5/5/08 Lecture 11 outline

• 1d Schrodinger equation for general potential. $H = \hat{p}^2/2m + V(\hat{x})$. To solve the equation, we want to solve for the energy eigenstates and eigenvalues, $H|E\rangle = E|E\rangle$. We write this in the x-basis (position space) as $\langle x|H|E\rangle = E\langle x|E\rangle$. Defining $\langle x|E\rangle \equiv \psi_E(x)$, this becomes:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi_E(x) = E\psi_E(x),$$

because $\hat{p} \to -i\hbar\frac{d}{dx}$ in position space. We solve this equation to determine the eigenvalues E and the eigenstates $\psi_E(x)$. The solution $\psi_E(x)$ is always a continuous function. It's derivative $\psi_E'(x)$ is continuous also, unless the potential has an infinite jump somewhere.

• Example of particle in a box, $V(x) = 0$ for $0 < x < L$ and infinite outside that range. Solutions are labeled by $n = 1, 2, 3\ldots$,

$$\psi_{E_n}(x) \equiv u_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \qquad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}.$$

Discuss also the solutions and their parity symmetry if we shift x so that $x = 0$ is the midpoint of the box.

Groundstate has $E_1 \neq 0$, related to uncertainty principle.

• The energy levels are quantized, because the particle is bound in the well. This is general. As long as $E < V(|x| \to infty)$, then $\psi(|x| \to \infty) \to 0$. Then the particle is bound in the well, and the energy levels are quantized. Qualitative example of particle in a finite well.

• the E_n are the possible outcomes of experiments if the energy is measured. Suppose that the system is in the state $\psi(x) = u_n(x)$. Measurement of the energy will then yield the corresponding E_n with 100% probability. On the other hand, the position is uncertain. E.g. the probability to measure in range from x_1 to x_2 is

$$\int_{x_1}^{x_2} |u_n(x)|^2 dx = \frac{x_2 - x_1}{L} - \frac{1}{2\pi n}\left(\sin(\frac{2\pi n x_2}{L}) - \sin(\frac{2\pi n x_1}{L})\right).$$

First term is what we'd expect on average classically. The second term goes away for $n \to \infty$, which is an example of the correspondence principle. It is straightforward to work out $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, $\langle p^2\rangle$ etc.. You will check these and the uncertainty principle in a HW problem.

The u_n form an orthonormal and complete basis of functions with the correct BCs: any wavefunction can be expanded as

$$\psi(x) = \sum_{n=1}^{\infty} c_n u_n(x) \qquad u_n \equiv \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L},$$

where

$$c_n = \int_0^L dx\ u_n(x)^* \psi(x).$$

Here is the physics: if one measures the energy, the probability of measuring E_n is $|c_n|^2$. If the wavefunction is properly normalized, $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$, then the above expression for c_n will imply that $\sum_n |c_n|^2 = 1$, so the energy probabilities properly sum to unity. The average expectation value of the energy is

$$\langle E \rangle = \sum_n E_n |c_n|^2 = \langle H \rangle = \int_{-\infty}^{\infty} \psi^*(x) H \psi(x).$$

After measuring energy E_n, the state of the system is changed: now it is fully in the corresponding eigenstate, $\psi(x) = u_n(x)$. Subsequent measurement of energy will give the same E_n, with 100% probability. This is a very important and general aspect of quantum mechanics, true for any observable: the initial wavefunction is in a superposition of eigenvectors of the observable. The coefficients of the superposition give the probability of measuring the corresponding eigenvalue. The measurement changes the state of the system: immediately afterward a measurement, the state is not in the superposition anymore, but rather it is fully in the eigenstate corresponding to the measured eigenvalue.

- The time dependence of the wavefunction is given by the Schrodinger equation,

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = H\psi.$$

Using the above form, we can immediately determine the solution of the Schrodinger equation. The wavefunction, as a function of time, is given by

$$\psi(x,t) = \sum_n c_n e^{-iE_n t/\hbar} \psi_n(x), \qquad \text{where} \qquad c_n = \int dx\ \psi_n^*(x) \psi(x, t=0).$$

Once we've expanded the initial wavefunction $\psi(x, t=0)$ in terms of the energy eigenstates (which is a useful thing to do in any case!), we can immediately write down the time dependence, as above! The S.E. is a partial differential equation, in x and t, and the solution above is the statement that we can use separation of variables, along with superposition (since the equation is linear).

• Even though the above t dependence looks so simple, it leads to very non-trivial t dependence when we compute different quantities, e.g. the position probability density $\rho(x,t) = |\psi(x,t)|^2$. This leads to nontrivial t dependence in general for measured quantities, and also for expectation values. We showed in the last lecture how quantum expectation values reproduce the classical equations of motion. For example, we have

$$\frac{d}{dt}\langle X\rangle = \frac{1}{i\hbar}\langle [X,H]\rangle = \langle P\rangle/m$$

where in the last line we used $H = P^2/2M + V(X)$. Likewise,

$$\frac{d}{dt}\langle P\rangle = \frac{1}{i\hbar}\langle [P,H]\rangle = \langle -\frac{\partial V(X)}{\partial X}\rangle.$$

• Note that if the system is in an energy eigenstate, $\psi(x,t) = e^{-iE_nt/\hbar}\psi_n(x)$, then all expectation values like $\langle x^n\rangle$ and $\langle p^n\rangle$ are time independent. This is called a stationary state.