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Tutorial 3 (Schrödinger equation for single qubits)
The Schrödinger equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = H |\psi(t)\rangle \tag{1}$$

describes how a quantum state $|\psi(t)\rangle$ governed by a Hamiltonian operator H evolves in time $t \in \mathbb{R}$. In this tutorial, we assume that H is a time-independent Hermitian matrix (not to be confused with the Hadamard gate). The formal solution of Eq. (1) is then

$$|\psi(t)\rangle = U_t |\psi(0)\rangle \quad \text{with} \quad U_t = \mathrm{e}^{-iHt/\hbar}.$$

U_t is the unitary *time evolution operator*. In quantum computing, U_t is used as quantum gate. In the following, we absorb the reduced Planck constant $\hbar$ into H, effectively setting $\hbar = 1$.

(a) Show that U_t is indeed unitary.

(b) Consider the Hamiltonian operator

$$H = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix}$$

acting on a single qubit, with the "frequency" parameters $\omega_1, \omega_2 \in \mathbb{R}$. Find U_t and $|\psi(t)\rangle$ for the initial state (i) $|\psi(0)\rangle = |0\rangle$ and (ii) $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$.

(c) We now add a small perturbation of strength ϵ to the Hamiltonian:

$$H = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} + \epsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Compute U_t and the "overlap" $\langle 1|\psi(t)\rangle$ between $|1\rangle$ and $|\psi(t)\rangle$ for the initial state $|\psi(0)\rangle = |0\rangle$.

Hint: Represent H in terms of the identity and Pauli-X and Z matrices: $H = \bar{\omega} I + \sqrt{\Delta\omega^2 + \epsilon^2}\,(\vec{v} \cdot \vec{\sigma})$ with $\Delta\omega = (\omega_1 - \omega_2)/2$ and suitable $\bar{\omega} \in \mathbb{R}$, $\vec{v} \in \mathbb{R}^3$, and then use the definition of $R_{\vec{v}}(\theta)$ from the lecture.

Solution

(a) First note that, for all $A \in \mathbb{C}^{n \times n}$,

$$\left(\mathrm{e}^{A}\right)^{\dagger} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(A^k\right)^{\dagger} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(A^{\dagger}\right)^k = \mathrm{e}^{(A^{\dagger})}.$$

Together with the property that H is Hermitian, i.e., $H^{\dagger} = H$ and thus $(-iHt)^{\dagger} = iHt$, one obtains

$$U_t^{\dagger} U_t = \mathrm{e}^{iHt} \mathrm{e}^{-iHt} = \mathrm{e}^{i(H-H)t} = \mathrm{e}^{0} = I.$$

(b) Since H is a diagonal matrix here, the matrix exponential e^{-iHt} can be computed by applying the exponential function to the diagonal entries:

$$U_t = \mathrm{e}^{-iHt} = \begin{pmatrix} \mathrm{e}^{-i\omega_1 t} & 0 \\ 0 & \mathrm{e}^{-i\omega_2 t} \end{pmatrix}.$$

We use vector notation to compute $|\psi(t)\rangle = U_t |\psi(0)\rangle$ for the two initial states:

$$U_t |0\rangle = \begin{pmatrix} \mathrm{e}^{-i\omega_1 t} & 0 \\ 0 & \mathrm{e}^{-i\omega_2 t} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{-i\omega_1 t} \\ 0 \end{pmatrix} = \mathrm{e}^{-i\omega_1 t} |0\rangle$$

and

$$U_t \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \begin{pmatrix} \mathrm{e}^{-i\omega_1 t} & 0 \\ 0 & \mathrm{e}^{-i\omega_2 t} \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{e}^{-i\omega_1 t} \\ \mathrm{e}^{-i\omega_2 t} \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\mathrm{e}^{-i\omega_1 t} |0\rangle + \mathrm{e}^{-i\omega_2 t} |1\rangle\right).$$

(c) Following the hint, we represent

$$H = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} + \epsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \bar{\omega} I + \Delta\omega Z + \epsilon X = \bar{\omega} I + \sqrt{\Delta\omega^2 + \epsilon^2}\,(\vec{v} \cdot \vec{\sigma})$$

with $\bar{\omega} = (\omega_1 + \omega_2)/2$, $\Delta\omega = (\omega_1 - \omega_2)/2$, the normalized vector

$$\vec{v} = \frac{1}{\sqrt{\Delta\omega^2 + \epsilon^2}} \begin{pmatrix} \epsilon \\ 0 \\ \Delta\omega \end{pmatrix}$$

and the Pauli vector $\vec{\sigma} = (X, Y, Z)$. Now using the properties of the generalized rotation operator (see lecture) leads to

$$U_t = \mathrm{e}^{-iHt} = \mathrm{e}^{-i\bar{\omega}t}\,\mathrm{e}^{-i\sqrt{\Delta\omega^2+\epsilon^2}\,(\vec{v}\cdot\vec{\sigma})t} = \mathrm{e}^{-i\bar{\omega}t}\left(\cos\!\left(\sqrt{\Delta\omega^2 + \epsilon^2}\,t\right) I - i \sin\!\left(\sqrt{\Delta\omega^2 + \epsilon^2}\,t\right)(\vec{v} \cdot \vec{\sigma})\right).$$

The overlap is then

$$\begin{aligned} \langle 1 | \psi(t) \rangle = \langle 1 | U_t | 0 \rangle &= -i\,\mathrm{e}^{-i\bar{\omega}t} \sin\!\left(\sqrt{\Delta\omega^2 + \epsilon^2}\,t\right) \langle 1 | (\vec{v} \cdot \vec{\sigma}) | 0 \rangle \\ &= -i\,\mathrm{e}^{-i\bar{\omega}t} \sin\!\left(\sqrt{\Delta\omega^2 + \epsilon^2}\,t\right) \frac{\epsilon}{\sqrt{\Delta\omega^2 + \epsilon^2}}, \end{aligned}$$

where we have used that $\langle 1 | I | 0 \rangle = 0$, $\langle 1 | Z | 0 \rangle = 0$, $\langle 1 | X | 0 \rangle = 1$.

The following figure visualizes the real and imaginary parts of the overlap as function of time, for parameters $\omega_1 = 1.05$, $\omega_2 = 0.95$ and $\epsilon = 0.05$. One recognizes a fast oscillation with frequency $\bar{\omega}$, enveloped by a slow oscillation with frequency $\sqrt{\Delta\omega^2 + \epsilon^2}$.