Intermediate Quantum Mechanics
Lecture 11 Notes (2/25/15)
Particle on a Line

Hamiltonian for a particle on a line

- Making the assumption that $\hat{H}$ is the energy operator and that $\hat{p} = \hbar\hat{k}$ is the momentum operator, the Hamiltonian for a particle on a line is given by:

$$\hat{H} \;=\; \frac{\widehat{p^2}}{2m} + V(\hat{x})$$

  We will see shortly the reason for the $\hat{H}$ and $\hat{p}$ operator assumptions.

- The kinetic energy term in the Hamiltonian is based on the non-relativistic energy-momentum relation: $E = p^2/2m$. We would, of course, prefer to base it on the relativistically correct energy-momentum relation: $E^2 = p^2c^2 + m^2c^4$ but, because this has two solutions: $E = \pm\sqrt{p^2c^2 + m^2c^4}$, it leads to issues involving negative energies and negative probabilities that have to be dealt with. For now, we will do as Schrodinger did and develop non-relativistic quantum mechanics.

- The second term is in the expression for the Hamiltonian is the potential energy. It is a function of the x-operator, $\hat{x}$. We will take $V(\hat{x})$ to be an analytic function. That is, it can be expressed as a power series: $V(\hat{x}) \;=\; v_0\hat{I} + v_1\hat{x} + v_2\widehat{x^2} + \cdots$.

Rate of change of the average position

- In order to find the rate of change of the average position, we use the Ehrenfest Theorem.

$$\frac{d}{dt}\langle\psi(t)|\hat{x}\,|\psi(t)\rangle \;=\; -\frac{i}{\hbar}\langle\psi(t)|[\hat{x},\hat{H}]\,|\psi(t)\rangle$$

- Since $[\hat{x},\widehat{x^n}] = 0$, we have $[\hat{x},V(\hat{x})] = 0$. Then only the $\widehat{p^2}/2m$ term in the Hamiltonian contributes to the commutation of $\hat{x}$ with $\hat{H}$.

- Now we calculate $[\hat{x},\widehat{p^2}]$:

$$\text{Use} \qquad [\hat{x},\hat{p}] = i\hbar \qquad \Rightarrow \qquad \hat{x}\hat{p} \;=\; [\hat{x},\hat{p}] + \hat{p}\hat{x} \;=\; i\hbar + \hat{p}\hat{x}$$

$$[\hat{x},\widehat{p^2}] \;=\; \hat{x}\hat{p}\hat{p} - \hat{p}\hat{p}\hat{x} \;=\; (i\hbar + \hat{p}\hat{x})\hat{p} - \hat{p}\hat{p}\hat{x}$$

$$=\; i\hbar\hat{p} + \hat{p}(i\hbar + \hat{p}\hat{x}) - \hat{p}\hat{p}\hat{x} \;=\; 2i\hbar\hat{p} + \hat{p}\hat{p}\hat{x} - \hat{p}\hat{p}\hat{x} \;=\; 2i\hbar\hat{p}$$

- We then have:

$$\frac{d}{dt}\langle\psi(t)|\hat{x}\,|\psi(t)\rangle \;=\; -\frac{i}{\hbar}\langle\psi(t)|[\hat{x},\hat{H}]\,|\psi(t)\rangle \;=\; -\frac{i}{\hbar}\langle\psi(t)|[\hat{x},\left(\frac{\widehat{p^2}}{2m} + V(\hat{x})\right)]\,|\psi(t)\rangle$$

$$=\; -\frac{i}{2m\hbar}\langle\psi(t)|[\hat{x},\widehat{p^2}]\,|\psi(t)\rangle \;=\; \frac{1}{m}\langle\psi(t)|\hat{p}\,|\psi(t)\rangle$$

Rate of change of the average momentum

- We'll now use the Ehrenfest Theorem to find the rate of change of the average momentum.
$$\frac{d}{dt}\langle\psi(t)|\hat{p}\,|\psi(t)\rangle \;=\; -\frac{i}{\hbar}\,\langle\psi(t)|[\hat{p},\hat{H}]\,|\psi(t)\rangle$$

- Since $[\hat{p},\hat{p^2}] = 0$, only the $V(\hat{x})$ term in the Hamiltonian contributes to the commutation of $\hat{p}$ with $\hat{H}$.

