4/17/08 Lecture 6 outline

• Last time: Fourier transforms,

$$\psi(x) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}\phi(p), \qquad \phi(p) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}\psi(x).$$

This is the Fourier transform and its inverse. The probability of finding particle in range from x to $x+dx$ is $P(x)dx = |\psi(x)|^2 dx$. The probability to find the particle having momentum in the range from p to $p+dp$ is $P(p)dp = |\phi(p)|^2 dp$.

• Last time: The time evolution of a free particle is given by

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} e^{i(px-Et)/\hbar}\phi(p), \qquad \phi(p) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}\psi(x,t=0)$$

where $E = p^2/2m$. Packet moves with velocity given by the group velocity, $v_g = d\omega/dk$, which for us is now $v_g = dE/dp = p/m$, which is indeed reasonable: the group velocity equals the particle's velocity. The spreading of wave packets is generally given by $d^2\omega/dk^2$, which for us is d^2E/dp^2, which is $1/m$ for a non-relativistic particle.

For example, suppose

$$\psi(x,t=0) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^{1/2} e^{i\bar{p}x/\hbar}\exp(-x^2/4\sigma^2) \to |\phi(p)|^2 = \frac{1}{\sqrt{2\pi}\tilde{\sigma}}\exp(-(p-\bar{p})^2/2\tilde{\sigma}^2),$$

which is of the Gaussian form, with average momentum $\bar{p}$. As an example, let's take $\bar{p} = 0$, so it's just a Gaussian, with zero average momentum. At time $t = 0$, it's width is σ. Plugging into above expression for time evolution, find that $\psi(x,t)$ again has the Gaussian form, but with $\sigma \to \sqrt{\sigma + it\hbar/2m\sigma}$. Gives a Gaussian probability, with $\sigma(t) = \sqrt{\sigma^2 + (\hbar t/2m\sigma)^2}$. This spreading of the packet is just like diffraction: the more the particle is localized, the more it will later spread out. E.g. an electron, localized initially in $\sigma = 10^{-10}m$ spreads to 1AU ($= 8 \times 60 \times 3 \times 10^8 m$) in $t \approx 9 \times 10^{-8}s$(!). Or 1 gram in $\sigma = 10^{-6}m$ spreads to $2 \times 10^{-6}m$ in $1.6 \times 10^{19}s$(!). Uncertainty principle again.

• Compute expectation values using probabilities, e.g.

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

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

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

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 classical mechanics, momentum and position are conjugate variables. Energy and time are conjugate variables. 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, $\frac{d}{dt}u = \frac{\partial}{\partial t}u + \{H, u\}$. 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 $\psi \sim e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}$.

• In quantum mechanics, the state of a system is given by a probability amplitude $|\psi(t)\rangle$, which is a is a vector in a space (the Hilbert space). The norm of that vector gives the probability. Position, momentum, energy, angular momentum are all replaced with operators, acting on the vectors in the Hilbert space. The eigenvalues of these operators are the observables. E.g. the allowed energies are the eigenvalues of the Hamiltonian operator, $H = p^2/2m + V(x)$, where p and x are operators. The quantum nature comes from commutation relations among these operators, in particular

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

where $[A, B] \equiv AB - BA$. The classical limit is $\hbar \to 0$, where the operators commute. The fact that they do not commute for $\hbar \neq 0$ means that one cannot simultaneously measure both the position and the momentum of a particle to arbitrary precision. This is the statement of the Heisenberg uncertainty principle, $\Delta x \Delta p_x \geq \hbar/2$. Again, this is related via $\vec{p} = \hbar\vec{k}$ to a basic property of Fourier transforms, $\Delta x \Delta k \geq \frac{1}{2}$.

• Let's discuss operators, vector spaces, and the Dirac bra-ket notation. To set the notation, consider a vector in K dimensions. We can expand it as $\vec{v} = \sum_{i=1}^{K} \widehat{e}_i v_i$, where $\widehat{e}_i$ are taken to be K orthonormal basis vectors.

• We're interested in complex vectors, and then the condition is $\widehat{e}_i \cdot \widehat{e}_j^* = \delta_{ij}$. Then $v_i = \vec{v} \cdot e_i^*$. Consider $\vec{v}$ as a matrix v, with 1 column and K rows. The inner product of two vectors v and w is then $\langle w|v\rangle \equiv w^\dagger v = \sum_{i=1}^{K} w_i^* v_i$. Note that this is a single, complex number, and that $\langle w|v\rangle^* = \langle v|w\rangle$. It follows that $\langle v|v\rangle$ is real, non-negative, and only vanishes if the vector $v = 0$.