QIP



$$\mathrm{Tr}\left\{\hat{\mathbf{O}}^{+}\hat{\mathbf{P}}_N\hat{\mathbf{U}}(T,0;\varepsilon)\hat{\mathbf{P}}_N\right\}$$

- desired gate operation : $\hat{\mathbf{O}}$
- actual evolution : $\hat{\mathbf{U}}(T,0;\varepsilon)$
- desired fidelity :

  $1-\epsilon$ where $\epsilon < 10^{-4}$

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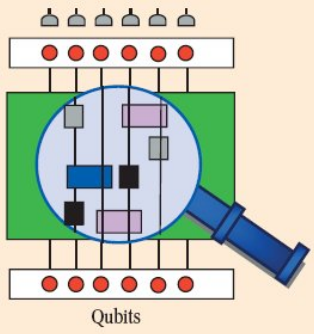

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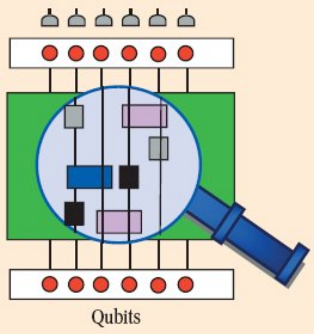

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- **best choice of $\hat{\mathrm{O}}$?**

why is OCT interesting for QI?

$$t = 0 \qquad\qquad\qquad t = T$$

$$|\varphi_{i,n}\rangle \quad n = 1, \ldots, N \qquad \rightsquigarrow \qquad |\varphi_{f,n}\rangle \quad n = 1, \ldots, N$$

obtain quantum gates via

1. N simultaneous state-to-state transitions

   Rangan & Bucksbaum, PRA 64, 033417 (2001)

   Tesch & de Vivie-Riedle, PRL 89, 157901 (2002)

2. optimization of unitary transformation

$$\frac{\partial \hat{\mathbf{U}}(t)}{\partial t} = -\frac{i}{\hbar}\hat{\mathbf{H}}(t)\hat{\mathbf{U}}(t) \qquad \hat{\mathbf{U}}(T) = e^{i\phi}\hat{\mathbf{O}}$$

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functionals

1. $\eta = \sum_{k=1}^{N} \left|\langle k|\hat{\mathbf{O}}^{+}\hat{\mathbf{U}}(T,0;\varepsilon)|k\rangle\right|^2 = F_{ss}$

2. $\tau = \sum_{k=1}^{N} \langle k|\hat{\mathbf{O}}^{+}\hat{\mathbf{U}}(T,0;\varepsilon)|k\rangle$

$\longrightarrow F_{re} = \mathfrak{Re}\left[\tau\right]$ or $F_{sm} = -\left|\tau\right|^2$

Palao & Kosloff, PRA 68, 062308 (2003)

➜ **optimization of gate operations**

functionals

or

how to convey the desired physics to the OCT algorithm

objective functionals / costs

$$J\left[\{\varphi_k(t), \varphi_k^*(t)\}, \varepsilon(t)\right] =$$

$$J_T\left[\{\varphi_k(T), \varphi_k^*(T)\}\right] + J_t\left[\{\varphi_k(t), \varphi_k^*(t)\}, \varepsilon(t)\right]$$

final-time target

intermediate-time target
time-dependent cost
state-dependent cost

functionals of the field $\boldsymbol{\varepsilon}(\mathbf{t})$

- explicitly
- implicitly through $\varphi_k(t)$, $\varphi_k(T)$

final-time objectives J_T

$$J_T = -\frac{\lambda_0}{N}\mathfrak{Re}\left[\mathrm{Tr}\left\{\hat{\mathbf{O}}^{+}\hat{\mathbf{P}}_N\hat{\mathbf{U}}(T,0;\varepsilon)\hat{\mathbf{P}}_N\right\}\right]$$

real-valued, phase-sensitive functional

- $\hat{\mathbf{O}}$ target operator
- λ_0 weight
- $N = \dim\{\hat{\mathbf{O}}\}$
- $\hat{\mathbf{P}}_N$ projector on subspace of $\hat{\mathbf{O}}$
- $\hat{\mathbf{U}}(T,0;\varepsilon)$ actual time evolution

