M. Otten

2024.05.28

Module 1: Simulating Neutral Atom Qubits with QuTiP

1 Introduction

In this multi-module software lab, you will write a neutral atom qubit simulator, find one- and two-qubit gates, and then use that simulator as a backend to run quantum computing experiments. Along the way, we will use Python libraries, including QuTiP, Numpy, Scipy, Matplotlib, and Qiskit, among others, and will explore topics in atomic-molecular-optical (AMO) physics, computational physics, and quantum information. The sections with 'Exercises' in the title should be completed and turned in as both an executable jupyter notebook and as a PDF printout of the previously executed notebook. Note that the modules in the software lab build upon each other; code in this first module will potentially be used in all further modules.

2 Introduction to QuTiP

This section provides a few brief introductions to QuTiP. These exercises need not be turned in, but provide a way to get comfortable with some of the tools you will use in later sections.

2.1 Operators and Expectation Values

This brief introduction to QuTiP is taken from the Phys799: Advanced Quantum Computing homework. If you are comfortable with basic operations in QuTiP, such as operators, expectation values, plotting on the Bloch sphere.

The Hamiltonian for a spin-1/2 in a magnetic field, $\boldsymbol{B}$, is given by

$$H = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\frac{1}{2} g \mu_B \boldsymbol{\sigma} \cdot \boldsymbol{B},$$

where g is the Landé g-factor, μ_B is the Bohr magneton, and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a vector of Pauli spin operators.

a) Write down the matrix and outer product (ket-bra) representations of the 3 Pauli spin operators and the identity operator.

b) Find the expectation value of the spin projection, $\langle \boldsymbol{\sigma} \rangle = (\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle)$, for each of the following quantum states in (1) Dirac braket notation, (2) matrix notation, and (3) on QuTiP:

   i) $|\psi\rangle = |0\rangle$

ii) $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$

iii) $|\psi\rangle = (\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}(1+i)|1\rangle)$

c) Plot the three states above on the Bloch sphere using QuTiP.

d) Evaluate the spin Hamiltonian in matrix form assuming the magnetic field points along the x-direction, $\boldsymbol{B} = (B_x, 0, 0)$. Find its eigenvalues and the corresponding eigenvectors.

e) Now define the spin Hamiltonian in QuTiP and use it to find the eigenvalues and eigenvectors. For this, use natural units (let h = 1 such that your Hamiltonian takes on units of frequency instead of energy), let g = 2, $\mu_B = 1.4$ MHz/gauss, and $B_x = 100$ gauss.

f) Using QuTiP, plot the spectrum (i.e. the eigenenergies) as a function of the magnetic field strength B_x. Make sure that your axes are labeled and have units.

2.2 Master Equation Evolution

We will make extensive use of the Lindblad Master equation and the `mesolve` function in QuTiP. Please follow the documentation at `https://qutip.readthedocs.io/en/qutip-5.0.x/guide/dynamics/dynamics-master.html`. An additional tutorial can be found at `https://nbviewer.org/urls/qutip.org/qutip-tutorials/tutorials-v5/time-evolution/003_qubit-dynamics.ipynb`. For coupled system dynamics, see `https://nbviewer.org/urls/qutip.org/qutip-tutorials/tutorials-v5/time-evolution/004_rabi-oscillations.ipynb`.

We will also use time-dependent Hamiltonians to represent the quantum gates, especially for two-qubit gates. The documentation at `https://qutip.readthedocs.io/en/qutip-5.0.x/guide/dynamics/dynamics-time.html` provides a good introduction to the time-dependent Hamiltonian features.

3 Neutral Atom Hamiltonian

Our overall goal is to simulate a neutral atom quantum computer. Before we get to implementing gates or interfacing with QuTiP, we will first look at the basic control knobs and interactions available. We will use the Lindblad master equation,

$$\frac{\partial \rho}{\partial t} = -i[H + H(t), \rho] + L(C)[\rho], \tag{1}$$

where H is the time-independent part of the Hamiltonian, $H(t)$ represents the time-dependent parts, and $L[C](\rho)$ represents decoherence from coupling with the environment. We are using unit such that $\hbar = 1$. We will use a simplified model, capturing some of the most important features of the neutral atom physics. Thought it is not necessary for this module, more information about the background AMO physics can be found at `https://mariannasafronova.com/phys626/` or, specifically related

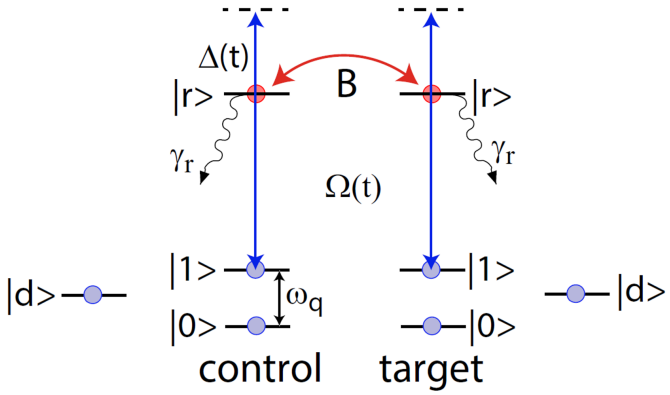

Figure 1: Reduced model for a pair of neutral atom qubits.

to atomic qubits, in Mark Saffman's book chapter `https://link.springer.com/chapter/10.1007/978-3-030-75436-5_13`. To simplify our physical model for the neutral atom qubit, we will use a four-level model, following Ref. M Saffman et al. "Symmetric Rydberg controlled-Z gates with adiabatic pulses". In: *Physical Review A* 101.6 (2020), p. 062309.

