CIQC Spring School 2022
Christiane Koch: Control of Open Quantum Systems

Problem Set

In order to provide interesting questions to all of you, this problem set covers **a lot** of material from the very basics to fairly advanced. As we go along, not only the complexity of the physics increases but also the required python programming skills. If you do not have the time to work through the complete set, feel free to pick that part of the problems that suits your own level and interests best. No matter where this puts you, enjoy the learning experience!

1. Recap of basics: Control of a two-level system

These problems are essential for anybody who is not familiar with a two-level system interacting with an external control. Even if you are, you might find the numerical part of the exercises useful as these will serve as a starting point for using python/jupyter notebooks. Moreover, the driven two-level system is always a good benchmark to test numerical methods needed for more complex problems.

Problem 1.1 – Interaction picture & rotating wave approximation (RWA)

Consider a two-level system with energies $E_g = -\hbar\omega_0/2$ und $E_e = \hbar\omega_0/2$. It interacts with a classical electric field in the so-called electric dipole approximation where the spatial dependence of the electric field can be neglected, $E(t) = E_0 \cos(\omega_L t + \phi(t))$ with ω_L the field frequency and $\phi(t)$ a time-dependent phase. The field frequency is (almost) resonant to the transition frequency between the two levels, $\omega_L = \omega_0 + \Delta$ with $|\Delta| \ll \omega_0$. Apply the unitary transformation

$$\mathbf{U} = \begin{pmatrix} \exp(i\vartheta/2) & 0 \\ 0 & \exp(-i\vartheta/2) \end{pmatrix}$$

to the time-dependent Schrödinger equation, i.e., calculate the transformed Hamiltonian appearing in $i\hbar\frac{\partial}{\partial t}|\tilde{\psi}\rangle = \tilde{\mathbf{H}}|\tilde{\psi}\rangle$ for

(a) $\vartheta = \omega_0 t$,

(b) $\vartheta = \omega_L t + \phi(t)$.

In both cases, invoke the rotating wave approximation where you neglect terms that oscillate with frequencies close to $2\omega_0$. When is this approximation justified?

(c) Sketch the electric field for $\phi(t) = 0$ and $\phi(t) = \alpha t^2$.

With which frequency does the reference frame rotate in these two cases?

Problem 1.2 – π-pulse

Consider the same two-level system as in problem 1.1(a) but now with modulated field amplitude $E_0(t) = E_0 S(t)$. Assume resonant excitation, i.e. $\Delta = 0$ and all population initially in the ground state, i.e., $c_g(t = 0) = 1$.

(a) Show that

$$c_g(t) = \cos\left[\frac{\Omega_0}{2}\int_0^t S(t')dt'\right] \quad \text{and} \quad c_e(t) = i\sin\left[\frac{\Omega_0}{2}\int_0^t S(t')dt'\right],$$

where $\Omega_0 = dE_0/\hbar$ (and d the dipole moment).

(b) For a Gaussian field envelope, $S(t) = \exp\left[-\frac{(t-t_0)^2}{2\sigma^2}\right]$ and $t_0 \gg \sigma$, how do you have to choose the pulse duration to ensure complete population inversion, i.e., $|c_g(T \gg t_0 + \sigma)|^2 = 0$ and $|c_e(T \gg t_0 + \sigma)|^2 = 1$, at the end of the pulse? Why is such a pulse called π-pulse? By analogy, what level populations would you expect for a $\pi/2$-pulse? *Hint:* $\int_{-\infty}^{\infty} \exp(-a^2x^2)dx = \sqrt{\pi}/a$ *for* $a > 0$

A python notebook for solving Problem 1.2 numerically (and also serving as first entry point for anyone who has not used such notebooks before) is found at hiips://gitlabph.physik.fu-berlin.de/ag-koch/resources/spring_school_2022 (exercise 1) *When you use binder for the first time, it may take a couple of minutes to load.*

Problem 1.3 – Dressed states
Consider the same two-level system as in problem 1.1(b) but now with modulated field amplitude $E_0(t)$. Recall the time-dependent phase $\phi(t) = \frac{\alpha}{2}t^2$ with $\alpha \geq 0$.

