Efficient Optimal Control for a Unitary Operation under Dissipative Evolution

Michael Goerz, Daniel Reich, Christiane P. Koch
Universität Kassel

March 20, 2014

DPG Frühjahrstagung 2014, Berlin
Session Q 43
Control Problem

Find a time-dependent control (e.g. laser pulse) that steers the system towards some desired goal (e.g. quantum gate)
Introduction: numerical optimal control

Control Problem

Find a time-dependent control (e.g. laser pulse) that steers the system towards some desired goal (e.g. quantum gate)

- define optimization functional
- for a guess pulse, solve the equation of motion numerically
- modify control pulse to improve value of optimization functional
Control Problem

Find a time-dependent control (e.g. laser pulse) that steers the system towards some desired goal (e.g. quantum gate)

- define optimization functional
- for a guess pulse, solve the equation of motion numerically
- modify control pulse to improve value of optimization functional
Introduction: numerical optimal control

Control Problem

Find a time-dependent control (e.g. laser pulse) that steers the system towards some desired goal (e.g. quantum gate)

- define optimization functional
- for a guess pulse, solve the equation of motion numerically
- modify control pulse to improve value of optimization functional

“optimal”: not limited to simple intuitive schemes, operate at the quantum speed limit
Gate optimization

$$\text{CPHASE} = \text{diag}(-1, 1, 1, 1)$$

$$\text{CNOT} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
\end{pmatrix}$$

**Goal:** Maximize

$$\mathcal{F} = \max_{d=1}^{d_0} \sum_{i=1}^{d_0} \left| \langle \Psi_i | \hat{O}^\dagger \hat{U}(T, 0, \epsilon) | \Psi_i \rangle \right|^2$$

Two-qubit gates:

$|00\rangle \hat{O} |00\rangle$

$|01\rangle \hat{O} |01\rangle$

$|10\rangle \hat{O} |10\rangle$

$|11\rangle \hat{O} |11\rangle$

$$\epsilon_{\text{new}}$$

$$\epsilon_{\text{old}}$$

$$t_0$$

$$\Delta \epsilon(t) \propto |\chi(t)| \left| \partial_\epsilon \hat{H} \right| \Psi(t)$$
Gate optimization

\[
\text{CPHASE} = \text{diag}(-1, 1, 1, 1)
\]

\[
\text{CNOT} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
\end{pmatrix}
\]

Goal: Maximize

\[
F = \frac{1}{d} \sum_{i=1}^{d} \Re \langle \psi_i | \hat{O}^\dagger \hat{U}(T, 0, \epsilon) | \psi_i \rangle
\]

Two-qubit gates: \( d = 4 \)
Gate optimization

\[
\text{CPHASE} = \text{diag}(-1, 1, 1, 1)
\]

\[
\text{CNOT} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
\]

Goal: Maximize

\[
F = \frac{1}{d} \sum_{i=1}^{d} \Re \langle \psi_i | \hat{O}^\dagger \hat{U}(T, 0, \epsilon) | \psi_i \rangle
\]

Two-qubit gates: \(d = 4\)

\[
\Delta \epsilon(t) \propto \langle \chi(t) | \partial_\epsilon \hat{H} | \psi(t) \rangle
\]
In the real world: decoherence
\[ \hat{\rho}(T) = \mathcal{D}(\hat{\rho}(0)); \quad \text{for example} \quad \frac{\partial \hat{\rho}}{\partial t} = \frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \mathcal{L}_D(\hat{\rho}) \]
\[ \hat{\rho}(T) = D(\hat{\rho}(0)); \text{ for example } \frac{\partial \hat{\rho}}{\partial t} = \frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \mathcal{L}_D(\hat{\rho}) \]

Lift \[ F = \frac{1}{d} \sum_{i=1}^{d} \Re \left( \psi_i \left| \hat{O}^\dagger \hat{U}(T, 0, \epsilon) \hat{P} \right| \psi_i \right) \] to Liouville space.