3.1 Four-Level System

One implementation of neutral atom quantum computers encodes the computational qubit in a specific, generally metastable hyperfine state of a neutral atom, such as rubidium or cesium. Interactions are provided by simultaneous excitation to specific, highly-excited Rydberg states, which can then decay back into the original qubit state, or into the manifold of all other hyperfine states. We can simulate this system using four states per atom, as shown in Fig. 3.1: two states for the computational qubit ($|0\rangle, |1\rangle$), one state for the Rydberg state ($|r\rangle$), and one state to represent the other possible hyperfine states ($|d\rangle$). First, we will start with a single four-level atom. Given this setup, we can now define a general Hamiltonian for this model,

$$H(t) = \frac{\Omega_{01}(t)}{2}\Big(|0\rangle\langle 1| + |1\rangle\langle 0|\Big) + \delta_1(t)|1\rangle\langle 1| + \frac{\Omega_r(t)}{2}\Big(|1\rangle\langle r| + |r\rangle\langle 1|\Big) + \Delta_r(t)|r\rangle\langle r|, \quad (2)$$

where $\Omega_{01}(t)$ represents the application of a laser pulse tuned to the $|0\rangle\langle 1$ transition, δ_1 is the detuning of the 0-1 laser, Ω_r represents the application of a separate laser pulse tuned to the $|0\rangle\langle r|$ transition, and Δ_r is the detuning of the 0-r laser.

The Rydberg state, $|r\rangle$, experiences decoherence mechanisms, whereas the $|0\rangle$, $|1\rangle$, and $|d\rangle$ states are considered stable for this model – their decay is sufficiently long to be negligible. The decay of the Rydberg state can be modeled with a set of Lindblad operators,

$$\mathcal{L}[\rho] = \sum_{j=\{0,1,d\}} L_j \rho L_j^\dagger - \frac{1}{2} L_j^\dagger L_j \rho - \frac{1}{2} \rho L_j^\dagger L_j \quad (3)$$

with collapse operators $L_j = \sqrt{b_{jr}\gamma_r}|j\rangle\langle r|$, where γ_r is the population decay rate of the Rydberg state and b_{jr} are the branching ratios the lower levels j. Together, the Hamiltonian of Eq. (2) and the Lindblad operators of Eq. (3) are implemented together in the Lindblad master equation (Eq. (1)) to represent a single neutral atom qubit.

3.2 Single Atom Exercises

The following exercises will explore various aspects of the single atom physics. As a tip, note that the Rydberg atom system is a four-level system and cannot be simply represented with Pauli matrices or raising and lowering operators. Instead, you can use the `basis()` function to represent kets, i.e., $|0\rangle$ = `basis(4,0)`, $|1\rangle$ = `basis(4,1)`, $|r\rangle$ = `basis(4,2)`, etc. You can then represent ket-bras (or operators) as $|r\rangle\langle r|$ = `basis(4,2) * basis(4,2).dag()`.

3.2.1 Exercise 1 - 0-1 Rabi Oscillations

For this exercise, we will take $\Omega_{01}(t)$ to be a constant, that is $\Omega_{01}(t) = 1$ MHz. We will set all of the other parameters in Eq.(2) to 0; that is $\delta_1(t) = 0$, $\Omega_r(t) = 0$, and $\Delta_r(t) = 0$. For the Lindblad terms, we take $\gamma_r = 1/(5\mu s)$, and the branching ratios to be $b_{0r} = 1/16, b_{1r} = 1/16, b_{dr} = 7/8$. Note that the actual lifetime is significantly longer.

Starting from the state $|0\rangle$, plot the populations of the $|0\rangle$, $|1\rangle$, $|r\rangle$, and $|d\rangle$ states over a time scale of 10s of microseconds. The population of $|1\rangle$ should follow the well-known Rabi oscillation formula, $P_1(t) = \sin^2(\frac{\Omega t}{2})$. Plot both the population of the $|1\rangle$ state and the Rabi oscillation formula together. Is there any decay?

3.2.2 Exercise 2 - Rydberg state lifetime

For this exercise, we will set all of the parameters in Eq.(2) to 0; that is $\Omega_{01}(t) = 0$, $\delta_1(t) = 0$, $\Omega_r(t) = 0$, and $\Delta_r(t) = 0$. For the Lindblad terms, we take $\gamma_r = 1/(5\mu s)$, and the branching ratios to be $b_{0r} = 1/16, b_{1r} = 1/16, b_{dr} = 7/8$.

