Optimal Control for Entangling Quantum Gates

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the quantum optimal control problem

quantum technology

steer quantum system in some desired way

\[ |\Psi^{(0)}\rangle \xrightarrow{\epsilon(t)} |\Psi^{tgt}\rangle \]

\(t_0\) to \(T\)

\(\epsilon(t)\): control field
the quantum optimal control problem

quantum technology

steer quantum system in some desired way

\[ |\psi(0)\rangle \rightarrow |\psi_{\text{tgt}}\rangle \]

\(\epsilon(t)\): control field

examples:

- **photo-chemistry**: form atomic bonds
- **medical imaging**: orient nuclear spin for max resolution
- **quantum networks**: prepare non-classical states
- **quantum computing**: apply logical operation ("gate")
optimizing quantum gates

\[ |\psi\rangle = \alpha_0 |0\ldots1\rangle + \cdots + \alpha_{2^N} |1\ldots1\rangle \]

reduce to two-qubit gates: \(4 \times 4\) matrix
|\psi\rangle = \alpha_0 |0 \ldots 1\rangle + \cdots + \alpha_{2^N} |1 \ldots 1\rangle

reduce to two-qubit gates: \(4 \times 4\) matrix

|\psi\rangle \rightarrow \hat{O} |\psi\rangle, \text{ e.g.} \quad \hat{O} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
optimizing quantum gates

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\[ \hat{O} = \begin{pmatrix}
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0 & 0 & 1 & 0
\end{pmatrix} \]

simultaneous targets (basis states)!
|ψ⟩ = α₀ |0...1⟩ + ... + α_{2N} |1...1⟩

N qubits

reduce to two-qubit gates: 4 × 4 matrix

Implementations:
- trapped atoms
- superconducting circuits
- NV centers
- quantum dots
- ...

optimizing quantum gates
logical subspace

e.g. trapped cesium atoms

$|r\rangle = |50^2 D_{3/2}\rangle$

1060 nm (1.17 eV) :

$|i\rangle = |7^2 P_{3/2}\rangle$

456 nm (2.72 eV) :

$|6^2 P_{1/2}\rangle$

895 nm (1.39 eV)

$|1\rangle = |6^2 S_{1/2}, F = 4\rangle$

9.2 GHz (0.04 meV)

$|0\rangle = |6^2 S_{1/2}, F = 3\rangle$

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logical subspace embedded in larger total Hilbert space!
numerical optimal control

analytical:

- geometric control – low dimension
- adiabatic schemes (e.g. STIRAP) – slow
- open quantum systems? noise? fundamental limits?
numerical optimal control

**analytical:**
- geometric control – low dimension
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**numerical:**
\[ |\Psi(0)\rangle \rightarrow |\Psi^{tgt}\rangle \quad \epsilon(t) \quad t_0 \rightarrow T \]
numerical optimal control

analytical:

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numerical:

\[
|\psi(0)\rangle \rightarrow |\psi(t_1)\rangle \rightarrow |\psi(t_2)\rangle \rightarrow |\psi(t_3)\rangle \rightarrow |\psi(t_4)\rangle \rightarrow |\psi(t_5)\rangle \rightarrow |\psi(t_6)\rangle \rightarrow |\psi^{tgt}\rangle
\]

\[t_0 \quad t_1 \quad t_2 \quad t_3 \quad t_4 \quad t_5 \quad t_6 \quad T\]
numerical optimal control

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\[ |\psi^{(0)}\rangle \rightarrow |\psi^{tgt}\rangle \]

\( t_0 \rightarrow t_1 \rightarrow t_2 \rightarrow t_3 \rightarrow t_4 \rightarrow t_5 \rightarrow t_6 \rightarrow T \)

minimize functional \( J_T \)

e.g. \( J_T = 1 - \frac{1}{d^2} \sum_{k=1}^{d} |\langle \psi_{k}^{tgt} | \psi_{k}(T) \rangle|^2 \)
numerical optimal control