Kallush & Kosloff, Phys. Rev. A 73, 032324 (2006),

\[ \Rightarrow F = \frac{1}{d^2} \sum_{j=1}^{d^2} \text{tr} \left[ \hat{O} \hat{\rho}_j(0) \hat{O}^\dagger \hat{\rho}_j(T) \right] \]
OCT for open quantum systems

\[ \hat{\rho}(T) = D(\hat{\rho}(0)); \quad \text{for example} \quad \frac{\partial \hat{\rho}}{\partial t} = \frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \mathcal{L}_D(\hat{\rho}) \]

Lift \[ F = \frac{1}{d} \sum_{i=1}^{d} \mathbb{R} \text{e} \left\langle \psi_i \left| \hat{O}^{\dagger} \hat{P} \hat{U}(T, 0, \epsilon) \hat{P} \right| \psi_i \right\rangle \] to Liouville space.

Kallush & Kosloff, Phys. Rev. A 73, 032324 (2006),

\[ \Rightarrow F = \frac{1}{d^2} \sum_{j=1}^{d^2} \text{tr} \left[ \hat{O} \hat{\rho}_j(0) \hat{O}^{\dagger} \hat{\rho}_j(T) \right] \]

\[ \hat{\rho}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{\rho}_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{\rho}_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \ldots \]

\[ d^2 \] matrices to propagate! (16 for two-qubit gate)
\[ \hat{\rho}(T) = D(\hat{\rho}(0)); \quad \text{for example} \quad \frac{\partial \hat{\rho}}{\partial t} = \frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \mathcal{L}_{D}(\hat{\rho}) \]

Lift \[ F = \frac{1}{d} \sum_{i=1}^{d} \Re \left< \psi_i \left| \hat{O}^\dagger \hat{P} \hat{U}(T, 0, \epsilon) \hat{P} \right| \psi_i \right> \text{ to Liouville space.} \]

Kallush & Kosloff, Phys. Rev. A 73, 032324 (2006),
Ohtsuki, New J. Phys. 12, 045002 (2010),
...

\[ \Rightarrow F = \frac{1}{d^2} \sum_{j=1}^{d^2} \text{tr} \left[ \hat{O} \hat{\rho}_j(0) \hat{O}^\dagger \hat{\rho}_j(T) \right] \]

Claim

We only need to propagate \textbf{three} matrices (independent of \(d\)), instead of \(d^2\).
A reduced set of density matrices

No need to characterize the full dynamical map! – much less information required to assess how well a desired unitary is implemented
No need to characterize the full dynamical map! – much less information required to assess how well a desired unitary is implemented

1. Do we stay in the logical subspace?
No need to characterize the full dynamical map!  
— much less information required to assess how well a desired unitary is implemented

1. Do we stay in the logical subspace?

\[ \hat{\rho}_3 = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]
No need to characterize the full dynamical map! — much less information required to assess how well a desired unitary is implemented

① Do we stay in the logical subspace?
② Are we unitary, and if yes, did we implement the right gate?

$$\hat{\rho}_1 = \frac{1}{20} \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix},$$

$$\hat{\rho}_2 = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix},$$

$$\hat{\rho}_3 = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$
A reduced set of density matrices

No need to characterize the full dynamical map! — much less information required to assess how well a desired unitary is implemented

1. Do we stay in the logical subspace?
2. Are we unitary, and if yes, did we implement the right gate?

\[ \hat{\rho}_1 = \frac{1}{20} \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \quad \hat{\rho}_3 = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]
No need to characterize the full dynamical map! — much less information required to assess how well a desired unitary is implemented

1. Do we stay in the logical subspace?
2. Are we unitary, and if yes, did we implement the right gate?

\[
\hat{\rho}_1 = \frac{1}{20} \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \quad \hat{\rho}_3 = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}
\]

E.g. \( \hat{O} = \text{diag}(-1, 1, 1, 1) \);
For \( \hat{U} = \text{diag}(e^{i\phi_{00}}, e^{i\phi_{01}}, e^{i\phi_{10}}, e^{i\phi_{11}}) \)

using just \( \hat{\rho}_1 \) will not distinguish \( \hat{U} \) from \( \hat{O} \). (\( \hat{U}\hat{\rho}_1\hat{U}^\dagger = \hat{O}\hat{\rho}_1\hat{O}^\dagger = \hat{\rho}_1 \))
No need to characterize the full dynamical map! — much less information required to assess how well a desired unitary is implemented