(a) Calculate the instantaneous eigenvalues of $\tilde{\mathbf{H}}$.

(b) Sketch the eigenvalues as a function of time, assuming the field to be slowly switched on and off.

(c) How can one achieve complete population inversion between the two levels with such a field?

Problem 1.4 – Chirped pulses
A notebook for solving this problem numerically is found at :
hiips://gitlabph.physik.fu-berlin.de/ag-koch/resources/spring_school_2022 (exercise 2)
Consider the same two-level system as in problem 1.3, assuming the modulation of the field amplitude to be Gaussian, $E_0(t) = E_0 \exp(-t^2/(2\tau^2))$ and take all population initially to be in the ground state. Calculate the time evolution numerically and plot the excited state population as a function of time.

(a) Choose a fixed pulse duration τ and vary the chirp α. How do you have to choose α to populate the excited state without oscillations?

(b) Keep the chirp α fixed and vary the pulse duration τ. How do you have to choose τ to populate the excited state without oscillations?

(c) Calculate the instantaneous eigenvalues and plot them as a function of time together with the diagonal elements of $\tilde{\mathbf{H}}$. Describe your observations.

2. Essential control concepts

Problem 2.1 – Frame transformations & RWA for more than two levels

(a) Consider a three-level system, where levels 1, 2 and levels 2, 3 are connected by a dipole transition. The system interacts with an electric field $E(t) = E_1 S_1(t)\cos(\omega_1 t) + E_2 S_2(t)\cos(\omega_2 t)$. Write down the Hamiltonian, and apply the following unitary transformation to the time-dependent Schrödinger equation,

$$\mathbf{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \exp(-i\omega_1 t) & 0 \\ 0 & 0 & \exp(-i(\omega_1 - \omega_2)t) \end{pmatrix}.$$

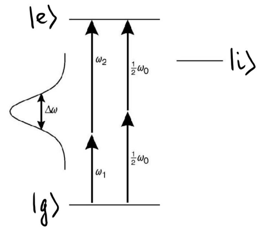
How does the transformed Hamiltonian differ from the Hamiltonian in the (standard) interaction picture (obtained with $\mathbf{U} = \exp(i/\hbar \mathbf{H}_0 t)$)?

(b) Assume that ω_1, ω_2 are near-resonant to the two transitions in the three-level system and take the so-called two-photon rotating wave approximation by neglecting terms that oscillate with sum frequencies while keeping those with difference frequencies. What does the Hamiltonian after the two-photon rotating wave approximation describe? Explain in particular the role of the one-photon and two-photon detunings. As specific examples, consider $E_2 > E_3 > E_1$ (λ-system), $E_3 > E_2 > E_1$ (ladder system), and $E_3 > E_1 > E_2$ (V-type system).

(c) Comparing the unitary transformations in Problems 1.1(a) and 2.1(a), devise a strategy for frame transformations and rotating-wave approximations for N-level systems.

Further reading: B. W. Shore: Manipulating Quantum Structures Using Laser Pulses, Cambridge Univ. Press 2011, in particular Ch. 13.2 & 15.3.1

Problem 2.2 – Spectral interference



Consider two-photon excitation from $|g\rangle$ to $|e\rangle$ mediated by the level $|i\rangle$ with a weak broadband pulse as sketched in the figure.

(a) Use second order perturbation theory to show that the two-photon absorption is determined by the quantity $S_2 = \left| \int_{-\infty}^{\infty} \varepsilon^2(t) e^{i\omega_0 t} dt \right|$.

(b) Show that S_2 can be rewritten as

$$S_2 = \left| \int_{-\infty}^{\infty} \tilde{\varepsilon}(\omega)\tilde{\varepsilon}(\omega_0 - \omega) d\omega \right| = \left| \int_{-\infty}^{\infty} A(\omega_0/2 + \Omega) A(\omega_0/2 - \Omega) e^{i[\Phi(\omega_0/2+\Omega)+\Phi(\omega_0/2-\Omega)]} d\Omega \right| ,$$

where $\tilde{\varepsilon}(\omega) = A(\omega)e^{i\Phi(\omega)}$ is the Fourier transform of $\varepsilon(t)$, and $A(\omega)$ and $\Phi(\omega)$ are the spectral amplitude and the spectral phase, respectively.

