Optimal Control of Quantum Gates under Decoherence

Michael Goerz, Daniel Reich, Sascha Trübelhorn, Giulia Gualdi, Christiane P. Koch

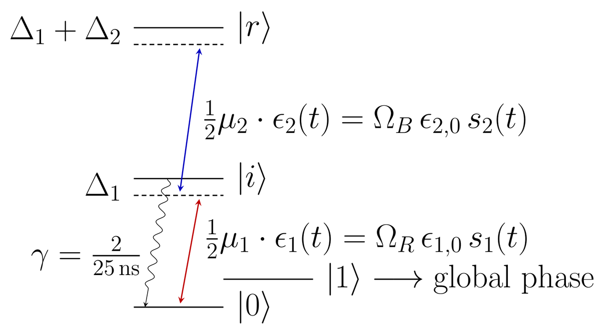
Quantum Dynamics and Control
UNIKASSEL VERSITÄT

Abstract

Optimal control theory provides a powerful method for the realization of entangling two-qubit gates under unitary evolution. This has been demonstrated e.g. for the implementation of a CPHASE gate for trapped neutral atoms [1, 2, 3]. In reality, however, every physical system suffers from decoherence. This could be relaxation due to spontaneous decay or dephasing due to noisy external fields. We therefore consider quantum systems whose dynamics is described by a master equation in Lindblad form. The Krotov optimization method [4] is adapted to operate in Liouville space so that the effect of decoherence is actively taken into account. We formulate the minimum number of optimization targets necessary to implement a unitary gate on the Hilbert space of the system, eliminating all redundancies of the density matrix description. The framework is applied to trapped neutral atoms, using realistic decoherence parameters.

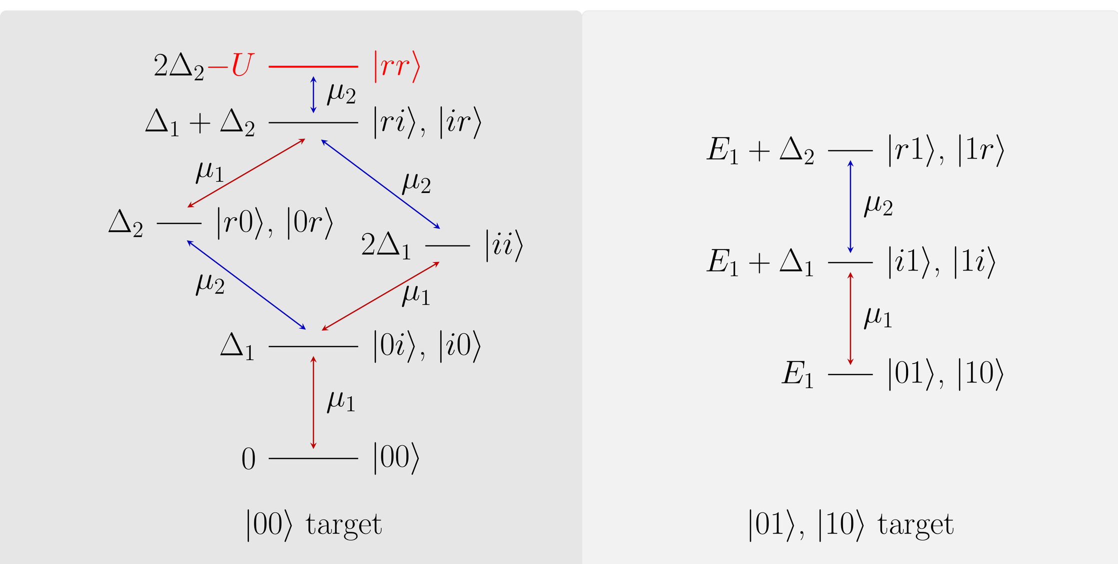
① Qubit Encoding in the Rydberg System

In RWA:
$$\hat{\mathbf{H}}_{1q}(t) = \begin{pmatrix} 0 & 0 & \frac{1}{2}\mu\epsilon_1(t) & 0 \\ 0 & E_1 & 0 & 0 \\ \frac{1}{2}\mu\epsilon_1(t) & 0 & \Delta_1 & \frac{1}{2}\mu\epsilon_2(t) \\ 0 & & \frac{1}{2}\mu\epsilon_2(t) & \Delta_2 \end{pmatrix}$$



with detunings Δ_1 for $|0\rangle \to |i\rangle$, Δ_2 for $|i\rangle \to |r\rangle$

$$\hat{\mathbf{H}}_{2q} = \hat{\mathbf{H}}_{1q} \otimes \mathbb{1} + \mathbb{1} \otimes \hat{\mathbf{H}}_{1q} - U\,|rr\rangle\langle rr| =$$



