Module 2: Finding Neutral Atom Qubit Gates

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I. 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.

II. FIDELITY

Before we can find good gates for neutral atom qubits, we must first define what we mean by 'good gates'. In quantum information, we generally measure the 'closeness' of two state via a measure known as *fidelity.* For two quantum states, ρ and σ, the fidelity can be calculated via

$$\mathcal{F}(\rho,\sigma) = \left(\mathrm{Tr}\sqrt{\rho\sqrt{\sigma}\rho}\right). \tag{1}$$

However, rather than *state* fidelity, we actually want to know with the fidelity of a gate operation is. There are multiple ways to measure this; either *process* fidelity or *gate* fidelity. We will focus on gate fidelity from now on, but do note that gate and process fidelity are related by the simple formula

$$\mathcal{F}_g = \frac{d\mathcal{F}_p + 1}{d+1}, \tag{2}$$

where $\mathcal{F}_g$ is the gate fidelity and $\mathcal{F}_p$ is the process fidelity, and $d = 2^n$ is the dimension of the computational Hilbert space with n qubits. Note that it is 2^n regardless of whether the physical qubit has 2, 3, 4 or any number m levels, as this fidelity only looks at the action on the computational Hilbert space – in short, we do not care what happens to the rest of the space.

Compared with state fidelity, gate fidelity is trickier to find. The gate acts on a state, but there are generally infinite possible input states. The gate can also incur noise, which makes a simple unitary description of general physical gates. Furthermore, in the case of many qubits, including neutral atom qubits, the dynamics happens in a space larger than that of the computational qubit. Generally, this involves an average of the state fidelities between the noisy and noise-free versions of the gate. The gate fidelity can be evaluated by random sampling of the gate action on input states in a d dimensional space. It is sufficient to sample a subset of $2d$ states in mutually unbiased bases [1]. We will instead use the method introduced in Ref. [2], which shows that the fidelity calculated from a reduced set of $d+1$ input states provides a good estimate of gate fidelity.

This set consist of the following states:

$$\rho_{B,i} = |\phi_i\rangle \langle\phi_i| \,, \quad i = 1, ..., d, \tag{3}$$
$$\rho_{TR} \quad = \tfrac{1}{d} \textstyle\sum_{i,j=1}^{d} |\phi_i\rangle \langle\phi_j| \tag{4}$$

where $|\phi_i\rangle$ are the computational basis states (i.e., $|00\rangle, |01\rangle$, etc), and ρ_{TR} is the superposition of all basis states (i.e., $|00\rangle + |01\rangle + \cdots$, appropriately normalized). According to Ref. [2], the average gate fidelity can be calculated with the arithmetic mean, modified geometric mean, or a combined measure of the two over $\mathcal{F}_j$, where $\mathcal{F}_j$ is the fidelity of state ρ_j with the expected output of the gate,

$$\mathcal{F}_{\text{unitary}}^{\text{arith}} \quad = \tfrac{1}{d+1} \left[\textstyle\sum_{i=1}^{d} \mathcal{F}_{B,i} + \mathcal{F}_{TR} \right], \tag{5}$$
$$\mathcal{F}_{\text{unitary}}^{\text{geom}} = \tfrac{1}{d+1} + (1 - \tfrac{1}{d+1}) \left[\textstyle\prod_{i=1}^{d} \mathcal{F}_{B,i} \cdot \mathcal{F}_{TR} \right], \tag{6}$$
$$\mathcal{F}_{\text{unitary}}^{\lambda} \quad = \lambda \mathcal{F}_{\text{unitary}}^{\text{geom}} + (1 - \lambda) \mathcal{F}_{\text{unitary}}^{\text{arith}}, \tag{7}$$

with

$$\lambda = 1 - \frac{1 - \prod_{i=1}^{d} \mathcal{F}_{B,i}}{1 - \prod_{i=1}^{d} \mathcal{F}_{B,i} \cdot \mathcal{F}_{TR}}. \tag{8}$$

We will use this method to measure the fidelity of our quantum gates, which will allow us to optimize the fidelity to obtain the best gates possible.