(c) Compare the two-photon absorption achieved with a transform-limited pulse, $\Phi(\omega) = 0$, to that achieved with phase-shaped pulses where the spectral phase is anti-symmetric, $\Phi(\omega_0/2 + \Omega) = -\Phi(\omega_0/2 - \Omega)$. What do you observe?

(d) Consider a phase shape consisting of a discontinuous step of π at frequency ω_s,

$$\Phi(\omega_0/2 + \Omega) + \Phi(\omega_0/2 - \Omega) = \begin{cases} 0 & \text{if} \quad \Omega \geq \Delta\omega_s \,, \\ 0 & \text{if} \quad \Omega \leq -\Delta\omega_s \,, \\ \pi & \text{if} \quad -\Delta\omega_s < \Omega < \Delta\omega_s \,, \end{cases}$$

where $\Delta\omega_s = \omega_s - \omega_0/2$. This phase shape can completely suppress the two-photon absorption depending on the value of ω_s [Meshulach & Silberberg, Nature 396, 239 (1998)]. Derive the step position, ω_s, from the condition $S_2 = 0$, assuming a Gaussian pulse. *Hint: This can be done analytically (error function!).*

Problem 2.3 – Compensating Stark shifts with chirps

Consider the same system as in Problem 2.2. For strong fields, time-dependent AC Stark shifts need to be taken into account. An effective two-level system is obtained by adiabatically eliminating the intermediate state and invoking a two-photon rotating-wave approximation,

$$\hat{\mathbf{H}}(t) = \begin{pmatrix} \omega_g^S(t) & \chi(t)e^{-i\varphi(t)} \\ \chi(t)e^{i\varphi(t)} & \Delta_{2P} + \omega_e^S(t) \end{pmatrix} ,$$

where $\omega_{g/e}^S(t)$ denotes the dynamic Stark shift of the ground and excited state, $\chi(t)$ the two-photon coupling, $\varphi(t)$ the temporal phase of the pulse and Δ_{2P} the two-photon detuning, $\Delta_{2P} = \omega_{eg} - 2\omega_L$. The two-photon coupling is given by

$$\chi(t) = -\frac{1}{4} E_0^2 |S(t)|^2 \frac{d_{ei} d_{ig}}{\omega_{ig} - \omega_L} ,$$

and the dynamic Stark shifts read

$$\omega_j^S(t) = -\frac{1}{2} E_0^2 |S(t)|^2 |d_{ij}|^2 \frac{\omega_{ij}}{\omega_{ij}^2 - \omega_L^2} , \quad j = g, e \,.$$

(a) Introduce the differential Stark shift, $\delta_\omega^S(t) = \omega_e^S(t) - \omega_g^S(t)$ and show that the Hamiltonian can be rewritten

$$\hat{\mathbf{H}}'(t) = \begin{pmatrix} -\frac{1}{2}[\delta_\omega^S(t) + \Delta_{2P} + \dot{\varphi}(t)] & \chi(t) \\ \chi(t) & \frac{1}{2}[\delta_\omega^S(t) + \Delta_{2P} + \dot{\varphi}(t)] \end{pmatrix} ,$$

(b) The two-level system can undergo Rabi cycling with e.g. a two-photon π-pulse corresponding to

$$\int_{-\infty}^{\infty} dt |\chi(t)| = \pi \,.$$

However, the π-pulse condition will only yield population inversion if the two-photon resonance is maintained [Trallero-Herrero et al, Phys. Rev. A 71, 013423 (2005)], i.e. if the diagonal elements of $\hat{\mathbf{H}}'(t)$ are zero. Which pulse parameter allows you to maintain resonance? How do you need to choose it?

(c) Evaluate the integral for the pulse parameter obtained in (b) assuming a Gaussian pulse envelope.

