L4 Quantum information and computing (QIC) 2022-23

Lecture 4: Rotation operators and the Rabi solution

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Aims of Lecture 4: To introduce the concept of single-qubit gates (qubit rotations) and then how they are implemented using external fields.

Qubit rotation

We can use the terms single-qubit gates and qubit rotation interchangeably, because apart from the global phase factor, all unitary single-qubit operations can be represented as a rotation of the Bloch vector. In quantum mechanics, the rotation operator (also called a generator of rotation) for a rotation by an angle Θ (not, in general, the same as the polar angle θ) about an axis defined by the unit vector $\hat{\boldsymbol{n}} = (n_x, n_y, n_z)$ is given by

$$\mathsf{R}_{\hat{\boldsymbol{n}}} \quad = \quad \mathrm{e}^{-\mathrm{i}\boldsymbol{J}\cdot\hat{\boldsymbol{n}}\Theta/\hbar} = \mathrm{e}^{-\mathrm{i}\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}\Theta/2} \ ,$$

where for a two-level system (equivalent to a spin-1/2), the angular momentum is given by $\boldsymbol{J} = \frac{1}{2}\hbar\boldsymbol{\sigma}$. To use this expression we need to evaluate the exponential of a matrix. Using a Taylor expansion and grouping even and odd terms we find that[1]

$$\mathsf{R}_{\hat{\boldsymbol{n}}} = \mathrm{e}^{-\mathrm{i}\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}(\Theta/2)} = \sigma_0 \cos\left(\frac{\Theta}{2}\right) - \mathrm{i}\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}} \sin\left(\frac{\Theta}{2}\right) \ .$$

Using this result we can write a **general rotation matrix**

$$\mathsf{R}_{\hat{\boldsymbol{n}}} = \begin{bmatrix} \cos\frac{\Theta}{2} - \mathrm{i}n_z \sin\frac{\Theta}{2} & (-\mathrm{i}n_x - n_y)\sin\frac{\Theta}{2} \\ (-\mathrm{i}n_x + n_y)\sin\frac{\Theta}{2} & \cos\frac{\Theta}{2} + \mathrm{i}n_z\sin\frac{\Theta}{2} \end{bmatrix} \ . \quad (4.1)$$

[1] For any Pauli spin matrix, σ_j, using $\sigma_j^{2m} = \sigma_0$ for any integer m, the Taylor expansion is

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}\sigma_j(\Theta/2)} &= \sigma_0 - \mathrm{i}\sigma_j\left(\frac{\Theta}{2}\right) - \frac{\sigma_j^2}{2!}\left(\frac{\Theta}{2}\right)^2 \\ &\quad + \mathrm{i}\frac{\sigma_j^3}{3!}\left(\frac{\Theta}{2}\right)^3 + \frac{\sigma_j^4}{4!}\left(\frac{\Theta}{2}\right)^4 + \ldots \\ &= \sigma_0 - \frac{\sigma_j^2}{2!}\left(\frac{\Theta}{2}\right)^2 + \frac{\sigma_j^4}{4!}\left(\frac{\Theta}{2}\right)^4 + \ldots \\ &\quad - \mathrm{i}\left[\sigma_j\left(\frac{\Theta}{2}\right) - \frac{\sigma_j^3}{3!}\left(\frac{\Theta}{2}\right)^3 + \ldots\right] \\ &= \sigma_0 \cos\left(\frac{\Theta}{2}\right) - \mathrm{i}\sigma_j \sin\left(\frac{\Theta}{2}\right) \ , \end{aligned}$$

where in the second line we rearranged the terms into even and odd series which correspond to cosine and sine respectively.