① Do we stay in the logical subspace?
② Are we unitary, and if yes, did we implement the right gate?

\[ \hat{\rho}_1 = \frac{1}{20} \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \hat{\rho}_2 = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \hat{\rho}_3 = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]

E.g. \( \hat{O} = \text{diag}(-1, 1, 1, 1) \);
For \( \hat{U} = \text{diag}(e^{i\phi_{00}}, e^{i\phi_{01}}, e^{i\phi_{10}}, e^{i\phi_{11}}) \)

using just \( \hat{\rho}_1 \) will not distinguish \( \hat{U} \) from \( \hat{O} \). (\( \hat{U}\hat{\rho}_1\hat{U}^\dagger = \hat{O}\hat{\rho}_1\hat{O}^\dagger = \hat{\rho}_1 \))
Efficient gate optimization in Liouville space

### Optimization States

\[
\hat{\rho}_1 = \frac{1}{20} \begin{pmatrix}
8 & 0 & 0 & 0 \\
0 & 6 & 0 & 0 \\
0 & 0 & 4 & 0 \\
0 & 0 & 0 & 2
\end{pmatrix}, \quad \hat{\rho}_2 = \frac{1}{4} \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1
\end{pmatrix}, \quad \hat{\rho}_3 = \frac{1}{4} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

- populations
- phases
- subspace

### Functional

\[
J_T = 1 - \sum_{j=1}^{3} \frac{w_j}{\text{tr}[\hat{\rho}_j^2(0)]} \text{tr} \left[ \hat{\mathbf{O}} \hat{\rho}_j \hat{\mathbf{O}}^\dagger \mathcal{D}[\hat{\rho}_j] \right]
\]

- Allow for different weights (\( \sum w_j = 1 \))
- \( J_T = 0 \) iff for all \( \hat{\rho}_j \): \( \mathcal{D}[\hat{\rho}_j] \equiv \) target state

  \( \Rightarrow \) implemented unitary gate \( \hat{\mathbf{O}} \).
Example 1

Optimization of a Diagonal Gate using Rydberg Atoms
Two trapped neutral atoms

Single-qubit Hamiltonian

\[
\hat{H}_{1q} = \begin{pmatrix}
0 & 0 & \frac{1}{2} \Omega_R(t) & 0 \\
0 & E1 & 0 & 0 \\
\frac{1}{2} \Omega_R(t) & 0 & \Delta_1 & \frac{1}{2} \Omega_B(t) \\
0 & 0 & \frac{1}{2} \Omega_B(t) & 0 
\end{pmatrix}
\]

In the RWA:

\[
\Delta_1
\]

\[
\Omega_B(t)
\]

\[
\Omega_R(t)
\]

\[
\tau = 25 \text{ ns}
\]

\[
|0\rangle |1\rangle
\]

\[
|i\rangle
\]

\[
|r\rangle
\]

Dipole-dipole interaction when both atoms in Rydberg state.

Only diagonal gates!
Two trapped neutral atoms

Single-qubit Hamiltonian

\[ \hat{H}_{1q} = \begin{pmatrix} 0 & 0 & \frac{1}{2}\Omega_R(t) & 0 \\ 0 & E1 & 0 & 0 \\ \frac{1}{2}\Omega_R(t) & 0 & \Delta_1 & \frac{1}{2}\Omega_B(t) \\ 0 & 0 & \frac{1}{2}\Omega_B(t) & 0 \end{pmatrix} \]

In the RWA:

\[ \Delta_1 = \Omega_{B}(t) \]
\[ \tau = 25 \text{ ns} \]

Two-qubit Hamiltonian

\[ \hat{H}_{2q} = \hat{H}_{1q} \otimes \mathbb{1} + \mathbb{1} \otimes \hat{H}_{1q} - U \ket{rr}ra{rr} \]

Dipole-dipole interaction when both atoms in Rydberg state.