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e.g. \( J_T = 1 - \frac{1}{d^2} \sum_{k=1}^{d} |\langle \psi^{tgt}_k | \psi_k(T) \rangle|^2 \)

\( \Rightarrow \) iterative scheme
Optimization Methods
gradient-free optimization

only evaluate fig. of merit $J_T$

$|\psi(0)\rangle$  $t_0$  $T$  $|\psi^\text{tgt}\rangle$

$\epsilon^{(0)}$
only evaluate fig. of merit $J_T$
only evaluate fig. of merit $J_T$
gradient-free optimization

only evaluate fig. of merit $J_T$
gradient-free optimization

only evaluate fig. of merit $J_T$

- any $J_T$
gradient-free optimization

only evaluate fig. of merit $J_T$

- any $J_T$
- good for small number of control parameters

$|\Psi(0)\rangle \rightarrow |\Psi^{tgt}\rangle$

$\epsilon^{(0)} \rightarrow \epsilon^{(1)} \rightarrow \epsilon^{(2)} \rightarrow \ldots$

$|\Psi(0)\rangle |\Psi^{tgt}\rangle$

$E_0 \uparrow$

$\epsilon \uparrow$

$\downarrow w$

$\text{time}$
gradient-free optimization

|ψ(0)⟩ → |ψtgt⟩

only evaluate fig. of merit $J_T$

- any $J_T$
- good for small number of control parameters

Nelder-Mead simplex:

$E_0$ $\epsilon$

$J_T$ $w$

$E_0$ $\epsilon$ $w$

time
gradient-free optimization

\[ |\psi^{(0)}\rangle \rightarrow \cdots \rightarrow |\psi^{tgt}\rangle \]

\[ \epsilon^{(0)} \rightarrow \epsilon^{(1)} \rightarrow \epsilon^{(2)} \]

only evaluate fig. of merit \( J_T \)

- any \( J_T \)
- good for small number of control parameters

Nelder-Mead simplex:

easy to use: scipy.optimize, Matlab, ...

\[ J_T \]

\[ E_0 \]

\[ \epsilon \]

\[ w \]

\[ \text{time} \]
control parameters: $\epsilon_i = \epsilon(t_i)$ for all points on time grid
GRAPE/LBFGS

- control parameters: $\epsilon_i = \epsilon(t_i)$ for all points on time grid

- $J_T \sim \langle \psi^{tgt} | \psi(T) \rangle = \langle \psi^{tgt} | \hat{U}_{nt} \ldots \hat{U}_1 | \psi_0 \rangle$
control parameters: $\epsilon_i = \epsilon(t_i)$ for all points on time grid

$J_T \sim \langle \psi^{tgt} | \psi(T) \rangle = \langle \psi^{tgt} | \hat{U}_n \cdots \hat{U}_1 | \psi_0 \rangle$

$$\frac{\partial J_T}{\partial \epsilon_i} = \langle \psi^{tgt} | \hat{U}^\dagger(t_i, T) \frac{\partial \hat{U}_i}{\partial \epsilon_i} \hat{U}(t_i, t_0) | \psi_0 \rangle$$

$$\left\langle \psi_{bw} \right|$$

$$\left| \psi_{fw} \right\rangle$$

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update scheme

$\Delta \epsilon_i \sim \frac{\partial J_T}{\partial \epsilon_i} \sim \langle \psi^{bw} | \frac{\partial \hat{U}_i}{\partial \epsilon_i} | \psi^{fw} \rangle$

$|\psi^{(0)}\rangle \rightarrow \frac{\partial \hat{U}_i}{\partial \epsilon_i} \rightarrow |\psi^{tgt}\rangle$
control parameters: $\epsilon_i = \epsilon(t_i)$ for all points on time grid

$J_T \sim \langle \Psi^{tgt} | \Psi(T) \rangle = \langle \Psi^{tgt} | \hat{U}_{nt} \ldots \hat{U}_1 | \Psi_0 \rangle$