A. Fidelity Exercises

1. *Implement Gate Fidelity*

First, implement the gate fidelities of eqs. (5), (6), (7): $\mathcal{F}_{\text{unitary}}^{\text{arith}}$, which uses the arithmetic mean; $\mathcal{F}_{\text{unitary}}^{\text{geom}}$, which uses the geometric mean; and $\mathcal{F}_{\text{unitary}}^{\lambda}$, which calculates a mixture of the two uses the mixture term λ. We will initially test this on a simple qubit system, and then move on to the large neutral atom system. `qutip` has a built in state fidelity function (`fidelity()`) which we can use to measure the state fidelities that go into our larger gate fidelity formula. Perform a few simple tests to verify that the code does what is expected, such as calculating the 'gate fidelity' between a set of density matrices and itself. Since all state fidelities should be one in this case, the gate fidelity should also be one. Change some of the states from this set; does the fidelity go down? Further exercises will perform more thorough tests, but it is always good to test for sanity before testing for proper physics.

2. *Exercise 1 - Test Gate Fidelity*

Even when things are checked for sanity, it is always better to check simple physics before going on to the real (more complicated) system. It is also instructive to perform multiple tests. We will first start with one qubit and a simple X gate on one qubit. Generate the set of test states needed. Generate the output states for the X gate. Test the gate fidelity between the target X gate and itself. Test the gate fidelity between the target X gate and other Pauli gates (Y, Z, I). Test the gate fidelity between the target X and an X rotation gate (`rx()` in `qutip`). Plot the fidelity as function of angle θ for the `rx()` gate. Qutip has a built in `average_gate_fidelity` function that works with the operators directly (whereas our function works directly with the states). How does our eq. (7) compare? Plot the arithmetic, geometric, and mixed fidelities and compare then with Qutip's build in function.

Perform the same tests using a random unitary (`rand_unitary()`). Are there any differences?

3. Exercise 2 - Optimizing Gate Fidelity

Given that we now have a working measure of the closeness between a target gate and some implementation, we can now optimize the fidelity to find the parameters of an operation so that it maximizes the fidelity (or minimizes the error). We will use `scipy.optimize.minimize` to do the optimization; see more details at `https://docs.scipy.org/doc/scipy-1.13.1/reference/generated/scipy.optimize.minimize.html`, which includes a small example.

It is known that any single-qubit gate can be decomposed into three rotation angles on two axes via Euler angles. We will use a sequence of Z X Z rotations here, which can be implemented via Qutip as something like `rz()*rx()*rz()`. Write a function which calculates the average gate fidelity, using our states method, between the Z X Z rotation gate and a random unitary for the three angles. Use `minimize` to find a set of optimal angles. Using a `callback` function, save the fidelity for each iteration. Plot the fidelity versus iteration number. Try with various solvers within `minimize` (i.e., Nelder-Mead, L-BFGS-B, Powell).

4. Exercise 3 - Test Gate Fidelity, Two-qubit gates

If implemented properly, the fidelity function should work just as well for two-qubit gates as it does for one qubit gates. Repeat the following tests above, using XX initially as a target. Compare with various two-qubit Pauli gates XX, XY, IZ, etc. Compare with two-qubit `tensor(rx(),rx())`. Create a 2D plot of angle θ_1 and angle θ_2 with the color being fidelity. Compare with a random two-qubit unitary. Try to optimize a six parameter gate, with `rz()*rx()*rz()` on each qubit. What is the maximum fidelity achievable with this two-qubit gate? Can you achieve a fidelity of 1? Why or why not?

III. NEUTRAL ATOM GATES

In this section, we will optimize the terms in our neutral atom Hamiltonian to obtain optimal parameters and fidelities for a set of single- and two-qubit gates. We will make use of the equations and you should (hopefully) be able to reuse your code from module one. Since we understand all of the physics now, we will jump right into the exercises. Note that, looking forward, the goal is to use the simulations of the gates as a backend simulator for Qiskit. As such, you should be designing your code with that in mind. That is, Qiskit may ask for a sequence of discrete gates which might need to be simulated gate by gate; the optimized gates we use here will be used there.