Only diagonal gates!
Optimization of a Rydberg gate

$\tau = 25 \text{ ns}, T = 75 \text{ ns}$

- full basis
Optimization of a Rydberg gate

\[ \tau = 25 \text{ ns}, \ T = 75 \text{ ns} \]

- **Full basis**
- **3 states**

Michael Goerz  ●  Uni Kassel  ●  Efficient OCT for a Unitary under Dissipation
Diagonal gates

\[ \hat{U} = \text{diag}(e^{i\phi_{00}}, e^{i\phi_{01}}, e^{i\phi_{10}}, e^{i\phi_{11}}) \]

only diagonal gates are possible

no coupling between \(|0\rangle, |1\rangle\)

\[ \tau = 25 \text{ ns} \]

\[ \Delta_1 \]
Diagonal gates

\[ \begin{align*}
\Delta_1 & \quad |i\rangle \\
\Omega_B(t) & \quad |r\rangle \\
\Omega_R(t) & \quad \tau = 25 \text{ ns} \\
\end{align*} \]

no coupling between \(|0\rangle, |1\rangle\)

\[ \hat{U} = \text{diag}(e^{i\phi_{00}}, e^{i\phi_{01}}, e^{i\phi_{10}}, e^{i\phi_{11}}) \]

only diagonal gates are possible

\[ \begin{align*}
\hat{\rho}_1 &= \frac{1}{20} \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \\
\hat{\rho}_2 &= \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \\
\hat{\rho}_3 &= \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}
\]
Diagonal gates

\[ \Omega_{B}(t) \]

\[ \Omega_{R}(t) \]

\[ \Delta_{1} \]

\[ r \]

\[ i \]

\[ 0 \]

\[ 1 \]

\[ \hat{U} = \text{diag}(e^{i\phi_{00}}, e^{i\phi_{01}}, e^{i\phi_{10}}, e^{i\phi_{11}}) \]

no coupling between \( |0\rangle \), \( |1\rangle \)

only diagonal gates are possible

\[ \hat{\rho}_{1} = \frac{1}{20} \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \quad \hat{\rho}_{2} = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \quad \hat{\rho}_{3} = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]
Optimization of a Rydberg gate

\[ \tau = 25 \text{ ns}, \ T = 75 \text{ ns} \]

- Black line: full basis
- Red line: 3 states

Gate error vs. OCT iteration
Optimization of a Rydberg gate

\[ \tau = 25 \text{ ns}, \ T = 75 \text{ ns} \]

- full basis
- 3 states
- 2 states

OCT iteration

gate error

0.05
0.10
0.15
0.20

Michael Goerz  •  Uni Kassel  •  Efficient OCT for a Unitary under Dissipation
Optimization of a Rydberg gate

$\tau = 25 \text{ ns}, T = 75 \text{ ns}$

- full basis
- 3 states
- 2 states
- 2 states (weighted)
Optimization of a Rydberg gate – asymptotic behavior

\[ \tau = 25 \text{ ns}, \ T = 75 \text{ ns} \]

- full basis
- 3 states
- 2 states
- 2 states (weighted)
Example 2

Optimization of a non-diagonal gate using transmon qubits
Two coupled transmon qubits

Cavity mediates
- driven excitation of qubit
- interaction between left and right qubit

left qubit

right qubit

\[
\begin{bmatrix}
|0\rangle \\
|1\rangle \\
|2\rangle \\
|3\rangle \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
|0\rangle \\
|1\rangle \\
|2\rangle \\
|3\rangle \\
\end{bmatrix}
\]
Two coupled transmon qubits

Cavity mediates
- driven excitation of qubit
- interaction between left and right qubit

Many gates possible, e.g. \(\sqrt{iSWAP}\):

\[
\hat{O} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\
0 & \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]
Optimization of a transmon gate

![Graph showing gate error vs. OCT iteration for a full basis]
Optimization of a transmon gate

![Graph showing gate error versus OCT iteration for full basis and 3 states]

- **Full Basis**
- **3 States**

Gate error

**OCT iteration**

Michael Goerz • Uni Kassel • Efficient OCT for a Unitary under Dissipation
Optimization of a transmon gate

![Graph showing gate error over OCT iteration for different quantum basis sets.]

