Problem Set 2

Geometric control is an established technique in the field of nuclear magnetic resonance (NMR) spectroscopy, and has been experimentally demonstrated. This worksheet will highlight some of the considerations that go into an experimental implementation of the theory contained in the lecture notes.

Problem 1: Preliminary calculations

Remind yourself of the following simple calculations which will be useful later:

(a) For $\mathcal{O} \in B(\mathcal{H})$, the set of operators on a Hilbert space such that $\mathcal{O}^2 = I$, show that $\exp(-\imath\theta\mathcal{O}) = \cos(\theta)I - \imath\sin(\theta)\mathcal{O}$.

(b) Explain why a general qubit may be written as $|\Psi\rangle = \cos(\theta)|0\rangle + \exp(\imath\phi)\sin(\theta)|1\rangle$

(c) Show that the density matrix corresponding to this state can be written as $\rho = \frac{1}{2}(I + \sin\theta\cos\phi\hat{\sigma}_x + \sin\theta\sin\phi\hat{\sigma}_y + \cos\theta\hat{\sigma}_z)$ for $\{\hat{\sigma}_k : k = x, y, z\}$ the set of Pauli matrices.

(d) Show that generic quantum gate can be expressed as $\hat{U} = \exp(-\frac{\imath\theta}{2}\mathbf{n}\cdot\sigma)$. Explain how this suggests a scheme for implementation of quantum process engineering.

(e) Alternately, show that the smaller set of gates $\{R^Z_\phi, R^X_{\frac{\pi}{2}}\}$ also suffice to generate all unitary U, for $R^J_\phi = \exp(-\frac{\imath\phi}{2}\sigma_J)$

Problem 2: Application to molecular control

A typical NMR system consists of a sample of liquid molecules, such as trichloroethylene, which contain hydrogen and carbon-13 atoms whose nuclei possess a magnetic moment $\mu = \mu I$. These moments precess around the axis of an external magnetic field. To a very good approximation, the Hamiltonian of this system may be shown to have the form $H = \mu \cdot \mathbf{B}$ where B is the externally applied magnetic field. Note this simple bilinear relationship, and the fact that there is no dissipation term means we may apply the techniques of geometric control to implement quantum logic gates.

(a) Let $\mathbf{B} = B\hat{\mathbf{z}}$, and naturally $\hat{U} = \exp[-\imath\hbar H(t)]$. Calculate the expectation (as a function of time) of the magnetic moment μ for the constant magnetic field. Illustrate on the Bloch sphere.
   - Hint: $\langle\mu\rangle = \mathrm{Tr}(\mu U\rho U^\dagger)$. Use the general form for ρ calculated above.

(b) Each nucleus precesses at Larmor frequency ω_j. Write down the unitary transformation that will put us in the multi-rotating frame of the nuclei.

(c) To induce a one-bit gate, we use a magnetic coil to apply a field of the form $B_{\mathrm{rf}} = B_x\cos[\omega(t - t_0)]\hat{\mathbf{x}} + B_y\sin[\omega(t - t_0)]\hat{\mathbf{y}}$. How does this look in the rotating frame?

If a magnetic field of the form $H_{\mathrm{grad}} = \mu \cdot B_{\mathrm{grad}} \cdot z\hat{z}$ is applied, then we find that the sample acquires a linear phase as a function of z. This can be used to carry out controlled decoherence, and to label parts of the density matrix with different phases.

Problem 3: Restricted control, Robustness

It is much easier in practice (for ease of calibration) to implement a general rotation around only one axis, coupled with a rotation around one axis, say $\hat{\mathbf{x}}$ which is always of a set angle. Although this requires a slightly more complicated pulse sequence, this is still sufficient for the creation of a universal set of gates.

(a) Show that $\exp\{-i\theta\hat{\mathbf{n}}\cdot\sigma\}$ can be written as

$$\exp\left\{\frac{-i\alpha}{2}\sigma_z\right\}\exp\left\{\frac{i\pi}{4}\sigma_x\right\}\exp\left\{\frac{i\beta}{2}\sigma_z\right\}\exp\left\{\frac{-i\pi}{4}\sigma_x\right\}\exp\left\{\frac{-i\theta}{2}\sigma_z\right\}\exp\left\{\frac{i\pi}{4}\sigma_x\right\}$$
$$\times\exp\left\{\frac{-i\beta}{2}\sigma_z\right\}\exp\left\{-\frac{i\pi}{4}\sigma_x\right\}\exp\left\{\frac{-i\alpha}{2}\sigma_z\right\}$$

where $\alpha = \tan^{-1}\left(\frac{\hat{n}_y}{\hat{n}_x}\right)$ and $\beta = \tan^{-1}\left(\frac{\hat{n}_x}{\hat{n}_z}\right)$

(b) Calibration in any experiment is never perfect, so control strategies should be robust to small systematic errors. Assume that a pulse to implement a rotation of $\frac{\pi}{2}$ actually implements a rotation of $\frac{\pi}{2} + \epsilon$. Show that the gate $U = \exp\left\{\frac{-i\pi}{4}\sigma_y\right\}\exp\left\{\frac{-i\pi}{2}\sigma_x\right\}\exp\left\{\frac{-i\pi}{4}\sigma_y\right\}$ is robust to order ϵ^2 under this error model.