A. Single Atom Exercises

1. *Exercise 1 - X gate*

For this exercise, we will take $\gamma_r = 1/(540\mu s)$, and the branching ratios to be $b_{0r} = 1/16, b_{1r} = 1/16, b_{dr} = 7/8$. We will take $\Omega_{01}(t)$ to be a Gaussian pulse,

$$\Omega_{01}(t) = \Omega_0 \exp\Big(\frac{-(t-t_0)^2}{2\sigma^2}\Big), \tag{9}$$

with Rabi frequency Ω_0, pulse center t_0, and pulse width σ. We will set all of the other parameters in to 0; that is $\delta_1(t) = 0$, $\Omega_r(t) = 0$, and $\Delta_r(t) = 0$. For a fixed pulse width $\sigma = 1\mu$s, plot the population of the $|1\rangle$ state versus time for various values of the Rabi frequency $\Omega_0 = \{0, 0.25, 0.5, 0.75, 1, 1.25, 1.5\}$ MHz. For a fixed Rabi frequency $\Omega_0 = 1$MHz, plot the population of the $|1\rangle$ state versus time for various values of the pulse width $\sigma = \{0.5, 1, 1.5, 2, 4, 8\}$ μs.

Next, we will perform a π pulse. Here, we do not necessarily need optimization to find the gate; we know that we need a pulse area of π. Integrate the Gaussian pulse, eq. (9), over time (from $-\infty$ to ∞) to find the pulse area A, and solve for the pulse width σ in terms of the Rabi frequency Ω_0. Find the pulse width for Ω_0 =1 MHz. Plot the population of the $|1\rangle$ versus time. Does the gate perform a π pulse, where initial state $|0\rangle$ goes to $|1\rangle$, and initial state $|1\rangle$ goes to $|0\rangle$.

Use the previously developed function for measuring fidelity to measure the fidelity of the π pulse compared with an X gate. Note that because the neutral atom simulation is done via a four-level system, and we want to compare the fidelity with respect to a two-level system, you will need to take the 2×2 computational subspace out of the 4×4 density matrix. In some cases we will see for two qubit gates, this may result in a density matrix that does not have trace one, due to leakage. What is the fidelity observed? What do you expect it to be? What error channels do we have that would affect the fidelity? For a fixed Rabi frequency Ω_0, try optimizing the pulse width σ. Is the optimal σ the same as the one we found with our analytic formula?

For the optimal parameters, and initial states of $|0\rangle$ and $|1\rangle$, plot the evolution of the state on the Bloch sphere.

2. *Exercise 2 - Z gate*

For this exercise, we will take $\gamma_r = 1/(540\mu s)$, and the branching ratios to be $b_{0r} = 1/16, b_{1r} = 1/16, b_{dr} = 7/8$. We will take $\delta_1(t)$ to be a constant during some time width, T

$$\delta_1(t) = \begin{cases} \delta_1 & \text{if } 0 \le t < T \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

We will set all of the other parameters in to 0; that is $\Omega_{01}(t) = 0$, $\Omega_r(t) = 0$, and $\Delta_r(t) = 0$. Starting from an initial superposition state, $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$, plot the evolution of the state over the Bloch vector under constant detuning for times $t = 0$ to $T = 20\mu$s. Does the state evolve around the Bloch sphere as expected? Optimize fidelity of the evolution with respect to a Z gate, using the detuning time T. Plot the fidelity as a function of the optimization iterations. What is the optimal detuning time T? What is the fidelity observed? What do you expect it to be? What error channels do we have that would affect the fidelity?

3. Exercise 3 - CZ gate

For this exercise, we will take $\gamma_r = 1/(540\mu s)$, and the branching ratios to be $b_{0r} = 1/16, b_{1r} = 1/16, b_{dr} = 7/8$. We take $\delta_1(t) = 0$ and $\Omega_{01}(t) = 0$. As opposed the single-atom exercises above, we now have to include the Rydberg blockade strength, B. We will take $B/2\pi = 100$MHz initially.

