4/19/07 Lecture 6 outline

• Today's lecture is on the Schrodinger equation, which is the primary equation of quantum mechanics. It's as central as $\vec{F} = m\vec{a}$ is to classical mechanics. As in that case, it gives a way to determine how systems evolve in time, given some initial state. We can motivate the Schrodinger equation from some general principles of classical mechanics: the notion of conjugate variables. Examples of conjugate variables are position and momentum. Energy and time are also conjugate variables.

Let's discuss that. But first, state the main message of today's lecture: the wavefunction evolves in space and time according to $\vec{p} = \hbar\vec{k}$ and $E = \hbar\omega$, even if the particle is not free.

Now, some classical mechanics. In the Hamiltonian description, consider motion in $(q, p)$ phase space. (Note: the uncertainty principle can be interpreted as saying that phase space is pixelated, with a basic pixel size $\Delta q\Delta p = \frac{1}{2}\hbar$. This is very useful in statistical mechanics! ) Recall Poisson brackets, $\{u, v\} \equiv \frac{\partial u}{\partial q^i}\frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i}\frac{\partial v}{\partial q^i}$. Note that: $\{u, p_i\} = \frac{\partial u}{\partial q_i}$. Also, $\frac{d}{dt}u = \frac{\partial}{\partial t}u + \{u, H\}$. These relations illustrate the statements that momentum generates translations in space, and energy generates translations in space.

• In quantum mechanics, these relations are related to $p = \hbar k$ and $E = \hbar\omega$ and that wavefunctions depend on position and time as $\psi \sim e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar}$. Related to uncertainty principles:

$$\Delta p\Delta x \geq \frac{\hbar}{2} \qquad \Delta E\Delta t \geq \frac{\hbar}{2}$$

• Illustrate this for expectation values in QM. Recall we compute expectation values using probabilities, e.g.

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} f(x)|\psi(x,t)|^2 dx, \qquad \langle F(p)\rangle = \int_{-\infty}^{\infty} F(p)|\phi(p)|^2 dp.$$

• We can now define more precisely what we mean by $\Delta x$ and $\Delta p$ in the uncertainty principle:

$$\Delta x \equiv \sqrt{\langle x^2\rangle - \langle x\rangle^2} \qquad \Delta p \equiv \sqrt{\langle p^2\rangle - \langle p\rangle^2}.$$

These always satisfy $\Delta x\Delta p \geq \frac{\hbar}{2}$. You can check that the gaussians have $\Delta x = \sigma$ and $\Delta p = \tilde{\sigma}$, according to the definitions used in lecture the other week.

• Can always compute either in position or momentum space, e.g.

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} \phi^*(p,t)f(i\hbar\frac{d}{dp})\phi(p,t)dp, \qquad \langle F(p)\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)F(-i\hbar\frac{d}{dx})\psi(x,t)dx,$$

where $\phi(p,t) = \phi(p)e^{-iE(p)t/\hbar}$. In position space, we replace $p \to -i\hbar\frac{d}{dx}$ and in momentum space we replace $x \to i\hbar\frac{d}{dp}$. This lead into the basic postulates of Q.M. Examples: use above gaussian wavefunction, $\langle p \rangle = p_0$ and $\langle x \rangle = p_0 t/m$. Expectation values satisfy expected classical relations , example of Ehrenfest's theorem.

• In QM, the statements about momentum and energy being the generators of translations in space and time can be written as

$$p \to -i\hbar\frac{\partial}{\partial x}, \qquad E \to i\hbar\frac{\partial}{\partial t}.$$

Leads to the Schrodinger equation

$$H\psi = i\hbar\frac{\partial}{\partial t}\psi$$

for time evolution of the wave function. $H$ is the Hamiltonian, $H = p^2/2m + V(x)$, which yields the energy. This says that a state of energy $E$ evolves in time as $\psi \sim e^{-iEt/\hbar}$, as for a free particle, i.e. $E = \hbar\omega$. A motivation: waves have the same frequency $\omega$ even in regions where the velocity changes, e.g light between materials of different index of refractions. In $H = p^2/2m + V(x)$, replace $p \to -i\hbar\frac{\partial}{\partial x}$. Or in 3d, $\vec{p} \to -i\hbar\nabla$.

• The momentum operator $p = -i\hbar\frac{d}{dx}$ is a Hermitian operator, $p^\dagger = p$. Show why. Implies that eigenvalues are always real. Implies its expectation value is always real. The $x$ operator is also Hermitian, $x^\dagger$ . The Hamiltonian operator is Hermitian (for real $V(x)$), so the energy eigenvalues are all real, and the expectation value of the energy is real.