Efficient Optimization of Quantum Gates in the Presence of Decoherence

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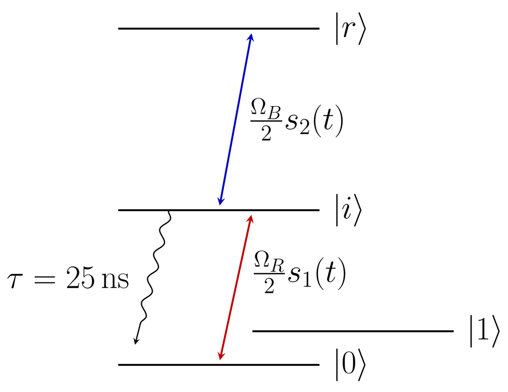
Abstract

Optimal control theory (OCT) represents a powerful tool for the implementation of quantum information tasks. For open systems, OCT is expected to find control solutions that are robust to decoherence. However, optimization of complex systems poses numerical challenges. Already in closed systems, the dimension of the Hilbert space scales exponentially with the size of the system, i.e., $d = 2^n$ for n qubits. The dimension of Liouville space is d^2, and according to common wisdom, optimization of a unitary operation requires propagation of a complete basis. Here, we show that for the optimization of unitary operations, it is not necessary to consider a complete set of basis states. Instead, a reduced set of states is sufficient. The minimal set consists of 3 states only.

To illustrate the efficient optimization of a unitary for an open quantum system, we consider the example of a Rydberg CPHASE gate with neutral trapped atoms [1]. The system Hamiltonian allows for diagonal gates only. We model the system dynamics with a master equation in Lindblad form and use optimal control theory, specifically Krotov's method [2], to find control pulses that implement the desired operation, and discuss the minimum number of states that needs to be accounted for in the optimization. For two transmon qubits coupled via shared cavity modes [3], also non-diagonal gates are possible. We give an outlook on the optimization of a CNOT gate on this system

① Rydberg gate: two trapped neutral atoms



$$\hat{\mathbf{H}}_{1q} = \begin{pmatrix} 0 & 0 & \frac{\Omega_R}{2}s_1(t) & 0 \\ 0 & E1 & 0 & 0 \\ \frac{\Omega_R}{2}s_1(t) & 0 & \Delta_1 & \frac{\Omega_B}{2}s_2(t) \\ 0 & & \frac{\Omega_B}{2}s_2(t) & \Delta_2 \end{pmatrix}$$

no coupling between $|0\rangle$, $|1\rangle \Rightarrow$ only diagonal gates

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

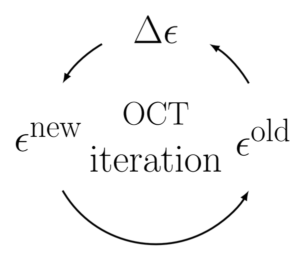
Two-qubit Hamiltonian: $\hat{\mathbf{H}}_{2q} = \hat{\mathbf{H}}_{1q} \otimes \mathbb{1} + \mathbb{1} \otimes \hat{\mathbf{H}}_{1q} - U\,|rr\rangle\langle rr|$
dipole-dipole interaction when both atoms in Rydberg state

Decoherence: $\frac{d\hat{\rho}}{dt} = -i[\hat{\mathbf{H}}, \hat{\rho}] + \mathcal{L}_D(\hat{\rho})$; $\quad \mathcal{L}_D(\hat{\rho}) = \gamma\left(\hat{\mathbf{A}}\hat{\rho}\hat{\mathbf{A}}^\dagger - \frac{1}{2}\left\{\hat{\mathbf{A}}^\dagger\hat{\mathbf{A}}, \hat{\rho}\right\}\right)$, $\quad \hat{\mathbf{A}} = |0\rangle\langle i|$

② Gate optimization in open quantum systems

- $\mathcal{H}$: Standard method: Krotov

$$J[\{\phi_k\}, \epsilon] = J_T[\{\phi_k(T)\}] + \lambda_a \int_0^T \frac{\Delta\epsilon^2(t)}{S(t)}\,\mathrm{d}t\,,$$