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- state-to-state transfer: $\hat{\mathbf{O}} = |\varphi_{\mathrm{target}}\rangle\langle\varphi_{\mathrm{target}}|$, $N = 1$
- single-qubit gate: $N = 2$, two-qubit gate: $N = 4$

cf. Palao & Kosloff, PRA 68, 062308 (2003)

intermediate-time objectives J_t

assumption: additive costs

$$J_t = \int_0^T \{g_a[\varepsilon(t)] + g_b[\varphi(t), \varphi^*(t)]\}\, dt$$

intermediate-time objectives J_t

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$$J_t = \int_0^T \left\{ g_a\left[\varepsilon(t)\right] + g_b\left[\varphi(t), \varphi^*(t)\right] \right\} dt$$

examples

$$g_a\left[\varepsilon(t)\right] = \lambda_a S(t)\left[\varepsilon(t) - \varepsilon_{\mathrm{ref}}(t)\right]^2$$

minimization of field intensity $(\varepsilon_{\mathrm{ref}}(t) = 0)$
or change in field intensity $(\varepsilon_{\mathrm{ref}}(t) = \varepsilon_{\mathsf{old}})$

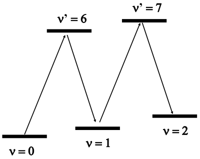
$$g_b\left[\varphi(t), \varphi^*(t)\right] = \lambda_b \langle \varphi(t) | \hat{\mathbf{D}}(t) | \varphi(t) \rangle$$

$\hat{\mathbf{D}}(t)$ target operator, λ_a, λ_b weights, $S(t)$ switch/shape function

time-dependent targets

$$g_b\left[\varphi(t), \varphi^*(t)\right] = \lambda_b \langle \varphi(t) | \hat{\mathbf{D}}(t) | \varphi(t) \rangle$$

prescribing a desired evolution



$$\begin{aligned} \hat{\mathbf{D}}(t) &= |6\rangle\langle 6|\Theta(T_1 - t) + \\ &\quad |1\rangle\langle 1|\Theta(t - T_1)\Theta(T_2 - t) + \\ &\quad |7\rangle\langle 7|\Theta(t - T_2)\Theta(T_3 - t) + \\ &\quad |2\rangle\langle 2|\Theta(t - T_3)\Theta(T - t) \end{aligned}$$

Ndong, Tal-Ezer, Kosloff, Koch, JCP 130, 124108 (2009)

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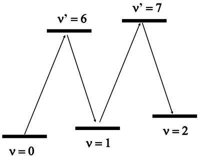

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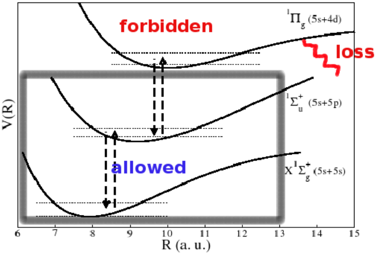
keeping the dynamics in a subspace



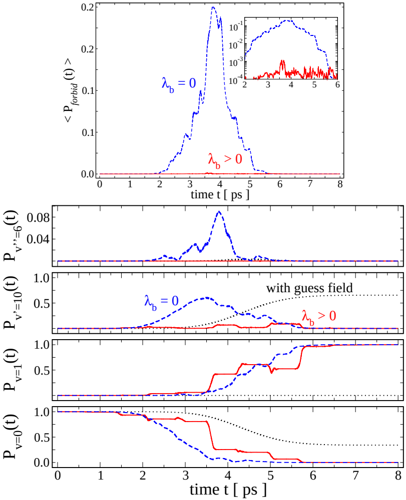
$$\hat{\mathbf{D}}(t) = \hat{\mathbf{P}}_{\text{allow}}$$

Palao, Kosloff, Koch, PRA 77, 063412 (2008)

optimal control in a subspace

model: 33 vibronic levels of Rb_2, 22 allowed

target: transition $v = 0 \longrightarrow v = 1$



standard OCT:

large amount of population in intermediate state can be further excited to forbidden subspace

OCT w/ state-dep. constraint:

population transfer via ladder-like process $\leftrightarrow$ short subpulses

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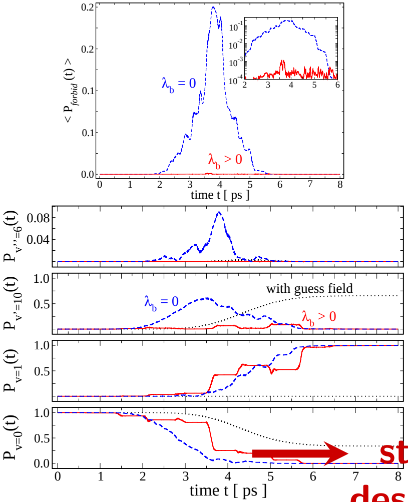


standard OCT:

large amount of population in intermediate state can be further excited to forbidden subspace