- We need to evaluate $[\hat{p},\hat{x^n}]$. We'll do this in the x-representation. Note that the commuter of two operators is independent of representation.
$$\langle x|[\hat{p},\hat{x^n}]\,|\psi\rangle \;=\; \langle x|\big(\hat{p}\hat{x^n} - \hat{x^n}\hat{p}\big)\,|\psi\rangle \;=\; -i\hbar\,\frac{d}{dx}\,[x^n\psi(x)] \,+\, i\hbar x^n\,\frac{d}{dx}\,\psi(x)$$
$$=\; -i\hbar\left[\frac{d}{dx}\,x^n\right]\psi(x) \,-\, i\hbar x^n\,\frac{d}{dx}\,\psi(x) \,+\, i\hbar x^n\,\frac{d}{dx}\,\psi(x) \;=\; -i\hbar\left[\frac{d}{dx}\,x^n\right]\psi(x)$$
$$\Rightarrow\qquad [\hat{p},\hat{x^n}] \;=\; -i\hbar\,\frac{d}{d\hat{x}}\,\hat{x^n}$$
Since: $\quad V(\hat{x}) \;=\; v_0\hat{I} + v_1\hat{x} + v_2\hat{x^2} + \cdots \qquad$ we have $\qquad [\hat{p},V(\hat{x})] \;=\; -i\hbar\,\frac{d}{d\hat{x}}\,V(\hat{x})$

- We then have:
$$\frac{d}{dt}\langle\psi(t)|\hat{p}\,|\psi(t)\rangle \;=\; -\frac{i}{\hbar}\,\langle\psi(t)|[\hat{p},\hat{H}]\,|\psi(t)\rangle - \frac{i}{\hbar}\,\langle\psi(t)|[\hat{p},\left(\frac{\widehat{p^2}}{2m} \,+\, V(\hat{x})\right)]\,|\psi(t)\rangle$$
$$=\; -\frac{i}{\hbar}\,\langle\psi(t)|[\hat{p},V(\hat{x})]\,|\psi(t)\rangle \;=\; -\langle\psi(t)|\left(\frac{d}{d\hat{x}}\,V(\hat{x})\right)\,|\psi(t)\rangle \;=\; \langle\psi(t)|F(\hat{x})\,|\psi(t)\rangle$$
where $\quad F(\hat{x}) \;=\; -\,\frac{d}{dx}V(\hat{x})$

Connection with classical physics

- We've now made the connection with classical physics. We've found that:
$$\frac{d}{dt}\langle\psi(t)|\hat{x}\,|\psi(t)\rangle \;=\; \frac{1}{m}\,\langle\psi(t)|\hat{p}\,|\psi(t)\rangle \qquad \text{and} \qquad \frac{d}{dt}\langle\psi(t)|\hat{p}\,|\psi(t)\rangle \;=\; \langle\psi(t)|F(\hat{x})\,|\psi(t)\rangle$$
$$\text{or} \qquad \dot{\overline{x}} \;=\; \frac{\overline{p}}{m} \qquad \text{and} \qquad \dot{\overline{p}} \;=\; \overline{F(x)}$$
These parallel the relations that we know from classical physics:
$$\dot{x} \;=\; \frac{p}{m} \qquad \text{and} \qquad \dot{p} \;=\; F(x)$$

- The association of $\hat{H}$ as the energy operator and $\hat{p} = \hbar\hat{k}$ as the momentum operator leads to a description at the macroscopic scale that is consistent with classical physics.

- In a sense, position, momentum and energy are emergent properties. At the microscopic scale, momentum specifies how rapidly the particle's wavefunction changes with position and energy specifies how rapidly the state of the particle changes with time. It is only when we average over many identical particles that position, energy and momentum take on their classical meanings.