- **full basis**
- **3 states**
- **3 states (weighted)**

**Gate Error** vs **OCT Iteration**
Optimization of a transmon gate – CPU time

- Number of propagations (equivalent to CPU time)
- Gate error

- Full basis
- 3 states
- 3 states (weighted)
Optimization of a transmon gate – CPU time

![Graph showing gate error against number of propagations (equivalent to CPU time). The graph compares full basis, 3 states, and 3 states (weighted) with different asymptotic regions.](image)

- **Full Basis**
- **3 States**
- **3 States (Weighted)**

Michael Goerz • Uni Kassel • Efficient OCT for a Unitary under Dissipation
Using pure states only

\[ \hat{\rho}_1 = \frac{1}{20} \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \quad \hat{\rho}_2 = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \quad \hat{\rho}_3 = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]
Using pure states only

\[ \hat{\rho}_1 = \frac{1}{20} \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \quad \hat{\rho}_2 = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \quad \hat{\rho}_3 = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]
optimization of a transmon gate – CPU time

![Graph showing the relationship between number of propagations and gate error for different basis sets. The graph includes three lines: full basis, 3 states, and 3 states (weighted). The x-axis represents the number of propagations equivalent to CPU time, while the y-axis represents gate error. The inset shows the asymptotic region, indicating that as the number of propagations increases, the gate error decreases.]
optimization of a transmon gate – CPU time

![Graph showing the optimization of a transmon gate over CPU time. The x-axis represents the number of propagations (equivalent to CPU time), and the y-axis represents the gate error. The graph compares different states: full basis, 3 states, 3 states (weighted), and 5 states. The asymptotic region is highlighted to show the convergence of the gate error with increasing number of propagations.]
Conclusion

- A set of three density matrices is sufficient for gate optimization: (independent of dimension of Hilbert space!)
  - one to check dynamical map on subspace
  - one to check the basis
  - one to check the phases

- Further reduction possible for restricted systems

- States can (should!) be weighted according to physical interpretation

⇒ Gate optimization in open quantum systems with large Hilbert spaces have become significantly more feasible.

Reference:
Conclusion

- A set of three density matrices is sufficient for gate optimization: (independent of dimension of Hilbert space!)
  - one to check dynamical map on subspace
  - one to check the basis
  - one to check the phases
- Further reduction possible for restricted systems
- States can (should!) be weighted according to physical interpretation

⇒ Gate optimization in open quantum systems with large Hilbert spaces have become significantly more feasible.

Reference:
In press: New Journal of Physics (special issue)
Conclusion

- A set of three density matrices is sufficient for gate optimization: (independent of dimension of Hilbert space!)
  - one to check dynamical map on subspace
  - one to check the basis
  - one to check the phases
- Further reduction possible for restricted systems
- States can (should!) be weighted according to physical interpretation

⇒ Gate optimization in open quantum systems with large Hilbert spaces have become significantly more feasible.

Reference:
In press: New Journal of Physics (special issue)

Thank you
Optimized dynamics of the Rydberg gate

![Graph showing population and field dynamics over time](image)

- **Population**
  - 00
  - r0
  - 0r
  - rr
  - int

- **Field (rel. units)**
  - $\Omega_R(t)$
  - $\Omega_B(t)$
  - guess

Parameters:
- Time (ns): 0, 20, 40, 60
- Field (rel. units): 0, 0.5, 1
- Population: 00, r0, 0r, rr, int
with dissipation, full basis

with dissipation, two states (weighted)

without dissipation, full basis

without dissipation, two states (weighted)
Two Coupled Transmon Qubits

J. Koch et al. PRA 76, 042319 (2007)

A. Blais et al. PRA 75, 032329 (2007)
Two Coupled Transmon Qubits

Full Hamiltonian

\[ \hat{H} = \omega_c \hat{a}^\dagger \hat{a} + \omega_1 \hat{b}_1^\dagger \hat{b}_1 + \omega_2 \hat{b}_2^\dagger \hat{b}_2 - \frac{1}{2} \left( \alpha_1 \hat{b}_1^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{b}_1 + \alpha_2 \hat{b}_2^\dagger \hat{b}_2^\dagger \hat{b}_2 \hat{b}_2 \right) + \\
\text{ } + g_1 (\hat{b}_1^\dagger \hat{a} + \hat{b}_1 \hat{a}^\dagger) + g_2 (\hat{b}_2^\dagger \hat{a} + \hat{b}_2 \hat{a}^\dagger) + \epsilon^* (t) \hat{a} + \epsilon (t) \hat{a}^\dagger \]