Problem 2.4 – Counterdiabatic driving

Consider the unitary transformation $\hat{\mathbf{U}}(t)$ that diagonalizes the Hamiltonian, $\hat{\mathbf{H}}(t) = \hat{\mathbf{H}}_0 + \hat{\mathbf{W}}(t)$, of a driven system. In the instantaneous eigenbasis, the time-dependent Schrödinger equation reads

$$i\hbar\frac{\partial}{\partial t}\left|\psi'(t)\right\rangle = \left(\hat{\mathbf{D}}(t) - i\hbar\hat{\mathbf{U}}(t)\frac{\partial\hat{\mathbf{U}}(t)}{\partial t}\right)\left|\psi'(t)\right\rangle ,$$

where $|\psi'(t)\rangle = \hat{\mathbf{U}}(t)\,|\psi(t)\rangle$. $\hat{\mathbf{D}}(t) = \hat{\mathbf{U}}(t)\hat{\mathbf{H}}(t)\hat{\mathbf{U}}^+(t)$ is the diagonal matrix containing the time-dependent eigenvalues of $\hat{\mathbf{H}}(t)$. Non-adiabatic transitions are caused by the off-diagonal elements of the second term in the parenthesis. The idea of counterdiabatic driving consists in adding an additional control $\hat{\mathbf{H}}_{CD}(t)$ to the Hamiltonian $\hat{\mathbf{H}}(t)$ that suppresses non-adiabatic transitions [Demirplak & Rice, J. Phys. Chem. A 107, 9937 (2003)].

(a) Show that this is equivalent to asking

$$\hat{\mathbf{H}}_{CD}(t) = i\hbar\frac{\partial\hat{\mathbf{U}}^+(t)}{\partial t}\hat{\mathbf{U}}(t)\,.$$

(b) Calculate the counterdiabatic term for a two-level system. It is useful to start in a rotating frame in which $\hat{\mathbf{H}}(t) = -\frac{\hbar}{2}\left(\Omega_0(t)\sigma_x - \Delta_L(t)\sigma_z\right)$ with $\Delta_L(t) = \omega_0 - \omega_L(t)$. Compare the counterdiabatic drive to the original drive in $\hat{\mathbf{W}}(t)$. Give an example how to realize the required time-dependence of the counterdiabatic term. *The comparison is best done in the lab frame. As to the pulse shape, you might want to take inspiration from Problem 1.*

(c) Calculate the counterdiabatic term for the Hamiltonian you have obtained in Problem 2.1(b), i.e., the so-called STIRAP-Hamiltonian. How practical is the counterdiabatic strategy in this case?

3. Optimal control warm-up

Problem 3.1 – Optimal control and variational calculus

One way to state the optimal control problem is to seek for the minimum (or maximum) of the target functional F under the constraint that the Schrödinger equation is obeyed. The latter can be included via a Lagrange multiplier $\langle\chi(t)|$,

$$J = F + 2\mathfrak{Re}\left[\int_0^T dt\left\langle\chi(t)\left|-\frac{\partial}{\partial t} + \frac{\hbar}{i}\hat{\mathbf{H}}[\Omega(t)]\right|\psi(t)\right\rangle\right] - \lambda\int_0^T dt|\Omega^2(t)|\,,$$

where $\hat{\mathbf{H}}$ depends on the yet unknown control $\Omega(t)$ and the last term is a regularization, introduced to keep $\Omega(t)$ finite [Zhu et al., J. Chem. Phys. 108, 1953 (1998)]. To optimize the transition from an initial to a target state, $F = |\langle\varphi_{\text{target}}|\hat{\mathbf{U}}(T,0)|\psi_{\text{initial}}\rangle|^2$ but one can also optimize e.g. the expectation value of some operator. Evaluate the extremum condition $\delta J = 0$ by calculating the variation of J with respect to $|\psi(t)\rangle$, $|\chi(t)\rangle$, and $\Omega(t)$. How does the choice of F enter the set of coupled equations you have obtained?

A notebook for solving the following problems is found at : hiips://gitlabph.physik.fu-berlin.de/ag-koch/resources/spring_school_2022 (exercise 3)

Problem 3.2 – Two-level system

Determine pulse shapes that optimize state-to-state transfer in a two-level system by working through the first notebook linked above. If you've worked through Problems 1.2-1.4 above, you know already several possible answers. Use this insight to initialize the optimization with different guess pulses. In particular, vary pulse duration, pulse amplitude, and use chirped pulses and check how the result depends on your initial guess. How do the optimizations differ when you start with an almost-optimal or far-from-optimal guess?