We will implement a CZ gate initially using the protocol described in Ref. [3]. This adiabatic rapid passage (ARP) pulse consist of two identical π pulses with time-dependent Rabi drive $\Omega_{1r}(t)$ and detuning $\Delta_r(t)$

$$\Omega_{1r}(t) = \Omega_{1r}\frac{e^{-(t-t_0)^4/\tau^4} - a}{1-a} \tag{11a}$$

$$\Delta_r(t) = -\Delta_r \cos\left(\frac{2\pi}{T}t\right), \tag{11b}$$

with t_0 the center of each pulse and $T/2$ the length of each pulse so the gate duration is T. The parameter $a = exp(-((t_0/\tau) * *4))$ is chosen so that $\Omega = 0$ at the beginning and end of each pulse. The pulse slope parameter was set to be $\tau = 0.175T$. Take the following initial parameter set: $T = 0.54\mu$s, $\Omega_{1r}/2\pi = 17$MHz, $\Delta_r/2\pi = 23$ MHz, $B/2\pi = 200$MHz and $\tau = 0.175T$. These parameters are consistent with Fig. 2 of Ref. [3]. With our simulation tools already set up, you should be able to reproduce the plots using an initial state of $|10\rangle$. Notably, plot the pulse shapes (Fig. 2(a)), and the populations of various states (Fig. 2(b) and 2(c)). Are you able to reproduce the results? Given this set of parameters, what is the fidelity of the gate, using the fidelity function we previously developed? Ref. [3] uses a slightly different fidelity function (so-called Bell state fidelity), so you might not get exactly the same number. For these parameters, try changing the $\gamma_r = \{1/(5\mu s), 1/(50\mu s), 1/(100\mu s), 1/(250\mu s), 1/(540\mu s), 1/(1000\mu s)\}$. How does the fidelity change with increasing lifetime? What about the leakage (that is, the total population of the $|r\rangle$ states)?

Using the optimization tools we have developed, find optimal parameters for various values of $B/2\pi = 50, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000$MHz. How does the fidelity change with increasing Rydberg blockade strength? How do the parameters change?

4. Bonus Exercise - Time-Optimal Gates

With all of the tools developed here, we should be able to explore not just ARP gates, but pretty much any gate pulse shape, and search for the highest fidelity version. Within the literature, there are quite a few different pulse shapes which can provide high fidelity, some of them higher fidelity than the ARP pulse studied above. One example is the so-called time-optimal gate [4].

$$\Omega_{1r}(t) = \Omega_{1r}\left[\frac{1}{1+e^{-(t-20\tau_{\rm e})/\tau_{\rm e}}} + \frac{1}{1+e^{-(t_{\rm gate}-20\tau_{\rm e}-t)/\tau_{\rm e}}} - 1\right] \tag{12}$$

with $\tau_{\rm e} = 1.825$ ns and $t_{\rm gate}$ the nominal gate duration. The phase profile is

$$\Delta_r(t) = \Delta_r t + a\sin[2\pi f(t-t_0)]e^{-[(t-t_0)/\tau]^4} \tag{13}$$

with $t_0 = t_{\rm gate}/2$ the midpoint, with Δ_r the detuning from ground-Rydberg resonance, a the amplitude of the phase modulation, f the modulation frequency, t_0 the midpoint of the pulse, and τ providing an envelope width. The parameters $\Omega_0, \Delta_0, a, f, \tau$ are chosen to optimize the fidelity for given V, τ_R values. Using the developed code, and perhaps referring to Table S2 of Ref. [4], find optimal parameters for a few values of the Rydberg blockade strength, $B/2\pi = 50, 100, 200, 300$MHz. Note that Ref. [4] assumes no error, so you may find slightly lower fidelities than those reported if you use our standard lifetime.

IV. CONCLUSION

In this module, you explored how to calculate gate fidelity and applied it to understanding single- and two-qubit gates. In the next module, we will perform some software engineering to use our neutral atom simulator and gates to provide a backend simulator for Qiskit.

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[4] C. Poole, T. Graham, M. Perlin, M. Otten, and M. Saffman, Architecture for fast implementation of qldpc codes with optimized rydberg gates, arXiv preprint arXiv:2404.18809 (2024).