

Lecture 11

The Hamiltonian Operator

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- So far we have not discussed systems that change in time.
- We will now develop a theory for how kets evolve in time, similar to Newton's laws of motion.
- We know classical systems subject to external forces evolve according to Newton's law $\vec{F} = m\vec{a}$.
- In QM, the Schrödinger equation plays the equivalent role to $\vec{F} = m\vec{a}$ in describing the time evolution of the quantum state $|\psi\rangle$.
- The first important point to keep in mind is that time is treated as a continuous parameter in QM. There is no operator that corresponds to time.
- How does a ket change in time?
- We need an operator that transforms a ket at one time to a ket at a different time.
- Let's use the approach we developed for rotations to construct an unitary operator that translates a state by an infinitesimal amount of time.
- Let's first review the properties of the infinitesimal translation operator.

- Operators corresponding to observables, such as angular momentum, linear momentum, position and energy all generate transformations of states in Hilbert space.
- Angular momentum, for example rotates kets. We will see later that the linear momentum operator will produce translations, and the energy operator will produce a translation of states in time.
- We can build continuous transformations by applying a series of infinitesimal transformations.
- The infinitesimal transformation operator has the basic form

$$U(\epsilon) = \mathbb{1} - i\epsilon G$$

where G is a Hermitian operator corresponding to the particular observable in question, e.g., angular momentum, and ϵ is the infinitesimal quantity, e.g., $d\phi$ for the case of rotations.

- There are two reasons for choosing $U(\epsilon)$ to have this mathematical form.
- First, we require that $\lim_{\epsilon \rightarrow 0} U(\epsilon) = \mathbb{1}$.
- Second, $U(\epsilon)$ should be unitary, that is, it should transform a state without changing its norm. Another way of saying this is that it should conserve probability. We therefore require that $UU^\dagger = \mathbb{1}$.

$$\begin{aligned} UU^\dagger &= (\mathbb{1} - i\epsilon G)(\mathbb{1} + i\epsilon G^\dagger) \\ G &= G^\dagger \quad G \text{ is a Hermitian operator} \\ &= \mathbb{1} + i\epsilon G - i\epsilon G + \epsilon^2 G^2 \end{aligned}$$

We see that terms of $\mathcal{O}(\epsilon)$ cancel. Neglecting terms of order $\mathcal{O}(\epsilon^2)$, $UU^\dagger = \mathbb{1}$, as required.

- Let the state of the system at time t be $|\psi(t)\rangle$.
- We define a unitary operator $U(t + \delta t, t)$, which translates the state $|\psi(t)\rangle$ in time to $|\psi(t + \delta t)\rangle$.

$$U(t + dt, t) = \mathbb{1} - i\Omega\delta t \quad (1)$$

where $\Omega = \Omega^\dagger$ is a Hermitian operator.

- We need to identify the physical observable that corresponds to the operator Ω .
- We note that Ω has units of frequency. We recall from the Planck-Einstein relationship in quantum theory that energy and frequency are related $E = \hbar\omega$.
- From classical mechanics, we also know that the Hamiltonian \mathcal{H} generates evolution in time.
- \mathcal{H} is equal to the total energy of the system.
- It is therefore natural to associate Ω with the total energy of the system.

$$\Omega = \frac{\mathcal{H}}{\hbar} \quad (2)$$

The Hamiltonian

- We rewrite eq.(1) as

$$U(t + \delta t, t) = \mathbb{1} - \frac{i\mathcal{H}\delta t}{\hbar} \quad (3)$$

- It is important to note that \mathcal{H} can be time dependent. In eq.(3) we are considering $\mathcal{H}(t)$, i.e., the Hamiltonian at time t .
- Applying the $U(t + \delta t, t)$ to $|\psi(t)\rangle$ we obtain

$$\begin{aligned} U(t + \delta t, t) |\psi(t)\rangle &= |\psi(t + \delta t)\rangle \\ \left(\mathbb{1} - \frac{i\mathcal{H}\delta t}{\hbar} \right) |\psi(t)\rangle &= |\psi(t + \delta t)\rangle \\ &= |\psi(t)\rangle + \frac{d}{dt} |\psi(t)\rangle \delta t + \mathcal{O}(\delta t^2) \end{aligned}$$

$$\mathcal{H} |\psi(t)\rangle = i\hbar \frac{d}{dt} |\psi(t)\rangle \quad (4)$$

Postulate 6

The time evolution of a quantum system is determined by the Hamiltonian or total energy operator $\mathcal{H}(t)$ through the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \mathcal{H}(t) |\psi(t)\rangle \quad (5)$$