\[ \text{ (1) } + \text{ (2) } + \text{ (3) } + \text{ (4) } + \text{ (5) } \]
Effective Hamiltonian

\[ \hat{H}_{\text{eff}} = \sum_{q=1,2} \sum_{i=0}^{N_q-1} (\omega_i^{(q)} + \chi_i^{(q)}) \hat{N}_i^{(q)} + \sum_{q=1,2} \sum_{i=0}^{N_q-1} g_{i}^{\text{eff} (q)} \epsilon(t)(\hat{C}_i^{+ (q)} + \hat{C}_i^{-(q)}) \]

\[ + \sum_{ij} J_{ij}^{\text{eff}} (\hat{C}_i^{-(1)} \hat{C}_j^{+(2)} + \hat{C}_i^{+(1)} \hat{C}_j^{-(2)}) . \]
Effective Hamiltonian

\[ \hat{H}_{\text{eff}} = \sum_{q=1,2} \sum_{i=0}^{N_q-1} \left( \omega_i^{(q)} + \chi_i^{(q)} \right) \hat{\Pi}_i^{(q)} + \sum_{q=1,2} \sum_{i=0}^{N_q-1} g_i^{\text{eff}}(q) \epsilon(t) \left( \hat{C}_i^{+(q)} + \hat{C}_i^{-(q)} \right) 
\]

\[ + \sum_{ij} J_{ij}^{\text{eff}} \left( \hat{C}_i^{-(1)} \hat{C}_j^{+(2)} + \hat{C}_i^{+(1)} \hat{C}_j^{-(2)} \right). \]

with

- \( \omega_i^{(q)} = i\omega_q - \frac{1}{2}(i^2 - i)\alpha_q, \quad g_i^{(q)} = \sqrt{i}g_q \)
- \( \hat{\Pi}_i^{(q)} = |i\rangle\langle i|_q, \quad \hat{C}_i^{+(q)} = |i\rangle\langle i-1|_q \)
- \( \chi_i^{(q)} = \frac{(g_i^{(q)})^2}{(\omega_i^{(q)} - \omega_{i-1}^{(q)} - \omega_c)} \)
- \( g_i^{\text{eff}}(q) = \frac{g_i^{(q)}}{(\omega_i^{(q)} - \omega_{i-1}^{(q)} - \omega_c)} \)
- \( J_{ij}^{\text{eff}} = \frac{1}{2}g_i^{\text{eff}}(1)g_j^{(2)} + \frac{1}{2}g_j^{\text{eff}}(2)g_i^{(1)} \)
<table>
<thead>
<tr>
<th>qubit frequency $\omega_1$</th>
<th>4.3796 GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>qubit frequency $\omega_2$</td>
<td>4.6137 GHz</td>
</tr>
<tr>
<td>drive frequency $\omega_d$</td>
<td>4.4985 GHz</td>
</tr>
<tr>
<td>anharmonicity $\alpha_1$</td>
<td>-239.3 MHz</td>
</tr>
<tr>
<td>anharmonicity $\alpha_2$</td>
<td>-242.8 MHz</td>
</tr>
<tr>
<td>effective qubit-qubit coupling $J$</td>
<td>-2.3 MHz</td>
</tr>
<tr>
<td>qubit 1,2 decay time $T_1$</td>
<td>38.0 µs, 32.0 µs</td>
</tr>
<tr>
<td>qubit 1,2 dephasing time $T_2^*$</td>
<td>29.5 µs, 16.0 µs</td>
</tr>
</tbody>
</table>

**Effective Hamiltonian**

$$\hat{H}_{\text{eff}} = \sum_{ijq} \left( (\omega_i^{(q)} + \chi_i^{(q)}) \hat{N}_i^{(q)} + g_i^{\text{eff}}(q) \epsilon(t)(\hat{C}_i^{+}(q) + \hat{C}_i^{-}(q)) + J_{ij}^{\text{eff}} (\hat{C}_i^{-}(1) \hat{C}_j^{+}(2) + c.c.) \right)$$