- Another connection with classical physics is through the conservation laws. In classical physics, we have that the energy of a closed system is conserved. In quantum mechanics we have from the Ehrenfest Theorem:

$$\frac{d}{dt}\langle\psi(t)|\hat{H}\,|\psi(t)\rangle \;=\; -\frac{i}{\hbar}\langle\psi(t)|[\hat{H},\hat{H}]\,|\psi(t)\rangle \;=\; 0$$

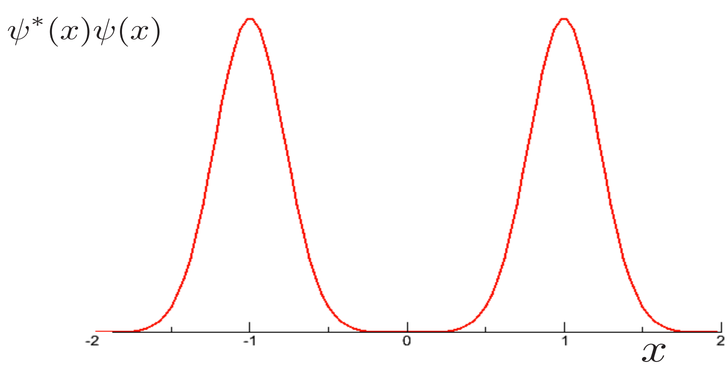
  Also, in classical physics, we have that the momentum of a free particle, $V(x) = 0$, is conserved. In quantum mechanics we have from the Ehrenfest Theorem:

$$\frac{d}{dt}\langle\psi(t)|\hat{p}\,|\psi(t)\rangle \;=\; -\frac{i}{\hbar}\langle\psi(t)|[\hat{p},\hat{H}]\,|\psi(t)\rangle \;=\; -\frac{i}{2m\hbar}\langle\psi(t)|[\hat{p},\hat{p^2}]\,|\psi(t)\rangle \;=\; 0$$

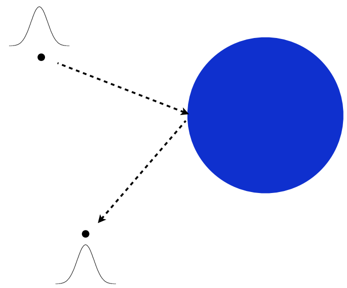
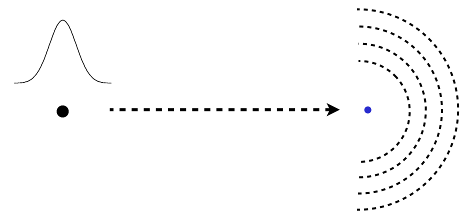
Classical potential

- From the above, we have $\dot{\overline{p}} = \overline{F(x)}$. However, correspondence with a classical situation requires the stronger condition that $\dot{\overline{p}} = F(\overline{x})$. Classically, the particle is located at $\overline{x}$ and the rate of change of momentum is given by the force at that point.

- In general, it is not the case that $\overline{F(x)} = F(\overline{x})$. This is shown by the following simple example. Take the case in which the position probability distribution is a double Gaussian peaked at $x = \pm 1$ while $F(x) = x^2$. Here, $\overline{x} = 0$ and $F(\overline{x}) = F(0) = 0$ with $\overline{F(x)} = \overline{x^2} \neq 0$.



- In order for the particle to behave classically, the feature size of the potential energy must be large compared to the feature size of the particle's wave packet. As shown in the left figure below. Then the particle nature of the wave packet dominates and it scatters off of the potential like a classical particle. If the feature size of the potential energy is small compared to the feature size of the wave packet, the wave nature of the packet dominates and and it scatters off of the potential like a classical wave as shown in the figure to the right. In the intermediate case, the wave packet scattering exhibits both particle and wave-like features.

Cauchy-Schwarz Inequality

- We now need to take a brief mathematical interlude to prove the Cauchy-Schwarz Inequality, a useful inequality of linear algebra. The Cauchy-Schwarz Inequality is based on the Triangle Inequality. We'll first derive these for the case of arrows (real vectors in physical space) and then extend this to the general case of abstract complex vectors.

