Phase 1: Simulate a Single-Qubit Hamiltonian to Reproduce Rabi Oscillations

Schrödinger Equation

Calculates how the system will evolve or change in time.

- Time-dependent Schrödinger equation (for time-independent H):

$$i\hbar\frac{d}{dt}\left|\psi(t)\right\rangle = H\left|\psi(t)\right\rangle .$$

- Rearranging:

$$\frac{d}{dt}\left|\psi(t)\right\rangle = -\frac{i}{\hbar}H\left|\psi(t)\right\rangle .$$

- With $\hbar = 1$ (simplifying convention):

$$\frac{d}{dt}\left|\psi(t)\right\rangle = -iH\left|\psi(t)\right\rangle .$$

- The formal solution:

$$\left|\psi(t)\right\rangle = e^{-iHt}\left|\psi(0)\right\rangle .$$

  The operator

$$U(t) = e^{-iHt}$$

is the **time evolution operator**.

Hamiltonian

A Hamiltonian is the mathematical description of the total energy of a system.

- It enables us to solve the Schrödinger equation.
- So the first step in any problem is identifying or calculating the Hamiltonian.

Wave Function

The wave function is the mathematical function describing the state of a particle.

General Form of a Two-State (Single Qubit) Hamiltonian

For a two-state system, any Hermitian matrix H can be written as:

$$H = a_0 I + a_x\sigma_x + a_y\sigma_y + a_z\sigma_z,$$

where a_n are real constants.

Pauli Matrices

Hermitian matrices represent observables (e.g., spin, position, energy). The Pauli matrices are:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Removing Imaginary Terms

We assume a Hermitian Hamiltonian, so no imaginary coefficients appear. Thus we can remove the σ_y term, giving:

$$H = a_0 I + a_x \sigma_x + a_z \sigma_z.$$

In matrix form:

$$H = \begin{pmatrix} a_0 & 0 \\ 0 & a_0 \end{pmatrix} + \begin{pmatrix} 0 & a_x \\ a_x & 0 \end{pmatrix} + \begin{pmatrix} a_z & 0 \\ 0 & -a_z \end{pmatrix}.$$

Combining terms:

$$H = \begin{pmatrix} a_0 + a_z & a_x \\ a_x & a_0 - a_z \end{pmatrix}.$$

Parameter Definitions

Let $\Omega = a_x$ represent the coupling strength, and define:

$$\Delta_1 = a_0 + a_z, \qquad \Delta_2 = a_0 - a_z,$$

which represent the self-energy of each state.

Final matrix form:

$$H = \begin{pmatrix} \Delta_1 & \Omega \\ \Omega & \Delta_2 \end{pmatrix}.$$

Expressing the Hamiltonian in the Pauli Basis

Every 2×2 Hermitian matrix can be uniquely expanded in the basis $\{I, \sigma_x, \sigma_y, \sigma_z\}$. Matching matrix elements gives:

$$\begin{aligned} H &= aI + b\sigma_x + c\sigma_y + d\sigma_z, && (1) \\ &= \begin{pmatrix} a+d & b-ic \\ b+ic & a-d \end{pmatrix}. && (2) \end{aligned}$$

Comparing with

$$\begin{pmatrix} \Delta_1 & \Omega \\ \Omega & \Delta_2 \end{pmatrix},$$

we obtain

$$c = 0, \qquad b = \Omega, \qquad a = \frac{\Delta_1 + \Delta_2}{2}, \qquad d = \frac{\Delta_1 - \Delta_2}{2}.$$

Define

$$E_{\text{avg}} := \frac{\Delta_1 + \Delta_2}{2}, \qquad \Delta := \frac{\Delta_1 - \Delta_2}{2}. \tag{3}$$

Then the Hamiltonian becomes

$$H = E_{\text{avg}} I + \Delta\sigma_z + \Omega\sigma_x \tag{4}$$

This decomposition is purely algebraic and makes no physical assumptions. It simply expresses H in the Pauli matrix basis.

Time Evolution via the Pauli Exponential Identity

Since I commutes with all operators,

$$e^{-iHt} = e^{-iE_{\text{avg}}t}\, e^{-i(\Delta\sigma_z+\Omega\sigma_x)t}. \tag{5}$$

Pauli-matrix exponential identity:

$$e^{-i(\vec{a}\cdot\vec{\sigma})t} = \cos(|\vec{a}|t)\, I - i\sin(|\vec{a}|t)\frac{\vec{a}\cdot\vec{\sigma}}{|\vec{a}|}, \tag{6}$$

valid for any real vector $\vec{a}$.