OCT w/ state-dep. constraint:

population transfer via ladder-like process $\leftrightarrow$ short subpulses

state-dep. constraint conveys desired physics to the algorithm

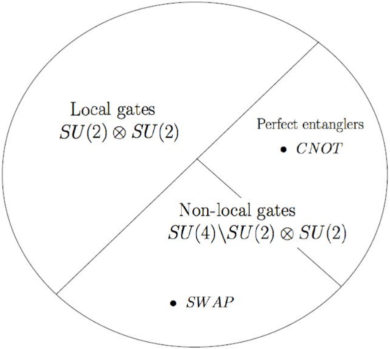
optimizing
for a
local equivalence class

classification of two-qubit gates

$G = SU(4)$ group of all two-qubit gates
$K = SU(2) \otimes SU(2)$ local gates
$G/K = SU(4)/SU(2) \otimes SU(2)$
non-local gates

$$\mathfrak{su}(4) = \mathfrak{k} \oplus \mathfrak{p}$$

Cartan decomposition of Lie algebras



$$\hat{\mathbf{U}} = \hat{\mathbf{k}}_1 e^{-\frac{i}{2}\sum_{j=x,y,z} c_j \hat{\boldsymbol{\sigma}}_j^1 \hat{\boldsymbol{\sigma}}_j^2} \hat{\mathbf{k}}_2$$

if

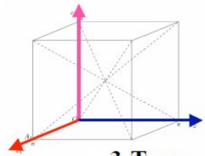
$$\hat{\mathbf{U}}_1 = \hat{\mathbf{k}}_1 \hat{\mathbf{U}}_2 \hat{\mathbf{k}}_2$$

then

$\hat{\mathbf{U}}_1$ and $\hat{\mathbf{U}}_2$ are in the same local equivalence class

Zhang, Vala, Sastry, Whaley, PRA 67, 042313 (2003)

Weyl chamber



3-Torus

Cartan decomposition

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

Local invariants

$$g_1 = \cos c_1 \cos c_2 \cos c_3$$

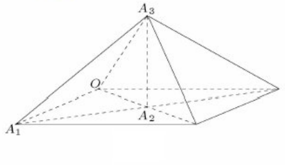
$$g_2 = \sin c_1 \sin c_2 \sin c_3$$

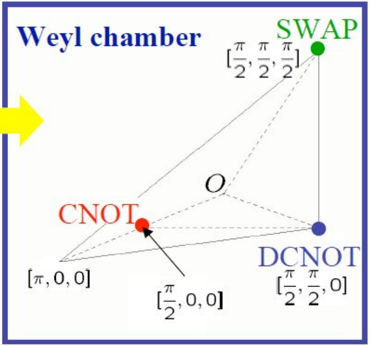
$$g_3 = 2(\cos^2 c_1 + \cos^2 c_2 + \cos^2 c_3) - 3$$

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

symmetry reduction

g_1,g_2 and g_3 are invariant with permutation of c_1, c_2, and c_3 with/without sign flips





There is a one-to-one correspondence between the points inside the Weyl chamber and local equivalence classes

local invariants

$$\hat{\mathbf{m}} = \hat{\mathbf{U}}_B^T \hat{\mathbf{U}}_B$$

$$\hat{\mathbf{U}}_B = \hat{\mathbf{Q}}^+ \hat{\mathbf{U}} \hat{\mathbf{Q}}$$ (i.e. $\hat{\mathbf{U}}$ in Bell basis)

$$\begin{aligned} g_1 &= \mathfrak{Re}\,\mathrm{Tr}[\hat{\mathbf{m}}]^2 / 16 \det(\hat{\mathbf{U}}) \\ g_2 &= \mathfrak{Im}\,\mathrm{Tr}[\hat{\mathbf{m}}]^2 / 16 \det(\hat{\mathbf{U}}) \\ g_3 &= \mathrm{Tr}[\hat{\mathbf{m}}]^2 - \mathrm{Tr}[\hat{\mathbf{m}}^2] / 4 \det(\hat{\mathbf{U}}) \end{aligned}$$

g_1, g_2, g_3 define local equivalence class $[\hat{\mathbf{U}}]$,
i.e. a class of two-qubit gates that are equivalent up to local (single-qubit) operations