System Parameters [5]

- $\Omega_R = 300 \cdot 2\pi$ MHz
- $\Omega_B = 25 \cdot 2\pi$ MHz
- $E_1 = 6.8$ GHz
- $\Delta_1 = 600$ MHz, 1200 MHz
- $\Delta_2 = 0$
- $U = 50$ MHz

Pulse Parameters

- $T = 50$ ns, 150 ns
- $\epsilon_{1,0} = 1$, $\epsilon_{2,0} = 12$

② Hilbert Space Optimization: Krotov Method

Minimize $J[\{\phi_k\}, \epsilon] = -F[\{\phi_k(T)\}] + \int_0^T g_a(\epsilon, t)\,\mathrm{d}t + \int_0^T g_b(\{\phi_k\}, t)\,\mathrm{d}t$

Update formula [6] for $\Delta\epsilon = \epsilon^{(1)} - \epsilon^{(0)}$,

$$\Delta\epsilon = \frac{S(t)}{\lambda_a} \mathfrak{Im} \left\{ \sum_k \left\langle \chi_k^{(0)}(t) \middle| \left(\frac{\partial \hat{\mathbf{H}}}{\partial \epsilon}\right)_{\epsilon^{(1)}} \middle| \phi_k^{(1)}(t) \right\rangle + \frac{1}{2}\sigma(t) \sum_k \left\langle \Delta\phi_k(t) \middle| \left(\frac{\partial \hat{\mathbf{H}}}{\partial \epsilon}\right)_{\epsilon^{(1)}} \middle| \phi_k^{(1)}(t) \right\rangle \right\},$$

with forward-propagated $|\phi_k(t)\rangle = \hat{\mathbf{U}}\,|\phi_k(0)\rangle$ and backward-propagated $|\chi_k(t)\rangle$, with $|\chi_k(T)\rangle$ given by the derivative of F with respect to the states, e.g. [4]

$$F_{\text{re}} = \frac{1}{N} \mathfrak{Re} \sum_{k=1}^{N} \left\langle \phi_k(0) \middle| \hat{\mathbf{O}}^\dagger \middle| \phi_k(T) \right\rangle \quad \Longrightarrow \quad |\chi_k(T)\rangle = \frac{\partial F}{\partial \langle \phi_k(T)|} = \frac{1}{N}\frac{1}{2}\hat{\mathbf{O}}\,|\phi_k(0)\rangle = \frac{1}{N}\frac{1}{2}\left|\phi_k^{\text{tgt}}\right\rangle$$

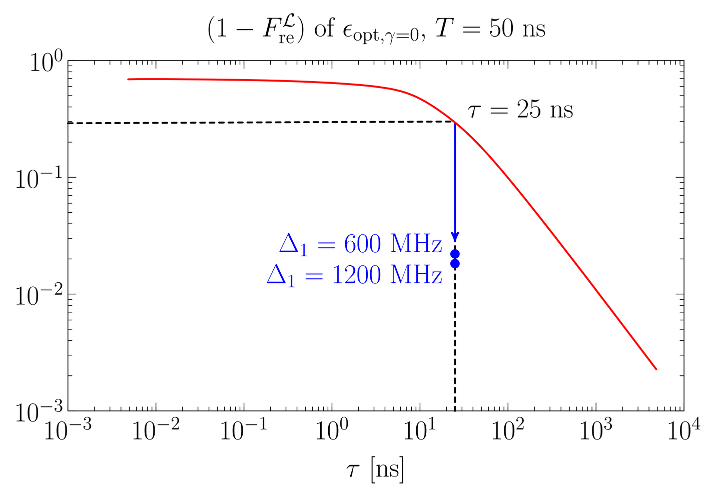
③ Decoherence in the Rydberg System

Master Equation in Lindblad form:

$$\frac{\partial}{\partial t}\hat{\rho} = -i\left[\hat{\mathbf{H}}, \hat{\rho}\right] + \sum_k \gamma_k \left(\hat{\mathbf{A}}_k \hat{\rho} \hat{\mathbf{A}}_k^\dagger - \frac{1}{2}\left\{ \hat{\mathbf{A}}_k^\dagger \hat{\mathbf{A}}_k, \hat{\rho} \right\} \right)$$
$$= -i\hat{\mathcal{L}}\hat{\rho}$$

