Homework assignment 2 - Density matrices and the physical implementation of quantum gates

Semiconducting & Superconducting Quantum Computers

Due: Oct. 1st, 2022

Problem 1 - The density matrix and the Werner states (15 pts / no collaboration)

Density matrices give a more general framework to describe quantum mechanics, especially in open systems, where quantum errors can occur, they provide an elegant way to describe qubit behavior. As a reminder, when a mixed quantum state is in the $|\psi_i\rangle$ state with probability p_i, the density matrix of the system is

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|.$$

a) We know that pure states evolve according to the Schrödinger equation, $i\hbar|\dot{\psi}\rangle = H|\psi\rangle$. Show that the time-evolution of the system described by the density matrix is

$$i\hbar\dot{\rho} = [H, \rho].$$

b) As an example, consider a free qubit described by the Hamiltonian $H = -\frac{1}{2}\hbar\omega_0\sigma_z$. At $t = 0$, we prepared the qubit in the pure $|-\rangle$ state. Express the time evolution of the density matrix, and calculate and plot the expectation value of $\langle\sigma_y\rangle(t) = \mathrm{Tr}\,(\rho\sigma_y)$.

c) Show that for a general state $\mathrm{Tr}\,(\rho) = 1$, but $\mathrm{Tr}\,(\rho^2) = 1$ only for pure states, and $\mathrm{Tr}\,(\rho^2) < 1$ for mixed states.

d) As a more advanced example, we consider the Werner states, which are a class of mixed states with a property that their amount of entanglement cannot be increased by any unitary transformation. The density matrix of a two-qubit Werner state can be written as

$$\rho_W = p \cdot |\psi_-\rangle\langle\psi_-| + (1-p)/4 \cdot I \otimes I,$$

where $|\psi_-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$ is the singlet Bell state, I is the identity operator for a single qubit and $p \in [0, 1]$ is a parameter. Write down the the density matrix in matrix form.

e) Plot the purity ($\mathrm{Tr}\rho_W^2$) of the state as a function of p. What is the physical meaning of purity?

f) Plot the degree of entanglement as a function of p. (Using Qutip is a good idea here.)

Problem 2 - Longitudinal ZZ coupling between qubits (20 pts / collaboration is encouraged)

In class, we discussed that the dipole-dipole interaction between qubits can lead to an XX coupling term. In the rotating frame of the qubits, this coupling can generate an iSWAP gate if the interaction is turned on for the appropriate time. However, such dipole-dipole coupling is not the only interaction scheme that exists between qubits. Another coupling that arises frequently in experimental architectures is the ZZ interaction. This interaction many times considered as residual, unwanted coupling and currently significant research effort is invested in reducing its effect.

a) When two qubits are coupled longitudinally, the full system Hamiltonian takes the following form in the lab frame

$$H_{\mathrm{LAB}} = -\frac{1}{2}\hbar\omega_A\sigma_{z,A} - \frac{1}{2}\hbar\omega_B\sigma_{z,B} + \hbar g\sigma_{z,A}\sigma_{z,B}, \tag{1}$$

where ω_A and ω_B are the qubit energies, g is the coupling strength, and $\sigma_{i,A}$ and $\sigma_{i,B}$ are the Pauli matrices acting on the two qubits. Use the usual unitary transformation $U = \exp\left[-i\left(\omega_A\sigma_{z,A} + \omega_B\sigma_{z,B}\right)t/2\right]$ to transfer the Hamiltonian to the rotating frame of the two qubits and show that the Hamiltonian in the rotating frame takes the following form

$$H_{\mathrm{ROT}} = UH_{\mathrm{LAB}}U^\dagger + i\hbar\dot{U}U^\dagger = \hbar g\sigma_{z,A}\sigma_{z,B}. \tag{2}$$

b) Express the unitary evolution of the system: $U_{\mathrm{ZZ}} = \exp\left[-iH_{\mathrm{ROT}}t/\hbar\right]$. Give the answer in a 4x4 matrix form in the qubit basis states.

c) When the interaction gate is turned on for the appropriate time t_{gate}, the unitary evolution can give rise to a perfect entangler controlled-phase (CZ) gate for ZZ coupling (in contrast to the iSWAP gate for XX coupling). The CZ gate corresponds to a phase shift of π on qubit B, when qubit A is excited, and has the following form

$$\mathrm{CZ} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

It is important to note that the unitary operation $U_{\mathrm{ZZ}}(t_{\mathrm{gate}})$ needs to be combined with single-qubit Z rotations (and a global phase factor) to generate the CZ gate:

$$\mathrm{CZ} = \exp[-i\pi/4]\left[R_A^z(-\pi/2) \otimes R_B^z(-\pi/2)\right] U_{\mathrm{ZZ}}(t_{\mathrm{gate}}). \tag{3}$$

Find t_{gate} so that the ZZ interaction and the combination of these single-qubit gates (and the global phase factor) gives the CZ gate.

d) As mentioned above, the ZZ coupling many times arises in quantum systems as a spurious interaction: even when we want to isolate two qubits from each other, the ZZ interaction still remains in the system and unwantedly entangles the two qubits. In this section, we will estimate the effect of this ZZ interaction on the qubit coherence.

