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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.

Exercise 3.1 (Properties of Pauli matrices and matrix exponential)
As usual, $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3) = (X, Y, Z)$ denotes the Pauli vector.

(a) Verify that the Pauli matrices anti-commute with each other, i.e.,

$$\{\sigma_1, \sigma_2\} = 0, \quad \{\sigma_2, \sigma_3\} = 0, \quad \{\sigma_3, \sigma_1\} = 0,$$

where $\{A, B\} = A\,B + B\,A$ denotes the *anti-commutator* of two matrices.

(b) Verify the following commutation relations (here $[A, B] = A\,B - B\,A$ denotes the *commutator* of two matrices):

$$[\sigma_1, \sigma_2] = 2i\sigma_3, \quad [\sigma_2, \sigma_3] = 2i\sigma_1, \quad [\sigma_3, \sigma_1] = 2i\sigma_2.$$

(c) Use the series expansion of the matrix exponential to derive that, for any $A \in \mathbb{C}^{n\times n}$ and unitary matrix $U \in \mathbb{C}^{n\times n}$,

$$\mathrm{e}^{U^\dagger A U} = U^\dagger\, \mathrm{e}^A\, U.$$

Remark: In case A is normal, one can combine this relation with the spectral decomposition to evaluate e^A, since the matrix exponential of a diagonal matrix is the pointwise exponential of the diagonal entries.

(d) Show that

$$HXH = Z \quad \text{and} \quad HZH = X,$$

where H denotes the Hadamard gate. (Since H is Hermitian and self-inverse, i.e., $H^2 = I$, H can thus be interpreted as base change matrix between the eigenvectors of X and Z.)

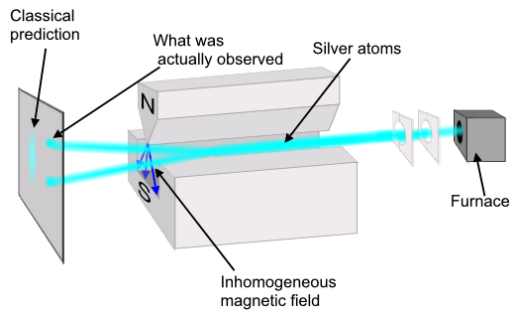
(e) Combine parts (c) and (d) to argue that

$$H R_x(\theta) H = R_z(\theta) \quad \text{for all } \theta \in \mathbb{R}.$$

Exercise 3.2 (The Stern-Gerlach experiment)

The Stern-Gerlach experiment is a fundamental experiment in the history of quantum mechanics, leading to the insight that electrons have an intrinsic, quantized spin degree of freedom. Otto Stern conceived the experiment in 1921, and conducted it together with Walther Gerlach in 1922.

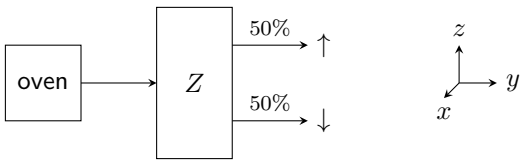
The setup is illustrated on the right. An oven (furnace) sends a beam of hot atoms through an inhomogeneous magnetic field, which causes the atoms to be deflected; the atoms are finally detected on a screen. The original experiment was conducted with silver atoms, but for our purpose it is simpler to discuss an analogous experiment with hydrogen atoms, which was performed in 1927.



https://commons.wikimedia.org/wiki/File:Stern-Gerlach_experiment.PNG

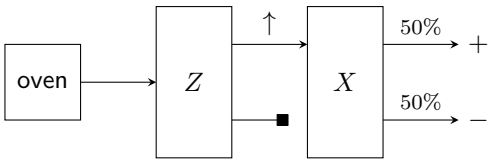
Based on classical physics, the electron orbiting around the proton in a hydrogen atom can be regarded as small magnetic dipole. One would then expect a continuous distribution of deflection angles, since the dipole axes are oriented randomly in space. Quantum mechanics predicts zero magnetic dipole moment for the hydrogen atom, and correspondingly the beam should not be deflected at all. Instead, a splitting into two beams was observed in the experiment.

We use the following schematic to summarize the Stern-Gerlach experiment:

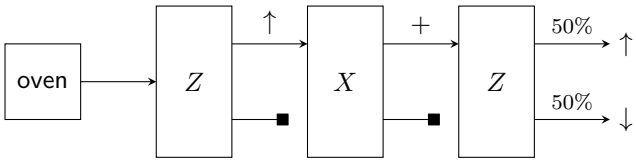


The coordinate system is chosen such that the beam propagates in y-direction. The inhomogeneous magnetic field (which we take to be oriented along the z-direction) splits the beam into two parts, one deflected up and the other down. Based on this description, one could hypothesize that each electron carries a classical bit of information, which specifies whether the atom goes up or down.

Now suppose we block the lower beam and send the upper beam through another inhomogeneous magnetic field, which is oriented along the x-direction. Classically, a dipole pointing in z-direction has zero moment in the x-direction, so one might expect that the final output is a single peak. Instead, experimentally one finds again two peaks, which we label $+$ and $-$:



Thus maybe each electron carries two classical bits of information, for selecting $\uparrow$ or $\downarrow$ and $+$ or $-$? If this was the case, and the electrons retained this information, then sending one beam of the previous output through another z-oriented field should result in a single beam deflected upwards. Instead, again two beams of equal intensity are observed:



Without any knowledge of quantum mechanics, it appears indeed challenging to invent a model explaining these observations.

Conversely, in the following we investigate the predictions of quantum mechanics when identifying the electronic spin as qubit, with $|0\rangle$ assigned to $\uparrow$ and $|1\rangle$ assigned to $\downarrow$. The inhomogeneous magnetic fields oriented along z- and x-direction measure the spin w.r.t. the eigenvectors of Pauli-Z (i.e., a standard measurement) and Pauli-X (equivalent to applying the Hadamard gate before the measurement and after the wavefunction collapse), respectively.

(a) Compute the eigenvalues and normalized eigenvectors of the Pauli-X, Y and Z matrices.

(b) Calculate the probabilities when measuring $|0\rangle$ with respect to the eigenvectors of X denoted $|+\rangle$, $|-\rangle$ (i.e., apply H before and after a standard measurement), and compare your results with the second schematic above.

(c) Explain the experimental observations of the third schematic setup. What would happen when orienting the last magnetic field along the x-direction instead of the z-direction?