Only consider relaxation from $|i\rangle \to |0\rangle$ with decay rate $\gamma = \frac{2}{\tau}$, $\tau = 25$ ns.

- Single qubit: $\hat{\mathbf{A}} = |0\rangle\langle i|$
- Two qubits: $\hat{\mathbf{A}}_1^{2q} = \hat{\mathbf{A}} \otimes \mathbb{1}$, $\hat{\mathbf{A}}_2^{2q} = \mathbb{1} \otimes \hat{\mathbf{A}}$



④ Optimization in Liouville Space

$$\Delta\epsilon(t) = \frac{S(t)}{\lambda_a} \mathfrak{Im} \left\{ \sum_{k=1}^{K} \left\langle\!\!\left\langle \Xi_k^{(1)}(t) \middle| \left(\frac{\partial \hat{\mathcal{L}}}{\partial \epsilon}\right)_{\epsilon^{(1)}} \middle| \rho_k^{(1)}(t) \right\rangle\!\!\right\rangle + \frac{1}{2}\sigma(t) \sum_{k=1}^{K} \left\langle\!\!\left\langle \Delta\rho_k(t) \middle| \left(\frac{\partial \hat{\mathcal{L}}}{\partial \epsilon}\right)_{\epsilon^{(1)}} \middle| \rho_k^{(1)}(t) \right\rangle\!\!\right\rangle \right\}$$

Questions:

1. **How many $\hat{\rho}_k$ need to be propagated? K for given Hilbert space dimension N?**
2. **How do the $\hat{\Xi}_k$ have to be constructed?**

Optimization in Liouville Space (cont.)

Direct Liouville Space Equivalent of Functional

$K = N^2$

Liouville equivalents of Hilbert space functionals [7], e.g.:

$$F_{\text{re}}^{\mathcal{L}} = \frac{1}{K} \mathfrak{Re} \sum_{k=1}^{K} \left\langle\!\!\left\langle \rho_k^{\text{tgt}} \middle| \rho_k(t) \right\rangle\!\!\right\rangle, \qquad F_{\text{sm}}^{\mathcal{L}} = \frac{1}{K^2} \left| \sum_{k=1}^{K} \left\langle\!\!\left\langle \rho_k^{\text{tgt}} \middle| \rho_k(t) \right\rangle\!\!\right\rangle \right|^2 \quad \Rightarrow \quad \hat{\Xi}_k = \frac{\partial \hat{\mathcal{L}}}{\partial \langle\!\langle \rho_k(T)|}$$

Unitary Optimization

$K = 2$

Given an evolution in Liouville space, what is the *most efficient* way to optimize a unitary evolution in Hilbert space?

$$F(\hat{\mathbf{U}}) = F_U\left(\left\{\hat{\rho}^{(i)}\right\}\right) + F_W\left(\left\{\hat{\rho}_W^{(i)}\right\}\right) + F_{TW}\left(\left\{\hat{\rho}_{TW}^{(i)}\right\}\right)$$

1. F_{TW}: The dynamical evolution in the *optimization subspace* corresponds to a dynamical map.
$$F_{TW} = 1 - \operatorname{tr}\left[\hat{\mathbf{P}}\hat{\rho}_W^{(1)}\hat{\mathbf{P}}\right]$$
2. F_W: The dynamical map is unitary.
$$F_W = \operatorname{tr}\left(\hat{\rho}_W^{(1)}(0)\right)^2 - \operatorname{tr}\left(\hat{\rho}_W^{(1)}(T)\right)^2 + \operatorname{tr}\left(\hat{\rho}_W^{(2)}(0)\right)^2 - \operatorname{tr}\left(\hat{\rho}_W^{(2)}(T)\right)^2$$
3. F_U: The unitary dynamical map corresponds to the target transformation.
$$F_U = \|\hat{\rho}_W^{(1)}(T) - \hat{\mathbf{O}}\hat{\rho}_W^{(1)}(0)\hat{\mathbf{O}}^\dagger\| + \|\hat{\rho}_W^{(2)}(T) - \hat{\mathbf{O}}\hat{\rho}_W^{(2)}(0)\hat{\mathbf{O}}^\dagger\|$$