Starting from the state $|r\rangle$, plot the populations of the $|0\rangle$, $|1\rangle$, $|r\rangle$, and $|d\rangle$ states over a time scale of 10s of microseconds. What do you observe? The state should decay smoothly as an exponential. The $|r\rangle$ state should decay with a lifetime of $1/5\mu s$. Does it? What happens to the $|0\rangle$, $|1\rangle$, and $|d\rangle$ states?

3.2.3 Exercise 3 - 0-r Rabi Oscillations

For this exercise, we will take $\Omega_r(t)$ to be a constant, that is $\Omega_r(t) = 10$ MHz. We will set all of the other parameters in Eq.(2) to 0; that is $\delta_1(t) = 0$, $\Omega_{01}(t) = 0$, and $\Delta_r(t) = 0$. For the Lindblad terms, we take $\gamma_r = 1/(5\mu s)$, and the branching ratios to be $b_{0r} = 1/16, b_{1r} = 1/16, b_{dr} = 7/8$.

Starting from the state $|1\rangle$, plot the populations of the $|0\rangle$, $|1\rangle$, $|r\rangle$, and $|d\rangle$ states over a time scale of 50 of microseconds. What do you observe? The population of the $|r\rangle$ state should oscillate according to the a damped version of the Rabi oscillation formula, $P_r(t) = \exp(-\gamma t)\sin^2(\frac{\Omega t}{2})$. What is γ for this exercise?

3.2.4 Exercise 4 - 0-1 Detuned Rabi Oscillations

For this exercise, we will take $\Omega_{01}(t)$ and $\delta_1(t)$ to be constant, that is $\Omega_{01}(t) = 1$ MHz and $\delta_1(t) = 1$ MHz. We will set all of the other parameters in Eq.(2) to 0; that is $\Omega_r(t) = 0$, and $\Delta_r(t) = 0$. For the Lindblad terms, we take $\gamma_r = 1/(5\mu s)$, and the branching ratios to be $b_{0r} = 1/16, b_{1r} = 1/16, b_{dr} = 7/8$.

Starting from the state $|0\rangle$, plot the populations of the $|0\rangle$, $|1\rangle$, $|r\rangle$, and $|d\rangle$ states over a time scale of 50 microseconds. What are the differences compared with exercise 1? Also plot the expectation value of $|0\rangle\langle 1| + |1\rangle\langle 0|$, which has the physical interpretation as the coherence between states $|0\rangle$ and $|1\rangle$. How does the coherence evolve? Redo this exercise with a smaller detuning, $\delta_1(t) = 100kHz$. How is the evolution different than with a larger detuning?

3.3 Two Atom Coupling

When two atoms are close enough, the can interact via the Rydberg blockade mechanism. Each atom will have its own, potentially independently controlled, Hamiltonian and Lindblad of Eqs. (2) and (3). In addition, there is a time-independent coupling that only affects the two atoms when they are both in their Rydberg states, represented by

$$H = B|rr\rangle\langle rr|, \tag{4}$$

where B is the Rydberg blockade strength.

3.4 Two Atom Exercises

3.4.1 Exercise 5 - Rydberg Blockade

For this exercise, we will take $\Omega_r^{(0)}(t)$ (where the superscript (0) means atom 0) to be a constant, that is $\Omega_r(t) = 10$ MHz. We will set all of the other parameters in Eq.(2) to 0; that is $\Omega_r^{(1)}(t) = 0$, $\delta_1^{(i)}(t) = 0$, $\Omega_{01}^{(i)}(t) = 0$, and $\Delta_r^{(i)}(t) = 0$. For the Lindblad terms, we take $\gamma_r = 1/(5\mu$ s), and the branching ratios to be $b_{0r} = 1/16, b_{1r} = 1/16, b_{dr} = 7/8$ for both atoms. We will use multiple values of the Rydberg blockade strength, B.

First, set the Rydberg blockade strength $B = 0$ MHz. Start with an initial state of $|10\rangle$. Plot the evolution of the population of the $|1\rangle$ and $|r\rangle$ states for qubit 0. Are they different than exercise 3? Now set the Rydberg blockade strength to $B = 400$ MHz and $B = 1$ MHz and plot the same populations. How do they compare? Try this same exercise with the initial state $|1r\rangle$. How do the results compare now? Plot comparisons between the same initial states with different blockade strengths, B, and the same blockade strengths with different initial states. Try again with no decay ($\gamma_r = 0$). Explain the various simulations.

4 Conclusion

In this module, you simulated the time dynamics of a single and of coupled neutral atom qubits. The code used for this module will serve as the basis for the physical

qubit simulator that we will eventually use to run quantum computing experiments. In the next module, we will explore how to tune the various knobs available (those in the Hamiltonian of Eq. (2)) to perform specific quantum gates, such as an X gate, a Z gate, a CZ gate, etc.