Note that $\mathsf{R}_{\hat{\boldsymbol{n}}}$ is **unitary**, i.e. $\mathsf{R}_{\hat{\boldsymbol{n}}}\mathsf{R}_{\hat{\boldsymbol{n}}}^\dagger = \sigma_0$ and the operator $|\psi'\rangle = \mathsf{R}|\psi\rangle$ preserves the norm of the state vector. The special case of rotation about the x, y, and z axes (see also Nielsen and Chang, Sec. 4.2) are given by

$$\begin{aligned} \mathsf{R}_x(\Theta) &= \mathrm{e}^{-\mathrm{i}(\Theta/2)\mathsf{X}} = \cos\tfrac{\Theta}{2}\mathsf{I} - \mathrm{i}\sin\tfrac{\Theta}{2}\mathsf{X} \\ &= \begin{pmatrix} \cos\frac{\Theta}{2} & -\mathrm{i}\sin\frac{\Theta}{2} \\ -\mathrm{i}\sin\frac{\Theta}{2} & \cos\frac{\Theta}{2} \end{pmatrix} \ . \end{aligned}$$

$$\begin{aligned} \mathsf{R}_y(\Theta) &= \mathrm{e}^{-\mathrm{i}(\Theta/2)\mathsf{Y}} = \cos\tfrac{\Theta}{2}\mathsf{I} - \mathrm{i}\sin\tfrac{\Theta}{2}\mathsf{Y} \\ &= \begin{pmatrix} \cos\frac{\Theta}{2} & -\sin\frac{\Theta}{2} \\ \sin\frac{\Theta}{2} & \cos\frac{\Theta}{2} \end{pmatrix} \ . \end{aligned}$$

$$\begin{aligned} \mathsf{R}_z(\Theta) &= \mathrm{e}^{-\mathrm{i}(\Theta/2)\mathsf{Z}} = \cos\tfrac{\Theta}{2}\mathsf{I} - \mathrm{i}\sin\tfrac{\Theta}{2}\mathsf{Z} \\ &= \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\frac{\Theta}{2}} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\frac{\Theta}{2}} \end{pmatrix} \ . \end{aligned}$$

Next, we shall look at how to implement these rotation using oscillatory electromagnetic (EM) fields.

Qubits in EM fields: the interaction Hamiltonian

In practice, qubit rotations are implemented by applying EM fields (lasers and microwaves) with angular frequency, ω, either resonant or detuned by $\Delta = \omega - \omega_0$ with respect to the qubit resonance, $\omega_0 = (E_1 - E_0)/\hbar$. The external field has the form

$$\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{E}}_0 \cos(\phi_{\mathrm{L}} - \omega t) \ ,$$

where $\phi_{\mathrm{L}} = \boldsymbol{k}\cdot\boldsymbol{r} + \phi_0$ is the phase. Note that this depends on the position of the qubit, $\boldsymbol{r}$, which is a problem if the qubit is delocalised or moves.

The field changes the coefficients, a and b, appearing in the state vector. The time evolution of the state vector is given by solving the Schrödinger equation, (see Appendix for derivation)

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi\rangle \quad = \quad \mathcal{H}_{\mathrm{int}}|\psi\rangle \ ,$$

where $\mathcal{H}_{\rm int}$ is known as the interaction Hamiltonian.[2] For a two-level system, using the vector form, the interaction Hamiltonian is a 2×2 matrix

$$\mathcal{H}_{\rm int} = \frac{\hbar}{2}\begin{pmatrix} \Delta & \Omega e^{-i\phi_L} \\ \Omega e^{i\phi_L} & -\Delta \end{pmatrix} ,$$

where Ω is known as the Rabi frequency (proportional to the amplitude of the EM field, $\Omega = \langle 1| - \boldsymbol{d}\cdot\boldsymbol{\mathcal{E}}_0|0\rangle/\hbar$, where $\boldsymbol{d}$ is the dipole moment of the qubit). The next step is to write this interaction in the form of a rotation.