- The spectrum of allowed energies of a quantum system corresponds to the eigenvalues of the Hamiltonian $\{E\}$. The corresponding eigenvectors $\{|E\rangle\}$ are referred to as energy eigenkets.
- We will begin our study of the Schrödinger equation first considering a time-independent Hamiltonian.

$$\mathcal{H} |E_n\rangle = E_n |E_n\rangle \quad (6)$$

- The Hamiltonian is a Hermitian operator, therefore the basis eigenkets form a complete and orthonormal basis.

Time-Independent Hamiltonians

- In the energy basis, the operator \mathcal{H} is diagonal

$$\mathcal{H} = \begin{pmatrix} E_1 & 0 & 0 & \cdots \\ 0 & E_2 & 0 & \cdots \\ 0 & 0 & E_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

- We can represent any time-dependent state $|\psi(t)\rangle$ in terms of the energy eigenvectors.

$$|\psi(t)\rangle = \sum_n c_n(t) |E_n\rangle$$

- **Important:** For a time independent Hamiltonian, the basis vectors are time independent. The time dependence of $|\psi(t)\rangle$ enters through the the coefficients $c(t)$.
- Solve for the time dependence of a particular $c_n(t)$.

$$i\hbar \frac{d}{dt} \sum_n c_n(t) |E_n\rangle = \mathcal{H} \sum_m c_m(t) |E_m\rangle$$

Time-Independent Hamiltonians

$$i\hbar \sum_n \frac{dc_n}{dt} |E_n\rangle = \sum_m c_m E_m |E_m\rangle$$

$$i\hbar \sum_n \frac{dc_n}{dt} \underbrace{\langle E_k | E_n \rangle}_{\delta_{kn}} = \sum_m c_m E_m \underbrace{\langle E_k | E_m \rangle}_{\delta_{km}}$$

$$i\hbar \frac{dc_k}{dt} = c_k E_k$$

$$\frac{dc_k}{c_k} = \frac{E_k}{i\hbar} dt$$

$$\ln c_k = -\frac{iE_k}{\hbar} t + \text{const.}$$

$$c_k(t) = c_k(t=0) \exp\{-iE_k t/\hbar\}$$

$$\boxed{|\psi(t)\rangle = \sum_n c_n(0) \exp\{-iE_n t/\hbar\} |E_n\rangle} \quad (7)$$

Time-Independent Hamiltonians

- For a time-independent Hamiltonian, the time dependence of $|\psi(t)\rangle$ is equal to the sum of energy eigenkets multiplied by a time-dependent phase factor.
- **Example:** Suppose we start from an energy eigenstate of the Hamiltonian $|\psi(0)\rangle = |E_m\rangle$. Calculate $|\psi(t)\rangle$, and the probability $|\langle\psi(0)|\psi(t)\rangle|^2$ that the system remains in the original state $|\psi(0)\rangle$.

$$|\psi(t)\rangle = c_m(0) \exp\{-iE_m t/\hbar\} |E_m\rangle$$

$$|\langle\psi(0)|\psi(t)\rangle|^2 = 1$$

$$|c_m(0)|^2 = 1 \quad \Rightarrow \quad c_m(0) = 1$$

$$|\langle\psi(0)|\psi(t)\rangle|^2 = |\exp\{-iE_m t/\hbar\} \langle E_m | E_m \rangle|^2 = 1$$