Zhang, Vala, Sastry, Whaley, PRA 67, 042313 (2003)

optimization target [Ô] instead of Ô

(old) functional to obtain Ô

$$J_T = -\frac{\lambda_0}{N}\mathfrak{Re}\left[\mathrm{Tr}\left\{\hat{\mathbf{O}}^{+}\hat{\mathbf{P}}_N\hat{\mathbf{U}}(T,0;\varepsilon)\hat{\mathbf{P}}_N\right\}\right]$$

(new) functional to obtain [Ô]

$$J_T = \Delta g_1{}^2 + \Delta g_2{}^2 + \Delta g_3{}^2 + \left(1 - \frac{1}{N}\mathrm{Tr}\left[\hat{\mathbf{U}}_N\hat{\mathbf{U}}_N^{+}\right]\right)$$

with $\Delta g_i{}^2 = \left|g_i(\hat{\mathbf{O}}) - g_i(\hat{\mathbf{U}})\right|^2$ and $g_i(\hat{\mathbf{O}})$ the local invariants of $\hat{\mathbf{O}}$

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remember:

$$J = J\left[\{\varphi_k(t), \varphi_k^*(t)\}, \varepsilon(t)\right]$$

to carry out variations, we need to express g_i in terms of $\varphi_k(t)$

functional based on local invariants

using the definition of the invariants and of the Bell basis and after quite some algebra

$$J_T = f_1^2 + f_2^2 + f_3^2 + f_4^2 + f_5$$

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$$J_T = f_1^2 + f_2^2 + f_3^2 + f_4^2 + f_5$$

$$
\begin{aligned}
f_1 &= \mathfrak{Re}\left[a_0 \det(\hat{\mathbf{U}})\right] - \frac{1}{16}\sum_{k,l} \vec{\alpha}_k^2\vec{\alpha}_l^2 + \vec{\beta}_k^2\vec{\beta}_l^2 - 2\vec{\alpha}_k^2\vec{\beta}_l^2 - 4\left(\vec{\alpha}_k\cdot\vec{\beta}_k\right)\left(\vec{\alpha}_l\cdot\vec{\beta}_l\right) \\
f_2 &= \mathfrak{Im}\left[a_0 \det(\hat{\mathbf{U}})\right] - \frac{1}{16}\sum_{k,l} 4\vec{\alpha}_k^2\left(\vec{\alpha}_l\cdot\vec{\beta}_l\right) - 4\vec{\beta}_k^2\left(\vec{\alpha}_l\cdot\vec{\beta}_l\right) \\
f_3 &= \mathfrak{Re}\left[b_0 \det(\hat{\mathbf{U}})\right] - \frac{1}{4}\sum_{k,l} \vec{\alpha}_k^2\vec{\alpha}_l^2 + \vec{\beta}_k^2\vec{\beta}_l^2 - 2\vec{\alpha}_k^2\vec{\beta}_l^2 - 4\left(\vec{\alpha}_k\cdot\vec{\beta}_k\right)\left(\vec{\alpha}_l\cdot\vec{\beta}_l\right) - \left(\vec{\alpha}_k\cdot\vec{\alpha}_l\right)^2 - \left(\vec{\beta}_k\cdot\vec{\beta}_l\right)^2 \\
&\quad +2\left(\vec{\alpha}_k\cdot\vec{\alpha}_l\right)\left(\vec{\beta}_k\cdot\vec{\beta}_l\right) + 4\left(\vec{\alpha}_k\cdot\vec{\alpha}_l\right)\left(\vec{\beta}_k\cdot\vec{\beta}_l\right) \\
f_4 &= \mathfrak{Im}\left[b_0 \det(\hat{\mathbf{U}})\right] - \frac{1}{4}\sum_{k,l} 4\vec{\alpha}_k^2\left(\vec{\alpha}_l\cdot\vec{\beta}_l\right) - 4\vec{\beta}_k^2\left(\vec{\alpha}_l\cdot\vec{\beta}_l\right) - 4\left(\vec{\alpha}_k\cdot\vec{\alpha}_l\right)\left(\vec{\alpha}_k\cdot\vec{\beta}_l\right) + 4\left(\vec{\beta}_k\cdot\vec{\beta}_l\right)\left(\vec{\alpha}_k\cdot\vec{\beta}_l\right)
\end{aligned}
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with $a_0 = \mathrm{Tr}^2\left(\hat{\mathbf{m}}_O\right)/16\det(\hat{\mathbf{O}})$ and $b_0 = \left[\mathrm{Tr}^2\left(\hat{\mathbf{m}}_O\right) - \mathrm{Tr}\left(\hat{\mathbf{m}}_O^2\right)\right]/4\det(\hat{\mathbf{O}})$