**Master Equation**

$$\mathcal{L}_D(\hat{\rho}) = \sum_{q=1,2} \left( \gamma_q \sum_{i=1}^{N-1} iD \left[ |i-1\rangle \langle i|_q \right] \hat{\rho} + \gamma_{\phi,q} \sum_{i=0}^{N-1} \sqrt{iD} \left[ |i\rangle \langle i|_q \right] \hat{\rho} \right),$$

with

$$D\left[ \hat{A} \right] \hat{\rho} = \hat{A} \hat{\rho} \hat{A}^\dagger - \frac{1}{2} \left( \hat{A}^\dagger \hat{A} \hat{\rho} + \hat{\rho} \hat{A}^\dagger \hat{A} \right)$$
### qubit properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>qubit frequency $\omega_1$</td>
<td>4.3796 GHz</td>
</tr>
<tr>
<td>qubit frequency $\omega_2$</td>
<td>4.6137 GHz</td>
</tr>
<tr>
<td>drive frequency $\omega_d$</td>
<td>4.4985 GHz</td>
</tr>
<tr>
<td>anharmonicity $\alpha_1$</td>
<td>-239.3 MHz</td>
</tr>
<tr>
<td>anharmonicity $\alpha_2$</td>
<td>-242.8 MHz</td>
</tr>
<tr>
<td>effective qubit-qubit coupling $J$</td>
<td>-2.3 MHz</td>
</tr>
<tr>
<td>qubit 1,2 decay time $T_1$</td>
<td>38.0 µs, 32.0 µs</td>
</tr>
<tr>
<td>qubit 1,2 dephasing time $T_2^*$</td>
<td>29.5 µs, 16.0 µs</td>
</tr>
</tbody>
</table>

- Near resonance of $\alpha_1$ with $\omega_1 - \omega_2$  

### Effective Hamiltonian

\[
\hat{H}_{\text{eff}} = \sum_{i} \left( (\omega_i^{(q)} + \chi_i^{(q)}) \hat{N}_i^{(q)} + g_i^{\text{eff}}(q) \epsilon(t) (\hat{C}_i^{+}(q) + \hat{C}_i^{-}(q)) + J_{ij}^{\text{eff}} (\hat{C}_i^{-}(1) \hat{C}_j^{+}(2) + \text{c.c.}) \right)
\]

### Master Equation

\[
\mathcal{L}_D(\hat{\rho}) = \sum_{q=1,2} \left( \gamma_q \sum_{i=1}^{N-1} iD \left[ |i-1\rangle\langle i|_q \right] \hat{\rho} + \gamma_{\phi,q} \sum_{i=0}^{N-1} \sqrt{iD} \left[ i\rangle\langle i|_q \right] \hat{\rho} \right),
\]

with
\[
D \left[ \hat{A} \right] \hat{\rho} = \hat{A} \hat{\rho} \hat{A}^\dagger - \frac{1}{2} \left( \hat{A}^\dagger \hat{A} \hat{\rho} + \hat{\rho} \hat{A}^\dagger \hat{A} \right)
\]
IBM Qubit – Poletto et al. PRL 109, 240505 (2012)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>qubit frequency $\omega_1$</td>
<td>4.3796 GHz</td>
</tr>
<tr>
<td>qubit frequency $\omega_2$</td>
<td>4.6137 GHz</td>
</tr>
<tr>
<td>drive frequency $\omega_d$</td>
<td>4.4985 GHz</td>
</tr>
<tr>
<td>anharmonicity $\alpha_1$</td>
<td>-239.3 MHz</td>
</tr>
<tr>
<td>anharmonicity $\alpha_2$</td>
<td>-242.8 MHz</td>
</tr>
<tr>
<td>effective qubit-qubit coupling $J$</td>
<td>-2.3 MHz</td>
</tr>
<tr>
<td>qubit 1,2 decay time $T_1$</td>
<td>38.0 µs, 32.0 µs</td>
</tr>
<tr>
<td>qubit 1,2 dephasing time $T_2^*$</td>
<td>29.5 µs, 16.0 µs</td>
</tr>
</tbody>
</table>

- Near resonance of $\alpha_1$ with $\omega_1 - \omega_2$
- Single frequency drive centered between two qubits