First, consider the density matrix of two qubits A and B, which can be expressed in the basis of $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ such as $\rho_{AB} = \rho_{11}|00\rangle\langle 00| + \rho_{12}|00\rangle\langle 01| + \ldots$:

$$\rho_{AB} = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{pmatrix}.$$

Show that the partial trace over qubit B takes the following form

$$\mathrm{Tr}_B\rho_{AB} = \begin{pmatrix} \rho_{11} + \rho_{22} & \rho_{13} + \rho_{24} \\ \rho_{31} + \rho_{42} & \rho_{33} + \rho_{44} \end{pmatrix}.$$

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e) Show that if the two qubits are in the unentangled state $\rho_{AB} = \rho_A \otimes \rho_B$, the reduced density matrix is equal to ρ_A, i.e., $\mathrm{Tr}_B\rho_{AB} = \rho_A$. On the other hand, if the states are the maximally entangled Bell states $|\psi_{\mathrm{Bell}}\rangle = (|00\rangle + |11\rangle)/\sqrt{2})$, $\mathrm{Tr}_B\rho_{AB}$ describes a classical mixed state, i.e., $\mathrm{Tr}_B\rho_{AB} = I/2$. Thus, from a single qubit perspective–roughly speaking–full entanglement means a fully mixed state and the loss of coherence.

f) Now focusing on two qubits coupled through ZZ interaction, we will show that this interaction reduces the purity of the qubit states. As a reminder, the ZZ coupling can be described by the following Hamiltonian in the rotating frame of the two qubits

$$H_{\mathrm{ROT}} = \hbar g \sigma_{z,A}\sigma_{z,B}, \tag{4}$$

Calculate the evolution of the density matrices ρ_{AB} and $\mathrm{Tr}_B\rho_{AB}$ if we initially prepared qubit A in state $|+\rangle$ and qubit B in state $|-\rangle$. Plot the concurrence and the purity of qubit A as a function of time on the same plot. What relationship do you see between these two quantities?

g) The coherence time of a qubit T_2 describes the decay of the off-diagonal term (ρ_{01}) in the density matrix. This can be an exponential or Gaussian decay depending on the noise, and for this problem we assume the latter one: $\rho_{01} \propto e^{-(t/T_2)^2}$. Find out the T_2 decoherence time of the qubit due to the ZZ interaction at short times ($t \ll T_2$, $gt \ll 1$).

Problem 3 - Simulating entangled state creation (15 pts / collaboration is encouraged)

In this problem, we will numerically simulate the iSWAP gate to create entangled states, and compare it with the theoretical expectations. Although this problem can be solved analytically in the absence of decoherence, the numerical approach will be useful for future systems with dephasing. Feel free to use and modify the shared QuTip codes or create your own.

a) First, we simulate the single-qubit gate. In the rotating frame and when the drive is on-resonant with the qubit frequency, the Rabi Hamiltonian takes the form of ($\hbar = 1$ from now)

$$H_{\mathrm{Rabi}} = \frac{1}{2}\Omega_I\sigma_x + \frac{1}{2}\Omega_Q\sigma_y,$$

where Ω_I and Ω_Q are the Rabi amplitudes. In this problem, we can consider a case when $\Omega_I = 0$, so that the rotation happens around the y axis. Assume that the Rabi frequency is $\Omega_Q = 1$. Simulate numerically the time evolution of the qubit after it is initialized in the $|0\rangle$ state, and find the gate time needed to create the $|+\rangle$ and $|-\rangle$ state based on the simulation. Extract the numerically obtained states for the two gate times, and compare it with the theoretically expected values. What is the fidelity of these states?

b) Using the gates calibrated above, assume that we initialized qubit A in the $|+\rangle$ and qubit B in the $|-\rangle$ state, and that both qubits have the same frequency. Now we can turn on the XX interaction between them, which, in the rotating frame, leads to the following Hamiltonian

$$H_{\text{int}} = \frac{1}{2} g \left[\sigma_{x,A}\sigma_{x,B} + \sigma_{y,A}\sigma_{y,B}\right].$$

This interaction generates the iSWAP gate as we simulated in examples in class (see notebook online). Again find numerically the gate time for doing the iSWAP gate and extract the states numerically (here, assume that the coupling rate is $g = 3$). What is the fidelity and concurrence of the states?