$(\alpha_k)_m = \mathfrak{Re}\left[\langle m|\varphi_k(T)\rangle\right]$, $(\beta_k)_m = \mathfrak{Im}\left[\langle m|\varphi_k(T)\rangle\right]$, $m = 1, \ldots, \dim(\mathcal{H})$

functional based on local invariants

$$J_T = f_1^2 + f_2^2 + f_3^2 + f_4^2 + f_5$$

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$$f_3 = \mathfrak{Re}\left[b_0 \det(\hat{\mathbf{U}})\right] - \frac{1}{4}\sum_{k,l} \vec{\alpha}_k^2\vec{\alpha}_l^2 + \vec{\beta}_k^2\vec{\beta}_l^2 - 2\vec{\alpha}_k^2\vec{\beta}_l^2 - 4\left(\vec{\alpha}_k\cdot\vec{\beta}_k\right)\left(\vec{\alpha}_l\cdot\vec{\beta}_l\right) - \left(\vec{\alpha}_k\cdot\vec{\alpha}_l\right)^2 - \left(\vec{\beta}_k\cdot\vec{\beta}_l\right)^2$$
$$+2\left(\vec{\alpha}_k\cdot\vec{\alpha}_l\right)\left(\vec{\beta}_k\cdot\vec{\beta}_l\right) + 4\left(\vec{\alpha}_k\cdot\vec{\alpha}_l\right)\left(\vec{\beta}_k\cdot\vec{\beta}_l\right)$$

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with $a_0 = \mathrm{Tr}^2\left(\hat{\mathbf{m}}_O\right)/16\det(\hat{\mathbf{O}})$ and $b_0 = \left[\mathrm{Tr}^2\left(\hat{\mathbf{m}}_O\right) - \mathrm{Tr}\left(\hat{\mathbf{m}}_O^2\right)\right]/4\det(\hat{\mathbf{O}})$

$(\alpha_k)_m = \mathfrak{Re}\left[\langle m|\varphi_k(T)\rangle\right]$, $(\beta_k)_m = \mathfrak{Im}\left[\langle m|\varphi_k(T)\rangle\right]$, $m = 1, \ldots, \dim(\mathcal{H})$

problem: J_T is 8th degree polynomial in $\{\vec{\alpha}_k, \vec{\beta}_k\}$, resp. $\{|\varphi_k\rangle\}$ $\curvearrowright$ non-convex

optimization of non-convex functionals

(old) functional to obtain Ô

$$J_T = -\frac{\lambda_0}{N}\mathfrak{Re}\left[\mathrm{Tr}\left\{\hat{\mathbf{O}}^{+}\hat{\mathbf{P}}_N\hat{\mathbf{U}}(T,0;\varepsilon)\hat{\mathbf{P}}_N\right\}\right]$$

quadratic

(new) functional to obtain [Ô]

$$J_T = \Delta g_1{}^2 + \Delta g_2{}^2 + \Delta g_3{}^2$$

non-convex

for non-convex functionals

- local optima may exist
- how to ensure monotonic convergence?
  $\longrightarrow$ 2nd order Krotov algorithm

Reich, Ndong, Koch, arXiv:1008.5126

application 1:
effective spin-spin model with polar molecules

effective spin-spin model

with trapped polar molecules

- two polar molecules with ${}^2\Sigma_{1/2}$ electronic ground states
- trapped e.g. in optical lattice
- near-resonant microwave driving induces strong dipole-dipole coupling