- We start with the case of arrows. The Triangle Inequality just says that the length of the sum of two sides of a triangle is greater than or equal to the length of the third side. I don't think that I need to prove this to you.

$$|\vec{X}| + |\vec{Y}| \geq |\vec{X} + \vec{Y}|$$

- If we square both sides of the Triangle Inequality we get:

$$|\vec{X}|^2 + |\vec{Y}|^2 + 2|\vec{X}||\vec{Y}| \geq \left|(\vec{X} + \vec{Y}) \cdot (\vec{X} + \vec{Y})\right| = |\vec{X}|^2 + |\vec{Y}|^2 + 2\vec{X} \cdot \vec{Y}$$

$$\Rightarrow \qquad |\vec{X}||\vec{Y}| \geq |\vec{X} \cdot \vec{Y}|$$

This is the Cauchy-Schwarz Inequality for arrows. For arrows, it is obviously true since $|\vec{A}||\vec{B}| \geq |\vec{A}||\vec{B}||\cos\theta|$

- Now we repeat the above for the case of general complex vectors. The Triangle Inequality becomes:

$$\sqrt{\langle X \,|\, X \rangle} + \sqrt{\langle Y \,|\, Y \rangle} \geq \sqrt{\big(\langle X| + \langle Y|\big)\big(\,|X\rangle + |Y\rangle\big)}$$

- We then square this and get the Cauchy-Schwarz Inequality as above:

$$\langle X \,|\, X \rangle + \langle Y \,|\, Y \rangle + 2\sqrt{\langle X \,|\, X \rangle \langle Y \,|\, Y \rangle} \geq \left|\big(\langle X| + \langle Y|\big)\big(\,|X\rangle + |Y\rangle\big)\right|$$

$$= \langle X \,|\, X \rangle + \langle Y \,|\, Y \rangle + \langle X \,|\, Y \rangle + \langle Y \,|\, X \rangle$$

$$\Rightarrow \quad \sqrt{\langle X \,|\, X \rangle \langle Y \,|\, Y \rangle} \geq \frac{1}{2}\left|\,\langle X \,|\, Y \rangle + \langle Y \,|\, X \rangle\right|$$

This is the Cauchy-Schwarz Inequality for a general complex vector space.

The Uncertainty Relation

- The standard deviation of a probability distribution is defined as:

$$\sigma_x^2 \;\equiv\; \overline{(x-\overline{x})^2} \;=\; \sum_i (x_i - \overline{x})^2 P(x_i) \;=\; \sum_i x_i^2 P(x_i) - 2\overline{x}\sum_i P(x_i) + \overline{x}^2 \sum_i P(x_i)$$

$$= \sum_i x_i^2 P(x_i) \;-\; \overline{x}^2 \;=\; \overline{x^2} \;-\; \overline{x}^2$$

- In a homework problem, using the Cauchy-Schwarz Inequality with $|X\rangle \equiv \hat{A}\,|\psi\rangle$ and $|Y\rangle \equiv i\hat{B}\,|\psi\rangle$, you showed that for any two Hermitian operators $\hat{A}$ and $\hat{B}$, we have:

$$\sigma_A \sigma_B \;\geq\; \frac{1}{2}\left|\langle\psi|\,[\hat{A},\hat{B}]\,|\psi\rangle\right|$$

- In the specific case of the operators $\hat{x}$ and $\hat{p}$, this gives the well know **Heisenberg Uncertainty Principle**:

$$\sigma_x \sigma_p \;\geq\; \frac{1}{2}\left|\langle\psi|\,[\hat{x},\hat{p}]\,|\psi\rangle\right| \;=\; \frac{\hbar}{2}$$

- You also showed in a homework problem that for Gaussian distributions the inequality is saturated and we have equality:

$$\sigma_x \sigma_p \;=\; \frac{\hbar}{2}$$

- For any distribution other than Gaussian:

$$\sigma_x \sigma_p \;>\; \frac{\hbar}{2}$$