$\frac{\partial J_T}{\partial \epsilon_i} = \langle \Psi^{tgt} | \hat{U}^\dagger(t_i, T) \frac{\partial \hat{U}_i}{\partial \epsilon_i} \hat{U}(t_i, t_0) | \Psi_0 \rangle$


library implementation: L-BFGS-B
Krotov’s method

- variational calculus, for continuous $\epsilon(t)$
Krotov’s method

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- extended functional: $J = J_T(\Psi) + \int_0^T J_t(\epsilon, \Psi) dt$
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- Krotov: separate dependency of states and field
  $(|\Psi(t)\rangle = \hat{U}(t, 0; \epsilon(t)) |\Psi_0\rangle)$
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- $\Rightarrow \epsilon^{(1)}$ that minimizes $J_T$ relative to $\epsilon^{(0)}$. 
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**update scheme**

\[
\Delta \epsilon(t) \sim \langle \chi^{bw} | \frac{\partial \hat{H}}{\partial \epsilon} | \psi^{fw}\rangle
\]

\[
|\psi^{(0)}\rangle \quad \bullet \quad \epsilon^{(1)} \quad \epsilon^{(0)} \quad \bullet \quad |\chi\rangle = \frac{\partial J_T}{\langle \Psi \rangle}
\]

Krotov’s method vs GRAPE

Krotov’s method

\[ \Delta \epsilon(t) \sim \langle \chi \mathbb{b}w \mid \partial \hat{H} \mid \psi \mathbb{f}w \rangle \]

\[ \mid \psi(0) \rangle \quad \epsilon^{(1)} \quad \epsilon^{(0)} \quad \mid \chi \rangle = \frac{\partial J_T}{\langle \psi \rangle} \]

\[ t_0 \quad t \quad T \]

GRAPe

\[ \Delta \epsilon_i \sim \frac{\partial J_T}{\partial \epsilon_i} \sim \langle \psi \mathbb{b}w \mid \partial \hat{U}_i \mid \psi \mathbb{f}w \rangle \]

\[ \mid \psi(0) \rangle \quad \partial \hat{U}_i \quad \partial \epsilon_i \quad \mid \psi \mathbb{t}g \rangle \]

\[ t_0 \quad \partial \epsilon_i \quad t \quad T \]

- sequential update
- continuous → discrete
- guaranteed monotonic convergence
- \( J_T \) only in boundary condition

- concurrent update
- inherently discrete
- parametrization through chain rule
Applications
progressively decrease gate duration
the quantum speed limit

- progressively decrease gate duration
- QSL is reached when objective can no longer be reached

progressively decrease gate duration
QSL is reached when objective can no longer be reached

example: optimization of entangling and local gates in superconducting transmon qubits

robustness to classical fluctuations

\[ \hat{H}_{2q} = \hat{H}_{1q} \Delta B(t) t = 150 \text{ ns} \]

\[ \hat{H}_{1q} \Delta R(t) \]

Quantum dynamics and control

\[ |0\rangle \hat{O} |\psi_{tgt}\rangle \]

\[ |1\rangle \hat{O} |\psi_{tgt}\rangle \]

\[ |2\rangle \hat{O} |\psi_{tgt}\rangle \]

\[ |3\rangle \hat{O} |\psi_{tgt}\rangle \]

\[ |4\rangle \hat{O} |\psi_{tgt}\rangle \]

\[ \ldots \]

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robustness to classical fluctuations

noise sources: fluctuation of Rydberg level, field amplitude
robustness to classical fluctuations

noise sources: fluctuation of Rydberg level, field amplitude

ensemble optimization

simultaneously optimize over multiple copies of the system with different noise realizations
robustness Rydberg gates

\[ \sigma_{\text{ryd}} \text{ (kHz)} \]

\[ \sigma_{\Omega} \text{ (\%)} \]

\[ \text{average gate error} \]

\[ \text{best analytic (800 ns)} \]

\[ \Rightarrow \text{ Goerz, Halperin, Aytac, Koch, Whaley. PRA 90, 032329 (2014)} \]
robustness Rydberg gates

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robustness Rydberg gates

- order of magnitude more robust!