Pulse update formula [2]:

$$\Delta\epsilon(t) = \frac{S(t)}{\lambda_a}\mathfrak{Im}\left\{\sum_{k=1}^{4}\left\langle\chi_k^{\text{old}}(t)\middle|\frac{\partial\hat{\mathbf{H}}}{\partial\epsilon^{\text{new}}}\middle|\phi_k^{\text{new}}(t)\right\rangle + \underbrace{\sigma(t)\sum_{k=1}^{4}\left\langle\Delta\phi_k(t)\middle|\frac{\partial\hat{\mathbf{H}}}{\partial\epsilon^{\text{new}}}\middle|\phi_k^{\text{new}}(t)\right\rangle}_{\text{for choices of } J_T \text{ requiring second order}}\right\},$$

with $|\chi_k(T)\rangle \equiv -\frac{\partial J_T}{\partial\langle\phi_k(T)|}$. For common J_T: $\quad |\chi_k(T)\rangle \propto \left|\phi_k^{\text{tgt}}\right\rangle$, $\quad \left|\phi_k^{\text{tgt}}\right\rangle \equiv \hat{\mathbf{O}}\,|\phi_k\rangle$

- $\mathcal{L}$: Lift e.g. $J_T = 1 - \frac{1}{d}\sum_{i=1}^{d}\mathfrak{Re}\left\langle\Psi_i\middle|\hat{\mathbf{O}}^\dagger\hat{\mathbf{P}}\hat{\mathbf{U}}(T,0,\epsilon)\hat{\mathbf{P}}\middle|\Psi_i\right\rangle$, $d = \dim(\mathcal{H}) = 4$

$$\Rightarrow J_T = 1 - \frac{1}{d^2}\sum_{j=1}^{d^2}\text{tr}\left[\hat{\mathbf{O}}\hat{\rho}_j(0)\hat{\mathbf{O}}^\dagger\,\hat{\rho}_j(T)\right] \qquad \hat{\rho}_j \text{ span entire Liouville space } (d^2 = 16)$$

Decoherence is taken into account explicitly in the optimization through the equations of motion!

③ Reduced set of density matrices

Claim: We only need to propagate **3** matrices, not **16**

No need to characterize the full dynamical map!

① Do we stay in the logical subspace?

② Are we unitary, and if yes, did we implement the *right* gate?

for two-qubit gate: $\hat{\rho}_1 = \frac{1}{20}\begin{pmatrix} 8&0&0&0\\0&6&0&0\\0&0&4&0\\0&0&0&2\end{pmatrix}$, $\hat{\rho}_2 = \frac{1}{4}\begin{pmatrix}1&1&1&1\\1&1&1&1\\1&1&1&1\\1&1&1&1\end{pmatrix}$, $\hat{\rho}_3 = \frac{1}{4}\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}$

- $(\hat{\rho}_1)_{ij} = \frac{2(d-i+1)}{d(d+1)}\delta_{ij}$: check that gate is diagonal in same basis as $\hat{\mathbf{O}}$

  Just looking at $\mathcal{D}(\hat{\rho}_1) = \hat{\mathbf{U}}\hat{\rho}_1\hat{\mathbf{U}}^\dagger$ cannot distinguish any two diagonal gates of the form $\hat{\mathbf{U}} = \text{diag}(e^{i\phi_{00}}, e^{i\phi_{01}}, e^{i\phi_{10}}, e^{i\phi_{11}})$
- $(\hat{\rho}_2)_{ij} = \frac{1}{d}$: "totally rotated state", check relative phases between maps of logical eigenstates

  Concept of total rotation: $\hat{\rho} = \sum_i \lambda_i\hat{\mathbf{P}}_i$; $\quad \hat{\rho}' = \hat{\mathbf{P}}_{TR}$ with $\forall i:\ \hat{\mathbf{P}}_{TR}\hat{\mathbf{P}}_i \neq 0$
- $(\hat{\rho}_3)_{ij} = \frac{1}{d}\delta_{ij}$: check CPTP map on logical subspace

$\hat{\rho}_1, \hat{\rho}_2, \hat{\rho}_3$ together ensure that map is unitary on logical subspace.