Effective Hamiltonian

$$\hat{H}_{\text{eff}} = \sum_{ijq} \left[ (\omega_i^{(q)} + \chi_i^{(q)})\hat{N}_i^{(q)} + g_i^{\text{eff}}(q)\epsilon(t)(\hat{C}_i^{+}(q) + \hat{C}_i^{-}(q)) + J_i^{\text{eff}}(\hat{C}_i^{-}(1)\hat{C}_j^{+}(2) + c.c.) \right]$$

Master Equation

$$\mathcal{L}_D(\hat{\rho}) = \sum_{q=1,2} \left[ \gamma_q \sum_{i=1}^{N-1} iD \left[ \left| i-1\right\rangle\langle i\left|_q \right. \right] \hat{\rho} + \gamma_{\phi,q} \sum_{i=0}^{N-1} \sqrt{iD} \left[ \left| i\right\rangle\langle i\right|_q \right] \hat{\rho} \right],$$

with $D \left[ \hat{A} \right] \hat{\rho} = \hat{A} \hat{\rho} \hat{A}^\dagger - \frac{1}{2} \left( \hat{A}^\dagger \hat{A} \hat{\rho} + \hat{\rho} \hat{A}^\dagger \hat{A} \right)$
Transmon Optimized Pulse

FIG. 9: Shape and spectrum of an optimized pulse, from optimization with 3 weighted states, with strong dissipation. The panels from top to bottom show the amplitude, complex phase, and spectrum of the optimized pulse $\mathcal{U}(t)$. The spectrum is shown in the rotating frame, with zero corresponding to the driving frequency $\omega_d$ of the field. The transition frequencies from the logical subspace are indicated by vertical dashed lines. These are $\frac{1}{\omega_1} = \frac{118.88}{MHz}$ and $\frac{1}{\omega_2} = \frac{358.18}{MHz}$ in red for the left qubit, and $\frac{2}{\omega_2} = \frac{115.20}{MHz}$ and $\frac{2}{\omega_2} = \frac{127.58}{MHz}$ in blue for the right qubit. The central peak in the spectrum has been cut off to show the relevant side-peaks, and would extend to a value of approximately 10.0. For all quantities, the values for the guess pulse are shown as a dotted line.

While the minimal number of states allows for determining whether a quantum gate has been implemented, it is insufficient to deduce bounds on the gate error [29]. Numerical and analytical bounds require $d + 1$, respectively $2d$, states in the reduced set, where $d$ is the dimension of the Hilbert space on which the optimization target is defined. Employing the sets of $d + 1$, respectively $2d$, states in quantum gate optimization is still significantly more efficient, both with respect to CPU time and memory requirements, than utilizing a full basis of Liouville space, with $d^2$ elements [9, 12, 23].

We have demonstrated the power of our approach in the optimization of a diagonal and a non-diagonal two-qubit gate. Specifically, we have optimized a controlled phase gate for trapped neutral atoms that are excited into a Rydberg state and subject to fast spontaneous emission from an intermediate state. The best performance was achieved by two states in the reduced set and a large weight of the Hilbert-Schmidt product for the state responsible for detecting phase errors. In the optimization of a $p$SWAP gate for two transmons coupled to the same transmission line cavity and subject to both energy relaxation and pure dephasing, we have found the best, and roughly identical, performance for the reduced sets consisting of $d + 1$, respectively $2d$, states. In all cases, the final gate error was limited by the decoherence rates. This confirms that employing a reduced set of states in quantum gate optimization is sufficient to determine the physical limit for the gate error.

The significant reduction in computational resources that we report here opens the door for a large-scale, systematic investigation of the fundamental limits of high-fidelity quantum gates in the presence of decoherence. Our approach is not tied to a specific decoherence model. It therefore allows to explore, using optimal control theory, settings for extended Hilbert spaces and beyond Markovian master equations, where a quantum system’s complexity may possibly be exploited for control.

Acknowledgments

We would like to thank Giulia Gualdi, Matthias M. M"uller, Felix Motzoi, Alireza Shabani and Birgitta Whaley for fruitful discussions and the Kavli Institute of Theoretical Physics at the University of California at Santa Barbara for hospitality. This research was supported in part by the Deutscher Akademischer Austauschdienst and by the National Science Foundation (Grant No. NSF PHY11-25915).
Transmon Population Dynamics

\[ \Psi(t = 0) = |01\rangle \]

\[ \Psi(t = 0) = |11\rangle \]