In our case,

$$\vec{a} = (\Omega,\, 0,\, \Delta), \qquad |\vec{a}| = \Omega_R := \sqrt{\Omega^2+\Delta^2}.$$

Thus

$$e^{-i(\Delta\sigma_z+\Omega\sigma_x)t} = \cos(\Omega_R t)\, I - i\sin(\Omega_R t)\left(\frac{\Omega}{\Omega_R}\sigma_x + \frac{\Delta}{\Omega_R}\sigma_z\right). \tag{7}$$

Combining everything, the time-evolution operator is

$$U(t) = e^{-iE_{\text{avg}}t}\left[\cos(\Omega_R t)\, I - i\sin(\Omega_R t)\left(\frac{\Omega}{\Omega_R}\sigma_x + \frac{\Delta}{\Omega_R}\sigma_z\right)\right]. \tag{8}$$

Time-Dependent State for an Initial $|0\rangle$

To understand how the system actually behaves, we apply the time evolution operator to a specific initial state. Here we choose

$$|\psi(0)\rangle = |0\rangle\,.$$

Using the identities

$$\sigma_x|0\rangle = |1\rangle\,, \qquad \sigma_z|0\rangle = |0\rangle\,,$$

we substitute into the expression for $U(t)$:

$$\begin{aligned}|\psi(t)\rangle &= U(t)\,|0\rangle && (9)\\ &= e^{-iE_{\text{avg}}t}\left[\cos(\Omega_R t)\,|0\rangle - i\sin(\Omega_R t)\left(\frac{\Omega}{\Omega_R}|1\rangle + \frac{\Delta}{\Omega_R}|0\rangle\right)\right]. && (10)\end{aligned}$$

Combining the $|0\rangle$ terms:

$$|\psi(t)\rangle = e^{-iE_{\text{avg}}t} \left[\left(\cos(\Omega_R t) - i\frac{\Delta}{\Omega_R} \sin(\Omega_R t) \right) |0\rangle - i\frac{\Omega}{\Omega_R} \sin(\Omega_R t) |1\rangle \right].$$

Thus the amplitudes are:

$$c_0(t) = e^{-iE_{\text{avg}}t} \left[\cos(\Omega_R t) - i\frac{\Delta}{\Omega_R} \sin(\Omega_R t) \right], \tag{11}$$

$$c_1(t) = -i\, e^{-iE_{\text{avg}}t} \frac{\Omega}{\Omega_R} \sin(\Omega_R t). \tag{12}$$

These coefficients tell us how the probability of being in each state evolves in time.

Measurement Probabilities

Once we have the amplitudes $c_0(t)$ and $c_1(t)$, the probabilities of finding the system in $|0\rangle$ or $|1\rangle$ are given by the magnitude squared of these coefficients:

$$P_0(t) = |c_0(t)|^2, \qquad P_1(t) = |c_1(t)|^2.$$

Since global phase does not affect probabilities, we obtain

$$P_1(t) = \frac{\Omega^2}{\Omega_R^2} \sin^2(\Omega_R t),$$

and

$$P_0(t) = 1 - P_1(t).$$

These expressions show that the probability of being in $|1\rangle$ increases and decreases in time in a smooth, oscillatory way. This back-and-forth behavior is what we refer to as *Rabi oscillations*: the qubit continuously moves between the two states under the action of the Hamiltonian.

Special case: $\Delta = 0$. If $\Delta = 0$, then the quantity

$$\Omega_R = \sqrt{\Omega^2 + \Delta^2}$$

reduces to just Ω. In this situation, the oscillations simplify to

$$P_1(t) = \sin^2(\Omega t), \qquad P_0(t) = \cos^2(\Omega t).$$

This special case is useful because the qubit fully transitions between $|0\rangle$ and $|1\rangle$ with 100% amplitude, making the oscillations especially easy to visualize and compare against simulation.

Bloch-Sphere Interpretation

The combination of σ_x and σ_z in the Hamiltonian can also be visualized on the Bloch sphere. A single qubit state corresponds to a point on this sphere, and the Hamiltonian determines how this point moves in time.

In our case, the Hamiltonian

$$\Delta\sigma_z + \Omega\sigma_x$$

causes the state to rotate around a fixed axis whose direction is set by the relative sizes of Ω and Δ. If $\Delta = 0$, the rotation axis lies purely along the x-direction; if $\Omega = 0$, the motion is around the z-axis. When both are present, the axis lies somewhere in between.

This gives a geometric picture of why the probabilities oscillate: the qubit state is literally rotating through the sphere, and the measurement outcomes change as the state moves.

Connection to the Quantum Circuit

In the notebook, we reproduce this continuous-time evolution by constructing single-qubit rotation gates whose combined effect matches the operator $U(t)$. By varying the evolution time t and measuring the qubit in the computational basis, we obtain empirical estimates of $P_0(t)$ and $P_1(t)$.

Comparing these results with the analytic predictions

$$P_1(t) = \frac{\Omega^2}{\Omega_R^2} \sin^2(\Omega_R t)$$

allows us to confirm that our circuit correctly simulates the Rabi dynamics generated by the Hamiltonian.