Micheli, Brennen, Zoller, Nature Phys. 2, 341 (2006)

$$\hat{\mathbf{H}}_{eff} = \frac{\hbar\Omega^2(t)}{8} \sum_{i,j=0}^{3} \hat{\boldsymbol{\sigma}}_i \hat{\mathbf{a}}_{ij}(x_0) \hat{\boldsymbol{\sigma}}_j$$

within 2nd order perturbation theory of the microwave field

- $\hat{\mathbf{a}}_{ij}(x_0)$ depends on distance between molecules, polarization and detuning of microwave field

two-qubit gates: the B-gate

the desired $\hat{\mathbf{U}}$

$$e^{i\frac{\pi}{4}\hat{\boldsymbol{\sigma}}_x\otimes\hat{\boldsymbol{\sigma}}_x}e^{i\frac{\pi}{8}\hat{\boldsymbol{\sigma}}_y\otimes\hat{\boldsymbol{\sigma}}_y} = \begin{pmatrix} 0.6533+0.2706i & 0 & 0 & 0.2706-0.6533i \\ 0 & 0.6533-0.2706i & 0.2706+0.6533i & 0 \\ 0 & 0.2706+0.6533i & 0.6533-0.2706i & 0 \\ 0.2706-0.6533i & 0 & 0 & 0.6533+0.2706i \end{pmatrix}$$

the Hamiltonian to generate a $\hat{\mathbf{U}}$ in [B]

$$\hat{\mathbf{H}} \sim \Omega^2(t)\begin{pmatrix} 9.4599 & 0 & 0 & 0.7299 \\ 0 & -9.4599 & 2.7671 & 0 \\ 0 & 2.7671 & -9.4599 & 0 \\ 0.7299 & 0 & 0 & 9.4599 \end{pmatrix}$$

two-qubit gates: CNOT

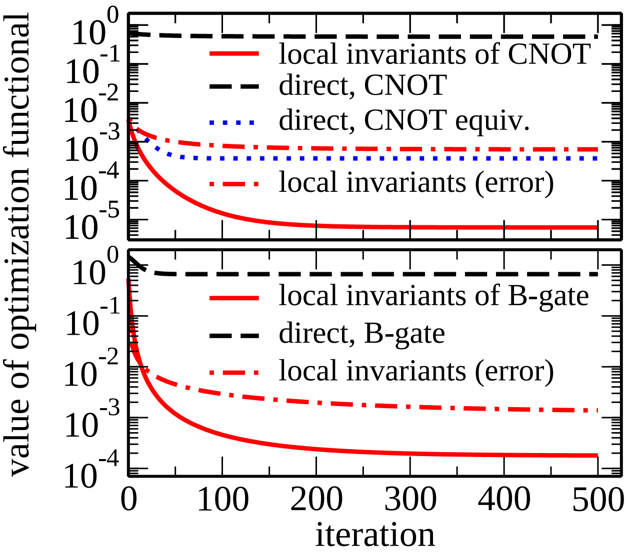
the desired $\hat{\mathbf{U}}$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

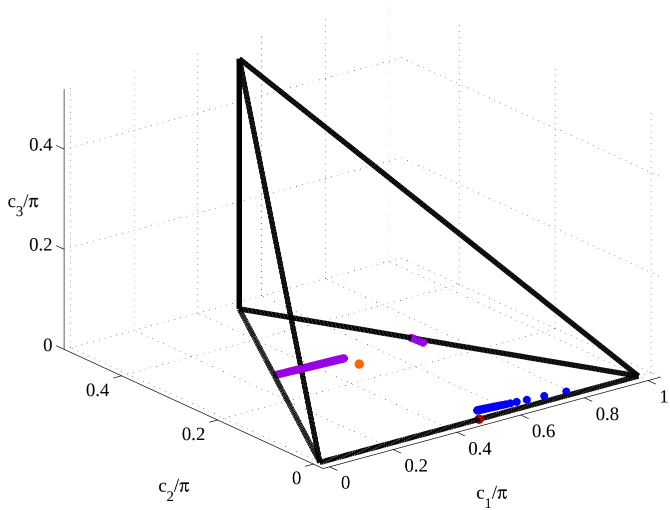
the Hamiltonian to generate a $\hat{\mathbf{U}}$ in [CNOT]

$$\hat{\mathbf{H}} \sim \Omega^2(t) \begin{pmatrix} 5.5056 & 0 & 0 & 0.0664 \\ 0 & -5.5056 & 0.2624 & 0 \\ 0 & 0.2624 & -5.5056 & 0 \\ 0.0664 & 0 & 0 & 5.5056 \end{pmatrix}$$

two-qubit gates with SrF molecules



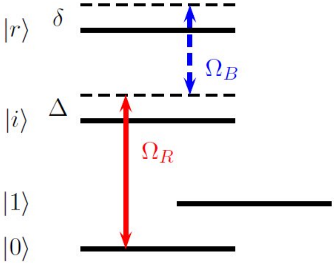
two-qubit gates with SrF molecules



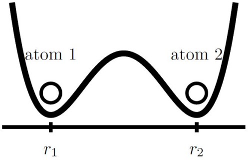
application 2:
Rydberg gate with cold atoms