The Rabi solution:

If the interaction Hamiltonian is time-independent then the solution to the Schrödinger equation is

$$|\psi(t)\rangle = \exp(-i\mathcal{H}_{\rm int}t/\hbar)|\psi(0)\rangle = \mathsf{R}|\psi(0)\rangle ,$$

where R has the form of a rotation matrix. To find the rotation matrix we rewrite the interaction in the form

$$\mathsf{R} = \exp(-i\mathcal{H}_{\rm int}t/\hbar) = \exp(-i\tfrac{1}{2}\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}\Theta) .$$

By writing the interaction Hamiltonian in terms of spin matrices

$$\mathcal{H}_{\rm int} = \frac{\hbar}{2}\left[\Delta\sigma_z + \Omega(\cos\phi_L\sigma_x + \sin\phi_L\sigma_y)\right] .$$

We construct the unit vector by normalising the coefficients of the Pauli matrices,

$$\hat{\boldsymbol{n}} = \frac{1}{(\Omega^2+\Delta^2)^{1/2}}\left[\Omega\cos\phi_L, \Omega\sin\phi_L, \Delta\right] ,$$

$\Omega_{\rm eff} = (\Omega^2+\Delta^2)^{1/2}$ is the normalisation factor. In this case the interaction Hamiltonian becomes

$$\mathcal{H}_{\rm int} = \frac{\hbar}{2}\Omega_{\rm eff}\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} .$$

By comparing the solution to the Schrödinger equation to a rotation matrix

$$e^{-i\mathcal{H}_{\rm int}t/\hbar} = e^{-i\Omega_{\rm eff}\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}t/2} = e^{-i\Theta\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}/2} ,$$

we find that the rotation angle is

$$\Theta = (\Omega^2+\Delta^2)^{1/2}t .$$

The factor $\Omega_{\rm eff} = (\Omega^2+\Delta^2)^{1/2}$ is known as the **effective Rabi frequency**. Substituting

$$\begin{aligned} n_x &= (\Omega/\Omega_{\rm eff})\cos\phi_L , \\ n_y &= (\Omega/\Omega_{\rm eff})\sin\phi_L , \\ n_z &= \Delta/\Omega_{\rm eff} , \end{aligned}$$

into the rotation matrix, eqn (4.1), we obtain[3]

$$\mathsf{R}_{\hat{\boldsymbol{n}}}(\Theta) = \begin{bmatrix} \cos\frac{\Theta}{2} - i\frac{\Delta}{\Omega_{\rm eff}}\sin\frac{\Theta}{2} & -i\frac{\Omega}{\Omega_{\rm eff}}e^{-i\phi_L}\sin\frac{\Theta}{2} \\ -i\frac{\Omega}{\Omega_{\rm eff}}e^{+i\phi_L}\sin\frac{\Theta}{2} & \cos\frac{\Theta}{2} + i\frac{\Delta}{\Omega_{\rm eff}}\sin\frac{\Theta}{2} \end{bmatrix} .$$

This is known as the **Rabi solution**. The three key parameters for driven qubits are: the Rabi frequency Ω, which characterises the strength of the coupling between the qubit and the field, the detuning, $\Delta = \omega - \omega_0$, and a phase of the field, ϕ_L.[4]

For the special case of zero detuning ($\Delta = 0$), the Rabi solution reduces to

$$\mathsf{R}(\theta_L, \phi_L) = \begin{bmatrix} \cos(\Omega t/2) & -ie^{-i\phi_L}\sin(\Omega t/2) \\ -ie^{+i\phi_L}\sin(\Omega t/2) & \cos(\Omega t/2) \end{bmatrix} ,$$

which corresponds to a rotation about a vector in the equatorial plane in the Bloch sphere. Note that we have switched to the notation $\mathsf{R}(\theta_L, \phi_L)$, where $\theta_L = \Omega t$ is the rotation angle and ϕ_L determines the direction in the xy plane about which we rotate. We shall explore this further in Lecture 5.

Summary:

What do you need to be able to do?