Evolution of Superposition of Energy Eigenstates

- We see that the time dependence of an energy eigenket is through the time-dependent phase factor $\exp\{-iE_m t/\hbar\}$. As we have noticed before, an overall phase factor does not affect the probability.
- We refer to an energy eigenstate as a **stationary state**, because a system that starts out in an energy eigenstate remains in that eigenstate.
- Let's consider a system that starts from a state that is not an energy eigenstate.

$$|\psi(0)\rangle = c_1(0) |E_1\rangle + c_2(0) |E_2\rangle$$

- In general, $|\psi(0)\rangle$ is not an eigenstate of \mathcal{H} .

$$\mathcal{H} |\psi(0)\rangle = E_1 c_1(0) |E_1\rangle + E_2 c_2(0) |E_2\rangle \neq \text{const.} |\psi(0)\rangle$$

- From the time-dependent state eq.(7) we derived, we can immediately write the expression for the $|\psi(t)\rangle$.

Evolution of Superposition of Energy Eigenstates

- We define the angular frequency $\omega_n := \frac{E_n}{\hbar}$.
- Let $c_n := c_n(0)$.

$$|\psi(t)\rangle = c_1(0)e^{-i\omega_1 t} |E_1\rangle + c_2(0)e^{-i\omega_2 t} |E_2\rangle$$

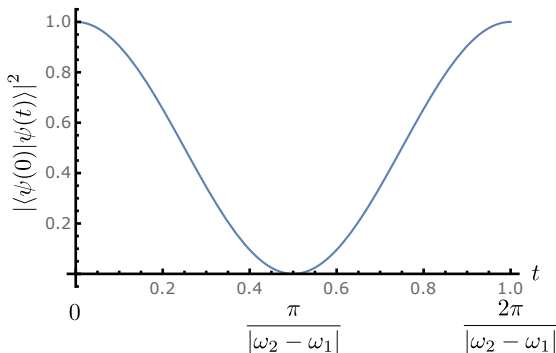
- Let's calculate the probability that the system remains in the initial state $|\psi(0)\rangle$.

$$\begin{aligned} |\langle\psi(0)|\psi(t)\rangle|^2 &= \left| \begin{pmatrix} c_1^* & c_2^* \end{pmatrix} \begin{pmatrix} c_1 e^{-i\omega_1 t} \\ c_2 e^{-i\omega_2 t} \end{pmatrix} \right|^2 \\ &= \left| |c_1|^2 e^{-i\omega_1 t} + |c_2|^2 e^{-i\omega_2 t} \right|^2 \\ &= |c_1|^4 + |c_2|^4 + |c_1|^2 |c_2|^2 (e^{i(\omega_2 - \omega_1)t} + e^{-i(\omega_2 - \omega_1)t}) \\ &= |c_1|^4 + |c_2|^4 + 2|c_1|^2 |c_2|^2 \cos[(\omega_2 - \omega_1)t] \end{aligned}$$

Evolution of Superposition of Energy Eigenstates

- Suppose we start from a normalized state where $|c_1|^2 + |c_2|^2 = 1$, and let $|c_1|^2 = |c_2|^2 = \frac{1}{2}$.

$$|\langle\psi(0)|\psi(t)\rangle|^2 = \frac{1}{2} [1 + \cos[(\omega_2 - \omega_1)t]]$$



Evolution of Superposition of Energy Eigenstates

- If the system does not start from an eigenstate, the probability evolves in time.
- What is the expectation value of the Hamiltonian?

$$\begin{aligned}\langle \psi(t) | \mathcal{H} | \psi(t) \rangle &= \begin{pmatrix} c_1^* e^{i\omega_1 t} & c_2^* e^{i\omega_2 t} \end{pmatrix} \begin{pmatrix} c_1 E_1 e^{-i\omega_1 t} \\ c_2 E_2 e^{-i\omega_2 t} \end{pmatrix} = E_1 |c_1|^2 + E_2 |c_2|^2 \\ &= P(E_1) E_1 + P(E_2) E_2\end{aligned}$$

where $P(E_n)$ is the probability to measure energy E_n .

- We note that the expectation value of the Hamiltonian is time independent, as it must. We see that, while the superposition evolves in time, the probability that the system is in states $|E_1\rangle$ or $|E_2\rangle$ is stationary.