$\sigma_{\text{ryd}}$ (kHz)

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robustness Rydberg gates

\[ \sigma_{\text{ryd}} \text{ (kHz)} \]

best analytic (800 ns)

\[ \sigma_{\Omega} \text{ (\%)} \]

OCT (800 ns)

OCT (100 ns)

⇒ Goerz, Halperin, Aytac, Koch, Whaley. PRA 90, 032329 (2014)
robustness to dissipation

just optimize density matrices!

\[ J^T = 1 - 3 \sum_{i=1}^{\infty} w_i \text{tr}[\hat{\rho}^2_i] \]

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

populations phases subspace

⇒ Goerz, Reich, Koch. NJP 16, 055012 (2014).

always 3 states, independent of dimension!

Alternative: MCWF trajectories
robustness to dissipation

just optimize density matrices!

\[ J_T = 1 - \sum_{i=1}^{3} \frac{w_i}{\text{tr}[^2_i]} \Re \left\{ \text{tr} \left[ \hat{\rho}_i^{\text{tgt}} \hat{\rho}_{i,n}(T) \right] \right\} \]
robustness to dissipation

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\[ J_T = 1 - \sum_{i=1}^{3} \frac{w_i}{\text{tr}[\hat{\rho}_i^2]} \text{Re} \left\{ \text{tr} \left[ \hat{\rho}_{i,\text{tgt}} \hat{\rho}_{i,n}(T) \right] \right\} \]
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populations \hspace{1cm} \text{phases} \hspace{1cm} \text{subspace}

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Alternative: MCWF trajectories
Quantum State Transfer and Entanglement Distribution among Distant Nodes

The basic idea of our scheme is to utilize strong coupling of atoms to a quantized transmission line (see text for explanation).

We consider a quantum network consisting of spatially separated nodes connected by quantum communication channels. Each node is a quantum system that stores quantum information and can exchange it with other nodes. Our scheme allows quantum transmission using photons (or any other means) to achieve efficient communication over long distances.

In this Letter we outline a scheme to implement this basic quantum transmission, which consists of the following steps:

1. A photon leaks out of the cavity, propagates to the first node, and enters the internal state of an atom.
2. By applying laser beams, one first transfers the internal state of an atom to a given node of the quantum network. By applying laser pulses, one can control the atom-cavity interaction, effectively switching off the dominant loss channel.
3. The photon wave packet entering a receiving cavity would "mimic" this time-symmetric outgoing pulse. If, on the other hand, we are able to drive the atom in a transmitting cavity in such a way that the photon wave packet and the outgoing pulse were already symmetric in time, the wave packet entering a receiving cavity would "mimic" this time-symmetric outgoing pulse.
4. The photon wave packet would be absorbed by the atom in a transmitting cavity in such a way that the photon wave packet and the outgoing pulse were already symmetric in time. The wave packet and the outgoing pulse would be transmitted through the network.

The distinguishing feature of our protocol is that by controlling the atom-cavity interaction, one can absolutely restore the original (unknown) superposition state of the atom, provided we would also reverse the timing of the laser pulses. If, on the other hand, we are able to "time reverse" this wave packet and send it back into the cavity; then this would be accomplished, let us consider that a photon leaks out of the cavity, and propagates away as a wave packet. Atoms and ions are particularly well suited for fast and internal-state-preserving transportation for fast and reliable communication over long distances. We propose a scheme to utilize photons for ideal quantum transmission between atoms located at trapped atoms or ions representing the nodes, with optical fibers or similar photon "conduits" providing the quantum channels.

The generated photons leak out of the cavity, propagate to a given node of the quantum network. By applying laser beams, one first transfers the internal state of an atom to the optical state of the cavity mode. The possibility of combining local quantum computation [11] is interesting from the perspective of distributed quantum cryptography [8], teleportation [9], and purification [10], and is a building block of communication in a distributed quantum network. Our scheme allows quantum transmission with optimal control for entangling quantum gates [16].