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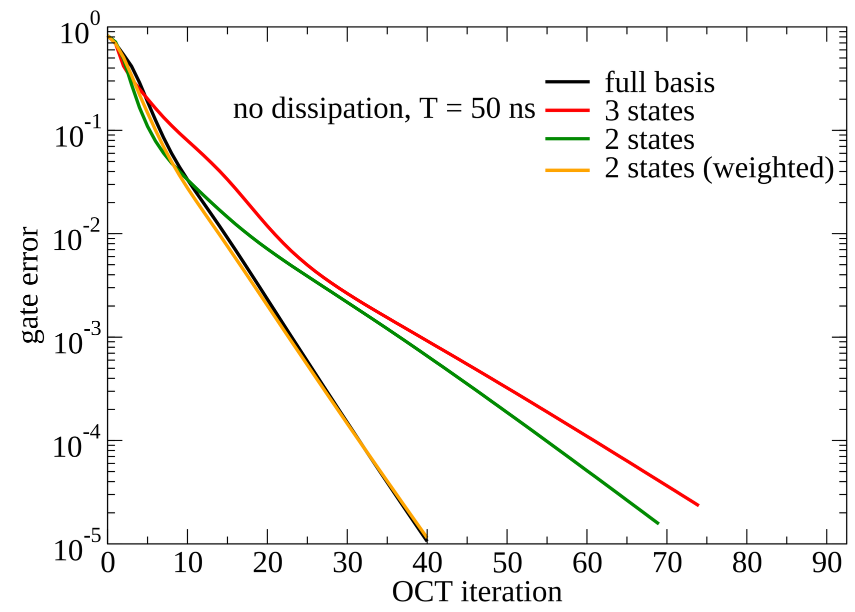
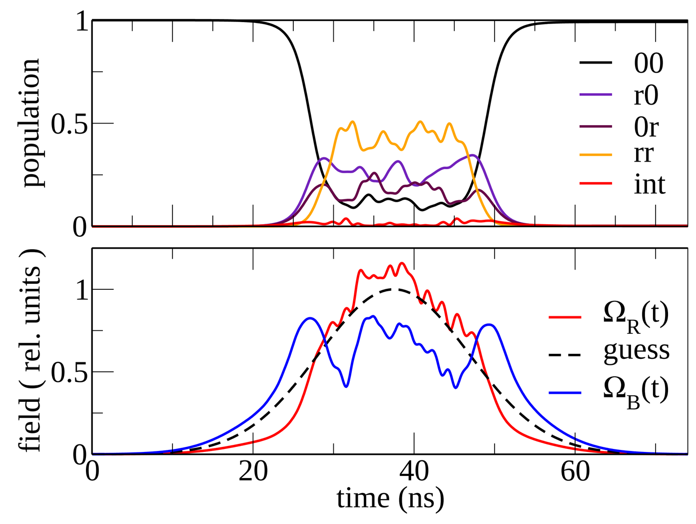
④ Rydberg CPHASE optimization results

Without dissipation

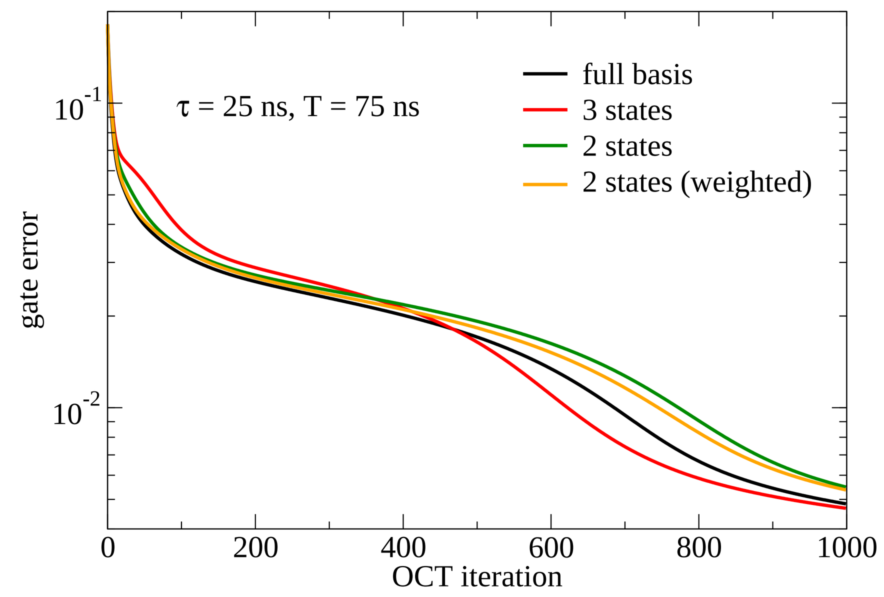
- only diagonal gates possible
  $\Rightarrow \hat{\rho}_1$ can be dropped
- $\hat{\rho}_2$, $\hat{\rho}_3$ can be weighted according to physical interpretation (implementing correct gate, staying in subspace)
- exponential convergence; weighted two states as good as full basis
- computational saving even for slower convergence