Only two(!) density matrices $\hat{\rho}_W^{(1)}$, $\hat{\rho}_W^{(2)}$ with completely non-degenerate, non-zero eigenvalues needed (in the optimization subspace); $\hat{\rho}_W^{(2)}$ is "totally rotated" with respect to $\hat{\rho}_W^{(1)}$: At least one eigenstate of $\hat{\rho}_W^{(2)}$ has non-zero projections onto *all* eigenstates of $\hat{\rho}_W^{(1)}$.

Local Invariants Functional

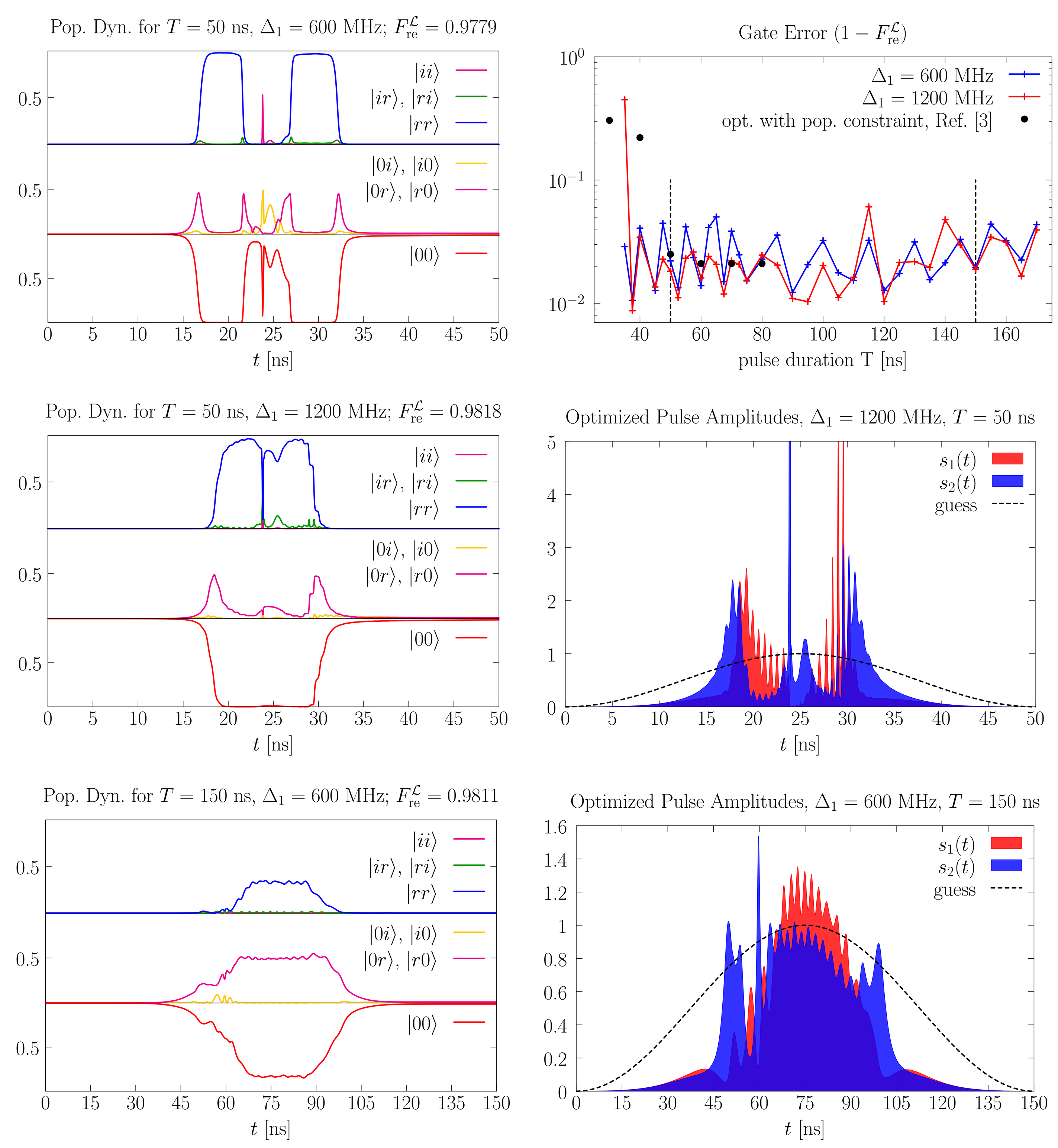
$K = N + 2$ ($K = 2$ for diag. gate)