We propose a scheme to utilize photons for ideal quantum transmission between atoms located at trapped atoms or ions representing the nodes, with optical fibers or similar photon "conduits" providing the quantum channels. Atoms and ions are particularly well suited for fast and internal-state-preserving transportation for fast and reliable communication over long distances. We propose a scheme to utilize photons for ideal quantum transmission between atoms located at trapped atoms or ions providing the quantum channels. Atoms and ions are particularly well suited for fast and internal-state-preserving transportation for fast and reliable communication over long distances.

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trajectory optimization

\[ \hat{H} = \hat{H}_1 + \hat{H}_2 + i\kappa (\hat{a}_1 \hat{a}_2^\dagger - \hat{a}_1^\dagger \hat{a}_2), \quad \hat{L} = \sqrt{2\kappa} (\hat{a}_1 + \hat{a}_2) \]

propagate with \( \hat{H}_{\text{eff}} = \hat{H} - \frac{i\hbar}{2} \hat{L}^\dagger \hat{L} \),

jump randomly with probability of \( \|\psi\| \)
Quantum State Transfer and Entanglement Distribution among Distant Nodes

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Abstract. In this Letter we outline a scheme to implement this basic quantum transmission between two spatially distant atoms \[1\].

The basic idea of our scheme is to utilize strong coupling of an atom there to a high-

Energy-levels of atoms or ions seem to be technically intractable. [5,6], since fast and internal-state-preserving transportation for fast and reliable communication over long distances of atoms or ions provides an attractive method for localizing trapped atoms or ions providing the quantum channels. Atoms and ions are particularly well suited for storing qubits in long-lived internal states, and recently proposed schemes for performing quantum gates between trapped atoms or ions representing the nodes, with optical fibers or similar photon "conduits" providing the quantum channels. Each node is a quantum system that stores quantum information in quantum bits and processes this information locally using quantum gates \[1\]. Exchange of quantum information between the nodes of the network is accomplished, let us consider that a photon leaks out of the cavity, effectively switching off the dominant loss channel for the atom in a transmitting cavity in such a way that the outgoing pulse were already symmetric in time, the wave packet and send it back into the cavity; then this would be responsible for decoherence in the communication process. For a physical picture of how this can be accomplished, let us consider that a photon leaks out of the cavity, propagating away as a wave packet. Imagine that we were able to "time reverse" this wave packet and send it back into the cavity; then this would restore the state of the first atom, provided we would also reverse the timing of the outgoing pulse.

The distinguishing feature of our protocol is that by sequentially addressing pairs of atoms (one at each node), as entanglements between arbitrarily located atoms can be created[1].

The possibility of combining local quantum computation [11] with quantum transmission between the nodes of the network opens the possibility for a variety of other interesting applications, such as building block of communication in a distributed quantum network. For example, quantum channels enable quantum transmission between two spatially distant atoms [7].

To date, no process has actually been identified for the generation of optical entanglement. One first transfers the internal state of an atom between a high-

The generated photons leak out of the cavity, propagate through the cavity, and are detected at the second cavity. If the detected photons do not coincide with the outgoing wave packet, the cavity is in the initial state, \(|g\rangle\), and the atom in the second cavity is also in the internal state \(|g\rangle\).

The action of each atom with the corresponding cavity mode is described by the Hamiltonian:

\[
\hat{H} = \hat{H}_1 + \hat{H}_2 + i\kappa(\hat{a}_1^{\dagger}\hat{a}_2 - \hat{a}_1\hat{a}_2^\dagger), \quad \hat{L} = \sqrt{2\kappa}(\hat{a}_1 + \hat{a}_2)
\]

propagate with 

\[
\hat{H}_{\text{eff}} = \hat{H} - \frac{i\hbar}{2}\hat{L}^\dagger\hat{L},
\]

jump randomly with probability of \(\|\Psi\|\).