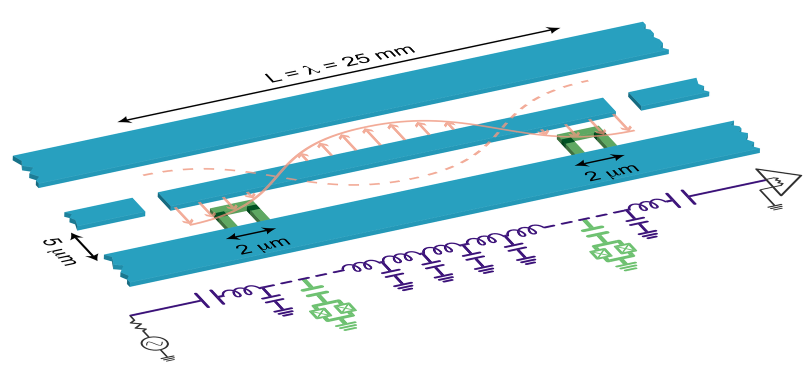
With dissipation



population dynamics / optimized pulses show double STIRAP-like behavior



⑤ Outlook: transmon two-qubit gate



superconducting qubits inside a transmission line resonator, Fig. from [4]

Parameters:

- $\omega_c = 8.3$ GHz
- $\omega_1 = 6.5$ GHz
- $\omega_2 = 6.6$ GHz
- $\alpha_1 = \alpha_2 = 150$ MHz
- $\omega_i^{(1,2)} = i\omega_{1,2} - (i^2 - i)\alpha_{1,2}$
- $J = 5$ MHz, $J_{ij} = \sqrt{ij}J$
- $g_1 = g_2 = 100$ MHz, $g_i^{(1,2)} = \sqrt{i}g_{1,2}$
- $g^{\text{eff}}\,|\epsilon(t)| < 50$ MHz (if possible)

$$\hat{\mathbf{H}} = \omega_c\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} + \omega_1\hat{\mathbf{b}}_1^\dagger\hat{\mathbf{b}}_1 + \omega_2\hat{\mathbf{b}}_2^\dagger\hat{\mathbf{b}}_2 - (\alpha_1\hat{\mathbf{b}}_1^\dagger\hat{\mathbf{b}}_1^\dagger\hat{\mathbf{b}}_1\hat{\mathbf{b}}_1 + \alpha_2\hat{\mathbf{b}}_2^\dagger\hat{\mathbf{b}}_2^\dagger\hat{\mathbf{b}}_2\hat{\mathbf{b}}_2) + J(\hat{\mathbf{b}}_1^\dagger\hat{\mathbf{b}}_2 + \hat{\mathbf{b}}_1\hat{\mathbf{b}}_2^\dagger) + g_1(\hat{\mathbf{b}}_1^\dagger\hat{\mathbf{a}} + \hat{\mathbf{b}}_1\hat{\mathbf{a}}^\dagger) + g_2(\hat{\mathbf{b}}_2^\dagger\hat{\mathbf{a}} + \hat{\mathbf{b}}_2\hat{\mathbf{a}}^\dagger) + \epsilon^*(t)\hat{\mathbf{a}} + \epsilon(t)\hat{\mathbf{a}}^\dagger$$