1. Write an identity for the rotation operator in terms of cosine and sine term.
2. Derive matrices for rotations about the x, y and z axes.
3. Rewrite the interaction Hamiltonian in terms of spin matrices.
4. Understand the significance of the terms in the Rabi solution.

[2] Note that Hamiltonians are **Hermitian** $\mathcal{H} = \mathcal{H}^\dagger$ but not usually unitary, so behave differently to rotation matrices. Any Hermitian matrix can be converted to a diagonal matrix with real eigenvalues, $D = U^\dagger\mathcal{H}U$, where U is a unitary operator.

[3] Note the sign of ϕ_L depends on whether $|0\rangle$ or $|1\rangle$ has higher energy. Other texts may use different sign conventions.

[4] Note that the sign of Ω term depends on our choice of field phase. Rather than $+\Omega$ at $\phi_L = 0$, some texts have $-\Omega$.

Appendix: Derivation of $\mathcal{H}_{\rm int}$

The Schrödinger equation describing the interaction between the qubit and the external field is,

$$\mathrm{i}\hbar\partial_t|\psi\rangle = (\mathcal{H}_0 + \mathcal{H}')|\psi\rangle \ ,$$

where $\mathcal{H}_0$ is the Hamiltonian for the quantum system and $\mathcal{H}'$ is the perturbation due to the EM field. We substitute a state vector of the form

$$|\psi(t)\rangle \quad = \quad a(t)|0\rangle \mathrm{e}^{-\mathrm{i}E_0 t/\hbar} + b(t)|1\rangle \mathrm{e}^{-\mathrm{i}E_1 t/\hbar} \ .$$

Using $\mathcal{H}_0|k\rangle = E_k|k\rangle$ we can cancel some terms on the left and right leaving

$$\mathrm{i}\hbar\left(\dot{a}(t)|0\rangle\mathrm{e}^{-\mathrm{i}E_0t/\hbar} + \dot{b}(t)|1\rangle\mathrm{e}^{-\mathrm{i}E_1t/\hbar}\right) = \mathcal{H}'|0\rangle a(t)\mathrm{e}^{-\mathrm{i}E_0t/\hbar} + \mathcal{H}'|1\rangle b(t)\mathrm{e}^{-\mathrm{i}E_1t/\hbar} \ .$$

Next, we take the inner product with $\langle 0|\mathrm{e}^{\mathrm{i}E_0t/\hbar}$ (or $\langle 1|\mathrm{e}^{\mathrm{i}E_1t/\hbar}$), and use the fact that the field couples states $|0\rangle$ and $|1\rangle$, i.e. $\langle 0|\mathcal{H}'|0\rangle = \langle 1|H'|1\rangle = 0$, we find

$$\begin{aligned}\mathrm{i}\hbar\dot{a}(t) &= \langle 0|\mathcal{H}'|1\rangle\mathrm{e}^{-\mathrm{i}\omega_0 t}\ b(t) \ ,\\ \mathrm{i}\hbar\dot{b}(t) &= \langle 1|\mathcal{H}'|0\rangle\mathrm{e}^{\mathrm{i}\omega_0 t}\ a(t) \ .\end{aligned}$$

The interaction is of the form $\mathcal{H}' = -\boldsymbol{d}\cdot\boldsymbol{\mathcal{E}}$ where $\boldsymbol{d} = -e\boldsymbol{r}$ is the electric dipole operator, and $\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{E}}_0\cos(\phi_{\rm L} - \omega t)$ is the electric part of the EM field. If the phase is zero at $t = 0$ then the laser is, $\phi_{\rm L} = \boldsymbol{k}\cdot\boldsymbol{r}$. We define a **Rabi frequency** (as a measure of the coupling between the field and the qubit) as $\Omega = -\langle 1|\boldsymbol{d}\cdot\boldsymbol{\mathcal{E}}_0|0\rangle/\hbar$[5]. If the state vectors are real such that $\Omega = -\langle 0|\boldsymbol{d}\cdot\boldsymbol{\mathcal{E}}_0|1\rangle/\hbar$ as well, then we can rewrite the coupled equations as