Problem 4: Two qubit gates

Interactions between nuclear spins are mediated through the molecular electrons, and give rise to an interaction Hamiltonian of Heisenberg form

$$H_I = \sum_{m,n} J_{m,n} \sigma^{(m)} \cdot \sigma^{(n)},$$

where $\sigma^{(m)} \cdot \sigma^{(n)} = \prod_{k,\ell=x,y,z} \sigma_k^{(m)} \sigma_\ell^{(n)}$ and $\sigma_k^{(n)}$ is an N-factor tensor product whose nth factor is σ_k, all others being the identity. E.g. for two qubits we have $\sigma_x^{(1)} = \sigma_x \otimes I$, $\sigma_x^{(2)} = I \otimes \sigma_x$, etc. This general interaction Hamiltonian is often simplified to $H_I = \sum_{m,n} J_{m,n} \sigma_z^{(m)} \sigma_z^{(n)}$, which is referred to as *Ising coupling Hamiltonian.* For the following problem you may assume the interaction Hamiltonian is of Ising form.

The coupling Hamiltonian is usually constant but we can implement single qubit rotations by applying suitable RF-fields, giving rise to a total control Hamiltonian that, in the multiply rotating frame, takes the form

$$H[B(t)] = \sum_n B_x^{(n)}(t) \sigma_x^{(n)} + B_y^{(n)}(t) \sigma_y^{(n)} + H_I$$

(a) Suggest a condition under which the Ising approximation is a sensible assumption. (Hint: Think rotating wave approximation)

(b) Suggest a simple scheme for implementing a $C_{\text{phase}} = \text{diag}(1, 1, 1, -1)$ gate.

(c) Suggest a simple scheme for implementing a C_{NOT} gate using four single qubit rotations and a C_{phase} gate. For the implementation of the single qubit gates, you may assume that the two-qubit coupling can be made negligible by ensuring that the amplitudes of the control fields, and hence single qubit control terms, are much larger than the inter-qubit coupling. (What happens when this assumption is not applicable?)

(d) Explain how you could implement an arbitary two-qubit gate using only C_{phase} gates and single qubit x, y or z rotations. (Hint: Recall the Cartan decomposition.)

Problem 5: Noise and decoherence

Incoherent interactions of a quantum system with the environment lead to relaxation effects. There are two main types: phase relaxation, which leads to a decay of the off-diagonal elements of the density operator, i.e., destroys the coherences, and population relaxation, which changes the diagonal elements of the density operator. For a two-level system there are three relaxation rates γ_{12} and γ_{21}, which describe the rate of population relaxation from state $|2\rangle$ to $|1\rangle$ and vice versa, and Γ_{12}, which describes the rate of decoherence of the off-diagonal elements ρ_{12} and ρ_{21} of the density matrix. The relaxation rates are usually temperature dependent.

As introduced in class, the master equation for the dissipative dynamics described above is given by ($\hbar = 1$):

$$\dot{\rho}(t) = -i[H, \rho(t)] + \mathcal{L}_D[\rho(t)]. \tag{0.1}$$

For a qubit system, the total dissipation operators takes the form

$$\mathcal{L}_D[\rho(t)] = \gamma_{12} \mathcal{L}[\sigma_-]\rho(t) + \gamma_{21} \mathcal{L}[\sigma_+]\rho(t) + \Gamma_{12}^d \mathcal{L}[\sigma_z]\rho(t)$$

where the individual Lindblad (super-)operators are given by

$$\mathcal{L}[V]\rho(t) = V\rho(t)V^\dagger - (V^\dagger V \rho(t) + \rho(t) V^\dagger V)/2$$

and $\sigma_+ = |2\rangle\langle 1|$, $\sigma_- = |1\rangle\langle 2|$ and $\sigma_z = (|1\rangle\langle 1| - |2\rangle\langle 2|)/\sqrt{2}$.

(a) Setting $\Gamma = (\gamma_{21} + \gamma_{12})/2 + \Gamma_{12}$, show that we have explicitly

$$\mathcal{L}_D[\rho(t)] = \begin{bmatrix} \gamma_{12}(-\rho_{11} + \rho_{22}) & -\rho_{12}\Gamma \\ -\rho_{12}^*\Gamma & \gamma_{21}(\rho_{11} - \rho_{22}) \end{bmatrix}$$

Under which conditions is the dissipative evolution unital, i.e., preserves the identity matrix?

(b) Use the result in from part (a) to show that dissipative master equation gives rise to an affine-linear evolution equation for the Bloch vector $\dot{\mathbf{s}}(t) = A\mathbf{s} + \mathbf{c}$ with

$$A = \begin{bmatrix} -\Gamma & -\alpha_z & \alpha_y \\ \alpha_z & -\Gamma & -\alpha_x \\ -\alpha_y & \alpha_x & -(\gamma_{12} + \gamma_{21}) \end{bmatrix}, \qquad \mathbf{c} = \begin{bmatrix} 0 & 0 & \gamma_{21} - \gamma_{12} \end{bmatrix}$$

where $\alpha = d_k d$ for $k = x, y, z$ determine the Hamiltonian $H = d/2(d_x\sigma_x + d_y\sigma_y + d_z\sigma_z)$.

(c) Show that for symmetric population relaxation $\gamma_{12} = \gamma_{21}$ the system will relax to the state $\mathbf{s}_\infty = \mathbf{0}$. What is the steady state in the case of asymmetric population relaxation? How about pure dephasing?