Rydberg gate: qubits

one-atom level scheme



optical tweezers



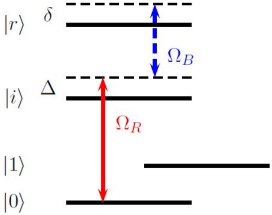
experiment of Gaetan et al., Nat. Phys. 5, 115 (2009)

one-atom Hamiltonian

$$
\begin{aligned}
\hat{\mathbf{H}}^{(1)} = \; & |0\rangle\langle 0| \otimes \left(\hat{\mathbf{T}}_{\hat{\mathbf{r}}} + V^0_{trap}(\hat{\mathbf{r}})\right) \\
& + |1\rangle\langle 1| \otimes \left(\hat{\mathbf{T}}_{\hat{\mathbf{r}}} + V^1_{trap}(\hat{\mathbf{r}})\right) \\
& + |i\rangle\langle i| \otimes \left(\hat{\mathbf{T}}_{\hat{\mathbf{r}}} + V^i_{trap}(\hat{\mathbf{r}}) - \Delta\right) \\
& + \varepsilon_{\mathbf{B}}(t) \left(|0\rangle\langle i| + |i\rangle\langle 0|\right) \otimes \mu(\hat{\mathbf{r}}) \\
& + |r\rangle\langle r| \otimes \left(\hat{\mathbf{T}}_{\hat{\mathbf{r}}} + V^r_{trap}(\hat{\mathbf{r}}) - \delta\right) \\
& + \varepsilon_{\mathbf{R}} \left(|i\rangle\langle r| + |r\rangle\langle i|\right) \otimes \mu(\hat{\mathbf{r}})
\end{aligned}
$$