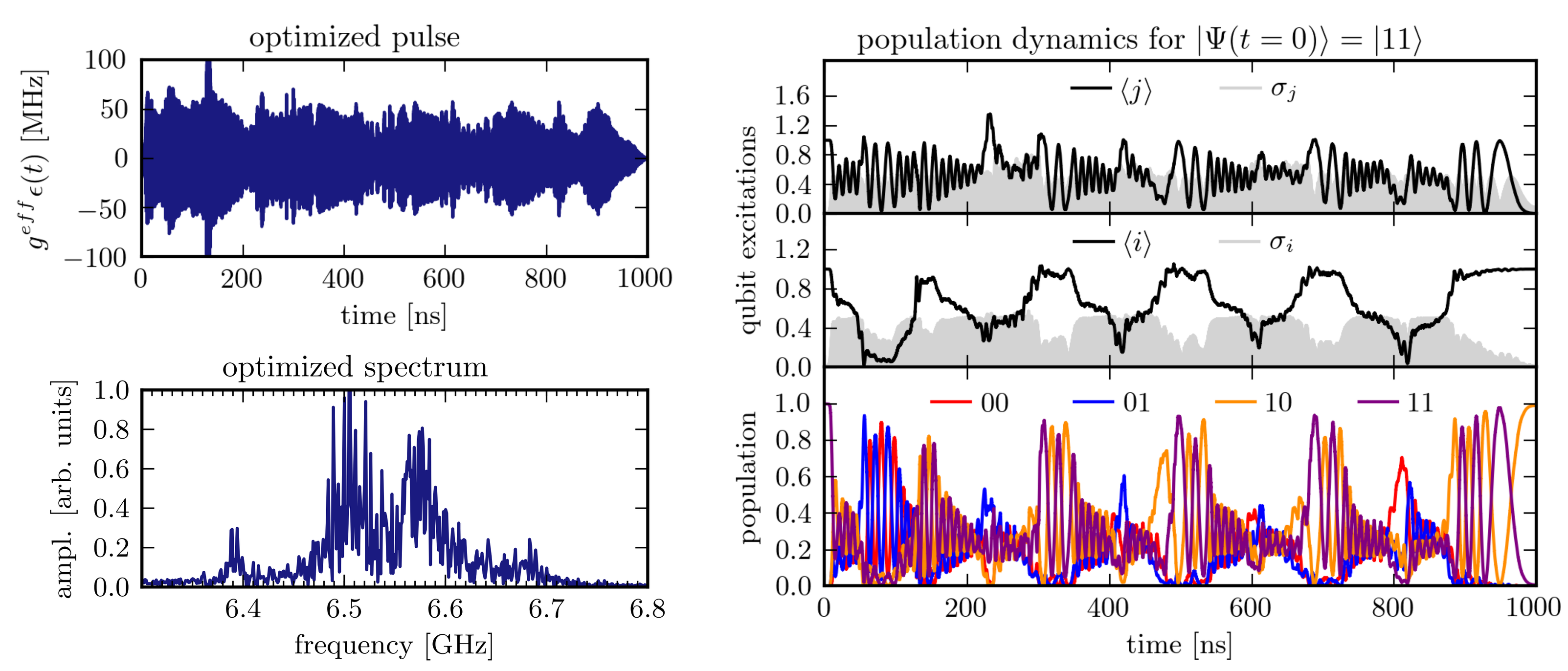
Schrieffer-Wolff transformation allows approximate diagonalization of Hamiltonian
$\Rightarrow$ reduced Hamiltonian after integrating out cavity

$$\hat{\mathbf{H}}_{\text{red}} = \sum_{q=1}^{2}\sum_{i=0}^{N_q-1}(\omega_i^{(q)} + \chi_i^{(q)})\hat{\mathbf{n}}_i^{(q)} + \sum_{q=1}^{2}\sum_{i=0}^{N_q-1}g_i^{\text{eff}\,(q)}\epsilon(t)(\hat{\mathbf{c}}_i^{+\,(q)} + \hat{\mathbf{c}}_i^{-\,(q)}) + \sum_{ij}J_{ij}^{\text{eff}}(\hat{\mathbf{c}}_i^{-\,(1)}\hat{\mathbf{c}}_j^{+\,(2)} + \hat{\mathbf{c}}_i^{+\,(1)}\hat{\mathbf{c}}_j^{-\,(2)})$$

$$g_i^{\text{eff}\,(1,2)} = \frac{g_i^{(1,2)}}{(\omega_i^{(1,2)} - \omega_{i-1}^{(1,2)} - \omega_c)}, \quad J_{ij}^{\text{eff}} = J_{ij} + \tfrac{1}{2}g_i^{\text{eff}\,(1)}g_j^{(2)} + \tfrac{1}{2}g_j^{\text{eff}\,(2)}g_i^{(1)}, \quad \chi_i^{(1,2)} = g_i^{\text{eff}\,(1,2)}g_i^{(1,2)}$$

Preliminary Optimization Result (CNOT):

$F = 99\%$



⑤ Conclusions & Next Steps

- A set of three density matrices is sufficient for gate optimization (independent of dimension of Hilbert space!): Since the goal is only to check whether a given unitary gate has been implemented, one does not need to span a full basis of the Hilbert space.
- Further reduction possible in special cases: If the Hamiltonian can only generate diagonal gates, $\hat{\rho}_1$ is automatically mapped correctly.
- States can be weighted according to physical interpretation. One may even change the relative weights between $\hat{\rho}_1$, $\hat{\rho}_2$, $\hat{\rho}_3$ dynamically.
- Success of optimization with reduced set of density matrices was demonstrated for the example of a CPHASE Rydberg gate. Optimal solutions match known STIRAP-like behavior in which the population in the decaying intermediary state is suppressed.
- It can be proven that $\hat{\rho}_1$, $\hat{\rho}_2$, $\hat{\rho}_3$ are sufficient to distinguish two unitaries in the logical subspace [5], but good convergence must still be shown numerically for Hamiltonian allowing non-diagonal gates.
- Superconducting qubits (transmons) provide rich dynamics and allow the realization of non-diagonal gates. They provide a suitable further testbed for the optimization with a reduced set of states.