The local invariants functional [2] allows to optimize for an equivalence class in the space of two-qubit gates, $\hat{\mathbf{U}} = \hat{\mathbf{k}}_1 \exp\left\{\frac{i}{2}(c_1\hat{\boldsymbol{\sigma}}_x^1\hat{\boldsymbol{\sigma}}_x^2 + c_2\hat{\boldsymbol{\sigma}}_y^1\hat{\boldsymbol{\sigma}}_y^2 + c_3\hat{\boldsymbol{\sigma}}_z^1\hat{\boldsymbol{\sigma}}_z^2)\right\}\hat{\mathbf{k}}_2$.

$$F_{\text{LI}} = \Delta g_1^2(\hat{\mathbf{U}}) + \Delta g_2^2(\hat{\mathbf{U}}) + \Delta g_3^2(\hat{\mathbf{U}}) - \frac{1}{N}\operatorname{tr}\left[\hat{\mathbf{U}}\hat{\mathbf{U}}^\dagger\right]; \qquad g_1, g_2, g_3 = \text{local invariants [8]}$$

The unitary evolution is analytically recovered from a set of N density matrices: $u_{ij} = \frac{(\rho_{jk})_{is}(T)}{\sqrt{(\rho_{kk})_{ss}(T)}}$.

⑤ Optimization Results for a Rydberg Gate



⑦ Conclusions & Outlook

We have shown that optimal control in Liouville space requires propagation of only two density matrices. This presents a significant speedup compared to previous approaches requiring propagation of N^2 density matrices.

Using $F_{\text{re}}^{\mathcal{L}}$, we have optimized a CPHASE Rydberg gate for varying pulse durations and two different detunings, taking into account decay from $|i\rangle$ to $|0\rangle$. The resulting optimized pulses show bang-bang type behavior for short gate times, and adiabatic behavior for long gate times. Using a larger detuning yields a suppression in the decaying state, and thus smaller errors for short pulse durations. The optimization success is comparable with earlier work [2, 3] in which the population in the decaying state was minimized to avoid dissipation.

In pending work, we examine the use of the local invariants functional, where the optimization via unitary reconstruction is essential. Besides a dramatic increase in efficiency, we expect an improvement in the gate fidelity due to the additional freedom given by the local equivalence class [2]. The optimization methods presented here are applicable to a wide range of other systems suffering from decoherence.

References

[1] M. H. Goerz, T. Calarco, and C. P. Koch, J. Phys. B **44**, 154011 (2011).

[2] M. M. Müller, D. M. Reich, M. Murphy, H. Yuan, J. Vala, K. B. Whaley, T. Calarco, and C. P. Koch, Phys. Rev. A **84**, 042315 (2011)

[3] M. M. Müller, H. Haakh, T. Calarco, C. P. Koch, and C. Henkel, Qu. Inf. Process. **10**, 771 (2011)

[4] J. P. Palao and R. Kosloff, Phys. Rev. A, **68**, 062308 (2003).

[5] T. Wilk, A. Gaëtan, C. Evellin, J. Wolters, Y. Miroshnychenko, P. Grangier, and A. Browaeys, Phys. Rev. Lett. **104**, 010502 (2010)

[6] D. M. Reich, M. Ndong, and C. P. Koch, arXiv:1008.5126.

[7] Y. Ohtsuki, New J. Phys. **12**, 045002 (2010)

[8] J. Zhang, J. Vala, S. Sastry, and K. B. Whaley, Phys. Rev. A **67**, 042313 (2003).