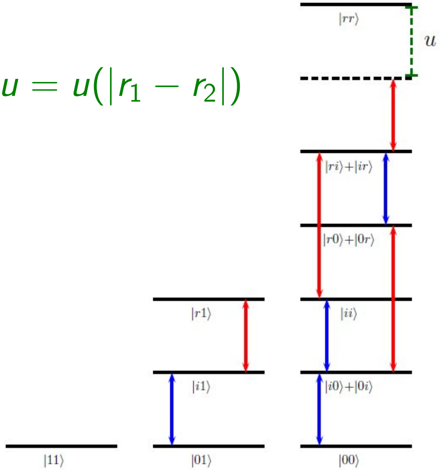
Rydberg gate: qubits

one-atom level scheme



two-atom level scheme

$$u = u(|r_1 - r_2|)$$



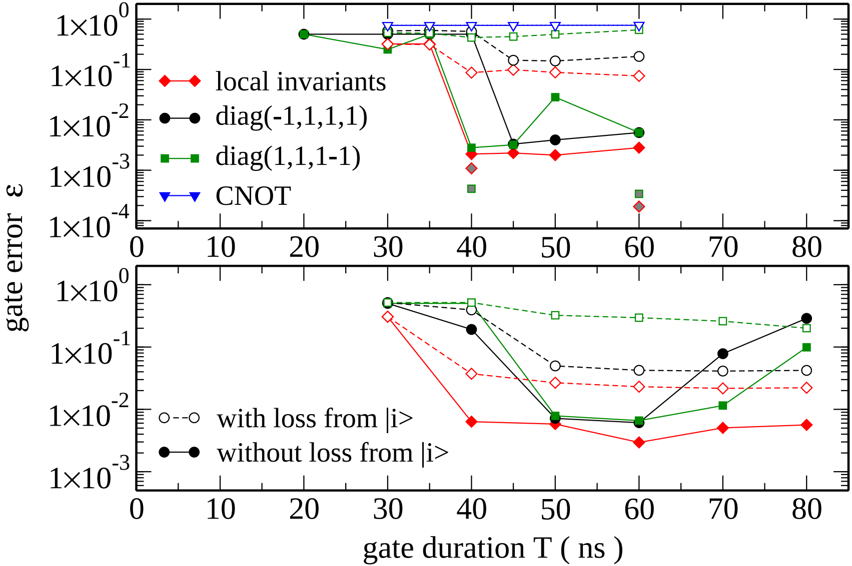
two-atom Hamiltonian

$$\begin{aligned}\hat{\mathbf{H}} &= \hat{\mathbf{H}}_1^{(1)} \otimes \mathbb{1}_{4,2} \otimes \mathbb{1}_{\hat{\mathbf{r}}_2} \\ &\quad + \mathbb{1}_{4,1} \otimes \mathbb{1}_{\hat{\mathbf{r}}_1} \otimes \hat{\mathbf{H}}_2^{(1)} \\ &\quad + \hat{\mathbf{H}}_{int}^{(1,2)} \\ \hat{\mathbf{H}}_{int}^{(1,2)} &= |rr\rangle\langle rr| \otimes \frac{u_0}{|\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2|^3}\end{aligned}$$

Jaksch et al., PRL 85, 2208 (2000)

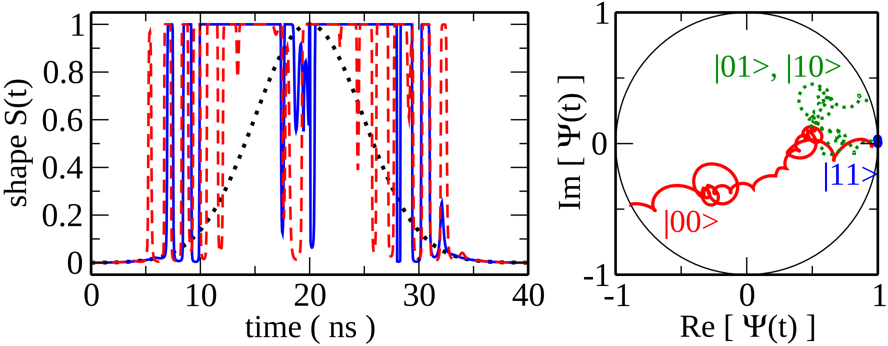
two-qubit Rydberg gates

identifying the quantum speed limit



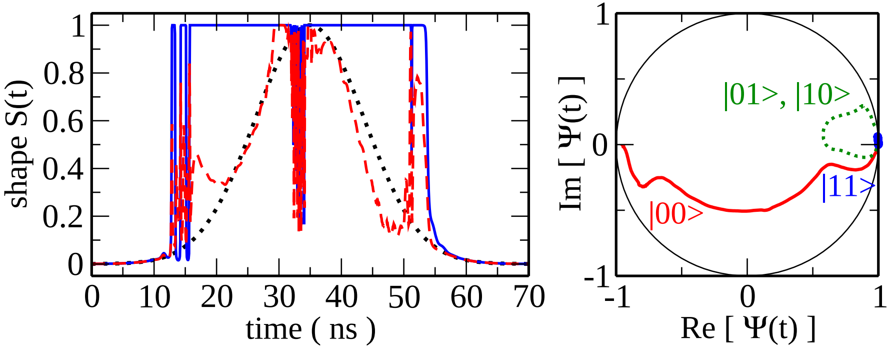
optimal pulse & phase dynamics

without spontaneous decay from $|i\rangle$



optimal pulse & phase dynamics

with spontaneous decay from $|i\rangle$
minimizing population in $|i\rangle$



summary

optimal control is an extremely versatile tool but you need to know how to ask questions!

- we derived a new class of optimization functionals suitable for quantum information purposes
- based on geometric classification of entangling operations (Cartan decomp. & Weyl chamber)
- requires optimization algorithm ensuring monotonic convergence – 2nd order Krotov method
- first results encouraging
- full power of approach still needs to be explored (more general Hamiltonians, decoherence)

where can we go from here?

1. optimize for an arbitrary perfect entangler
   - problem: no simple inversion of $g_1, g_2, g_3 \longrightarrow c_1, c_2, c_3$
   - solution: define ellipsoid in g-space containing almost all of the Weyl chamber
2. optimize for a specified trajectory in the Weyl chamber
3. include decoherence
4. ...