

4/24/07 Lecture 7 outline

- Last time we wrote down the Schrodinger equation. Write it out again, for 3d:

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = H\psi \equiv \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right) \psi(\vec{x}, t).$$

- Make some aside comments on some general consequences. First aside: particles don't disappear in QM. Indeed, probability density $\rho = |\psi(\vec{x}, t)|^2$, and probability current density $\vec{J} = \frac{\hbar}{2mi}(\psi^* \nabla \psi - (\nabla \psi^*)\psi)$ satisfies a conservation equation, $\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$ (since the potential V is real). This follows from the Schrodinger equation:

$$\frac{\partial \rho}{\partial t} = \frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} (-(H\psi)^* \psi + \psi^* H\psi) = -\nabla \cdot \vec{J}.$$

- For general real potential V , can show (using Schrodinger equation)

$$\frac{d}{dt} \langle \vec{x} \rangle = \int d^3x \vec{x} \frac{\partial \rho}{\partial t} = \int d^3x \vec{J} = \frac{1}{m} \langle \vec{p} \rangle.$$

$$\frac{d}{dt} \langle \vec{p} \rangle = \frac{d}{dt} \int d^3x \psi^* \frac{\hbar}{i} \nabla \psi = - \int \psi^* \nabla V \psi = \langle \vec{F} \rangle.$$

Which is are examples of Ehrenfest's theorem: the expectation values satisfy the classical relations (modulo caveats below). More generally, for any observable u , the Schrodinger equation implies

$$\frac{d}{dt} \langle u \rangle = \left\langle \frac{\partial}{\partial t} u \right\rangle + \frac{1}{i\hbar} \langle [u, H] \rangle,$$

which is of the same form as the statements about classical mechanics, where the statement applies to the expectation values, and the Poisson brackets are replaced with commutators,

$$\{A, B\} \rightarrow \frac{1}{i\hbar} [A, B] \quad \text{where} \quad [A, B] \equiv AB - BA.$$

This is a general statement about quantum mechanics. In particular, get

$$\frac{d}{dt} \langle p \rangle = \left\langle -\frac{\partial V}{\partial x} \right\rangle$$

which is similar to the classical equation of motion, except that in general

$$\langle F(x) \rangle = \left\langle \frac{-\partial V}{\partial x} \right\rangle \neq F(\langle x \rangle) = -\frac{\partial}{\partial \langle x \rangle} V(\langle x \rangle).$$

This is approximately true (leading the Ehrenfest's theorem) only if the potential is slowly varying and Δx is not too big.

- In QM, we replace observables, like position, momentum, energy, angular momentum, etc. with linear operators. These operators act on the wavefunction. We have already seen this with $E \rightarrow i\hbar \frac{\partial}{\partial t}$, which according to the S.E. is $E \rightarrow H$. And $p \rightarrow -i\hbar \frac{\partial}{\partial x}$. The general rule is that the Poisson brackets of classical mechanics are replaced with commutators of the operators in quantum mechanics:

$$[A, B] = i\hbar\{A, B\},$$

where $[A, B] \equiv AB - BA$. In your HW, you will do some checks that this makes sense. In particular,

$$[x, p_x] = i\hbar, \quad [y, p_y] = i\hbar, \quad [z, p_z] = i\hbar.$$

The classical limit is $\hbar \rightarrow 0$, where the operators commute.

- When we measure the observable, we measure an eigenvalue of the corresponding operator. The measurement process alters the state of the system: the final state is the eigenvector corresponding to the measured eigenvalue.

- If two operators do not commute, such as position and momentum above, they both can not be measured simultaneously. Leads to the Heisenberg uncertainty principle, $\Delta x \Delta p_x \geq \hbar/2$.

- Example: free particle in a box, between $x = 0$ and $x = L$. Energy eigenvectors $u_n(x) = \sqrt{\frac{2}{L}} \sin(n\pi x/L)$, with eigenvalue $E_n = \hbar^2 \pi^2 n^2 / 2mL^2$, for $n = 1, 2, 3, \dots$. Note groundstate energy $E_1 \neq 0$, connect to uncertainty principle.