$$\begin{aligned}\mathrm{i}\dot{a}(t) &= \Omega\cos(\phi_{\rm L} - \omega t)\ \mathrm{e}^{-\mathrm{i}\omega_0 t}\ b(t)\\ \mathrm{i}\dot{b}(t) &= \Omega\cos(\phi_{\rm L} - \omega t)\ \mathrm{e}^{\mathrm{i}\omega_0 t}\ a(t)\end{aligned}$$

where $\omega_0 = (E_1 - E_0)/\hbar$. Now we expand the cosine and use that for $\omega \sim \omega_0$, we can neglect terms in $\omega + \omega_0$ (known as **rotating wave approximation**) Integrating $\mathrm{e}^{\mathrm{i}(\omega+\omega_0)t} + \mathrm{e}^{\mathrm{i}(\omega-\omega_0)t}$ we get

$$\frac{\mathrm{e}^{\mathrm{i}(\omega+\omega_0)t}}{\mathrm{i}(\omega+\omega_0)} + \frac{\mathrm{e}^{\mathrm{i}(\omega-\omega_0)t}}{\mathrm{i}(\omega-\omega_0)} \ .$$

As $\omega + \omega_0 \sim 10^{15}$ and $\omega - \omega_0 \sim 10^7$ we can neglect the $\omega + \omega_0$ term, giving

$$\begin{aligned}\mathrm{i}\dot{a}(t) &= \tfrac{1}{2}\Omega\mathrm{e}^{-\mathrm{i}\phi_{\rm L}}\mathrm{e}^{\mathrm{i}\Delta t}\ b(t)\\ \mathrm{i}\dot{b}(t) &= \tfrac{1}{2}\Omega\mathrm{e}^{\mathrm{i}\phi_{\rm L}}\mathrm{e}^{-\mathrm{i}\Delta t}\ a(t) \ .\end{aligned}$$

[5] As $\boldsymbol{d} = -e\boldsymbol{r}$ the real frequency is positive.

where $\Delta = \omega - \omega_0$ is the **detuning**.

Finally, we transform into a **rotating frame** by make a change of variable, $\tilde{a} = a\mathrm{e}^{-\mathrm{i}(\Delta/2)t}$, $\tilde{b} = b\mathrm{e}^{\mathrm{i}(\Delta/2)t}$. This removes the explicit time dependence and we obtain,

$$\begin{aligned}\mathrm{i}\dot{\tilde{a}} &= \tfrac{1}{2}\Delta\tilde{a} + \tfrac{1}{2}\Omega\mathrm{e}^{-\mathrm{i}\phi_{\rm L}}\ \tilde{b}\\ \mathrm{i}\dot{\tilde{b}} &= \tfrac{1}{2}\Omega\mathrm{e}^{\mathrm{i}\phi_{\rm L}}\ \tilde{a} - \tfrac{1}{2}\Delta\tilde{b} \ .\end{aligned}$$

We can rewrite these coupled equations in the form of a Schrödinger equation,

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi\rangle \quad = \quad \mathcal{H}_{\rm int}|\psi\rangle$$

with

$$\mathcal{H}_{\rm int} \quad = \quad \frac{\hbar}{2}\left(\begin{array}{cc}\Delta & \Omega\mathrm{e}^{-\mathrm{i}\phi_{\rm L}}\\ \Omega\mathrm{e}^{\mathrm{i}\phi_{\rm L}} & -\Delta\end{array}\right) \ ,$$

and

$$|\psi\rangle \quad = \quad \left(\begin{array}{c}\tilde{a}\\ \tilde{b}\end{array}\right) \ .$$

We shall omit the tildes from now on.