Problem 3.3 – Three-level system
Determine pulse shapes that optimize the transfer from state 1 to 3 (where dipole transitions connect levels 1 and 2 and levels 2 and 3) by working through the second notebook linked above. Check again how the initial guess influences the optimized pulse that you obtain. In addition to pulse duration and amplitude, vary also the timing of the two pulses.

4. Optimal control of open quantum systems

Problem 4.1 – Three-level system with decay
Consider the three-level system as in Problem 3.2 but now with decay of level 2 characterized by the decay rate 2γ ("bonus" exercise in the second notebook linked above).

(a) Optimize population transfer from level 1 to 3 as described in the online documentation. Vary the parameter λ_a. How does this affect the convergence of the algorithm?

Hint: It is sufficient to use the same value of λ_a for all four field components.

(b) Vary the guesses for pump and Stokes fields (Ω_{P1}, Ω_{P2}, Ω_{S1}, Ω_{S2}). How do these affect your optimized pulses?

(c) Vary the overall duration T. How does this affect your optimized pulses?

For the remaining problems, you need to assemble your own scripts based on the examples
hiips://qucontrol.github.io/krotov/v1.2.1/09_examples.html
for using the python krotov package :
hiips://github.com/qucontrol/krotov

Problem 4.2 – Fast qubit reset (Example "Optimization of Dissipative Qubit Reset")
Calculate the pulse shape to reset a qubit to its ground state in the shortest possible time with the highest possible fidelity. In order to do reach the minimum time required for this task, we separate the environment into strongly and weakly coupled degrees of freedom. The former are represented by a single two-level system, whereas the coupling to the latter are described by a master equation in Lindblad form. Vary the overall duration and record the reset fidelity for the respective optimizations.
Further reading: Basilewitsch et al., New J. Phys. 19, 113042 (2017).
Basilewitsch et al., Phys. Rev. Research 3, 013110 (2021).

Problem 4.3 – Gate optimization (Example "Optimization of a Dissipative Quantum Gate")
Consider two superconducting qubits with base frequency $\omega_{1/2}$, anharmonicity $\delta_{1/2}$, and effective coupling J. The external control is exerted via a shared transmission line resonator which, in the dispersive limit, can be integrated out. The resulting Hamiltonian reads

$$\hat{\mathsf{H}} = \left(\omega_1 - \frac{\delta_1}{2}\right)\hat{\mathsf{b}}_1^+\hat{\mathsf{b}}_1 + \frac{\delta_1}{2}\left(\hat{\mathsf{b}}_1^+\hat{\mathsf{b}}_1\right)^2 + \left(\omega_2 - \frac{\delta_2}{2}\right)\hat{\mathsf{b}}_2^+\hat{\mathsf{b}}_2 + \frac{\delta_2}{2}\left(\hat{\mathsf{b}}_2^+\hat{\mathsf{b}}_2\right)^2 + J\left(\hat{\mathsf{b}}_1^+\hat{\mathsf{b}}_2 + \hat{\mathsf{b}}_1\hat{\mathsf{b}}_2^+\right)$$
$$+\Omega(t)\cos(\omega_d t)\left(\hat{\mathsf{b}}_1 + \hat{\mathsf{b}}_1^+ + \hat{\mathsf{b}}_2 + \hat{\mathsf{b}}_2^+\right).$$

Use optimal control to determine pulse shapes $\Omega(t)$ that implement an $\sqrt{i\mathrm{SWAP}}$.

(a) As explained in the example, the propagation of three density matrices is sufficient for the gate optimization. Run the optimization with the weights given in the example as well as with equal weights and compare the convergence of the optimization.

(b) Determine the shortest possible duration for which the gate error is solely due to qubit decay and dephasing. Which parameter(s) of the Hamiltonian are responsible for this limit?

Further reading: Goerz et al., New J. Phys. 16, 055012 (2014)
Goerz et al., npj Quantum Inf. 3, 37 (2017)