Quantum State Transfer and Entanglement Distribution among Distant Nodes

We consider a quantum network consisting of spatially separated nodes of a quantum network. The transmission protocol employs special laser pulses that excite an atom inside an optical cavity at the sending node so that its state is mapped into an atom there with unit probability. The generated photons leak out of the cavity, propagate through the network, and arrive at the first node to the optical state of the cavity mode. The transmission protocol is applied to any of the nodes of a quantum network. By applying laser pulses that excite an atom inside an optical cavity at the sending node so that its state is mapped into an atom there with unit probability, we can implement quantum transmission with photons (or any other means) to achieve efficient quantum transmission between two spatially separated nodes of a quantum network. Each node is a quantum system that stores quantum information. A photon packet entering a receiving cavity would "mimic" this time asymmetric outgoing pulse. If, on the other hand, we are able to drive the atom in a transmitting cavity in such a way that the outgoing pulse were already symmetric in time, the wave packet and send it back into the cavity; then this would be accomplished, let us consider that a photon leaks out of the cavity at the second node. Finally, the optical field at the second node is transferred to the internal state of the second cavity as a wave packet along the transmission line, and enter the detector. The distinguishing feature of our protocol is that by controlling the atom-cavity interaction, one can absolutely restore the original (unknown) superposition state of the atom, provided we would also reverse the timing of the atom-cavity interaction.

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propagate with \(\hat{H}_{\text{eff}} = \hat{H} - \frac{i\hbar}{2} \hat{L}^{\dagger} \hat{L}\), jump randomly with probability of \(\|\Psi\|\)
optimization in the Weyl chamber

- for two-qubit gates: many quantum gates are useful
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- which are most robust with respect to dissipation?
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- Cartan decomposition of any $4 \times 4$ unitary

$$\hat{A} = e^{i \frac{1}{2} (c_1 \hat{\sigma}_x \hat{\sigma}_x + c_2 \hat{\sigma}_y \hat{\sigma}_y + c_3 \hat{\sigma}_z \hat{\sigma}_z)}$$
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\]

- optimize for arbitrary perfect entangler
optimization for a perfect entangler

PE optimization for superconducting transmon qubits

optimization for a perfect entangler

PE optimization for superconducting transmon qubits

optimization for a perfect entangler

PE optimization for superconducting transmon qubits

much lower errors and much better convergence $\Rightarrow$ faster gates

design landscape exploration

two transmon qubits with shared transmission line
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design landscape exploration

two transmon qubits with shared transmission line

optimal choice of parameters?
two transmon qubits with shared transmission line

optimal choice of parameters?

\[ T = 200 \text{ ns} \]
\[ T = 50 \text{ ns} \]
\[ T = 10 \text{ ns} \]
design landscape exploration

two transmon qubits with shared transmission line

\[
\begin{align*}
L &= \lambda = 25 \text{ mm} \\
\omega_1 &\quad g &\quad \omega_2 \\
\alpha_1 &\quad g &\quad \alpha_2
\end{align*}
\]

optimal choice of parameters?

Identification of new QuaDiSQ regime

hybrid optimization schemes

combine gradient-free and gradient-based optimization in multiple stages
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⇒ Faster convergence
⇒ Cleaner pulses

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Bridging the gap to experiment:
spectral constraints, Hamiltonian estimation, noise source, . . .
summary

- OCT: toolbox for quantum engineering
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- optimization methods
  - gradient-free
  - gradient-based: GRAPE, Krotov’s method

- applications
  - quantum speed limit
  - robustness w.r.t. fluctuations → ensemble optimization
  - robustness w.r.t. dissipation: density matrix optimization, trajectories, advanced functionals
  - design landscape explorations
  - bridging the gap to experiment: hybrid optimization schemes, filters
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quantum dynamics and control
www.qnet-library.net

QNET
github.com/mabuchilab/QNET

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