Intermediate Quantum Mechanics
Lecture 8 Notes (2/16/15)
The Schrodinger Equation

Time evolution in classical physics

- In classical physics, the state of a particle is specified by giving its position and momentum. The particle state then evolves in time according to Newton's Law, $F = -\dfrac{dV(x)}{dx}$.
- Once the state is specified and the Hamiltonian (potential energy, $V(x)$) is known, the state of the particle for all times both future and past is uniquely determined. The state of the system traces out a trajectory in phase space.
- Classical physics is reversible, if the direction of time is changed, the system will retrace the trajectory that it followed. We know where the system came from. This is summarized by saying that information is conserved.
- Two systems that are in distinct states (different positions and/or momenta) remain in distinct states. Two phase space trajectories never cross.

Conservation of inner product

- In correspondence with the situation in classical physics, a postulate of quantum mechanics is that the inner product of two states remains invariant (constant) with time.
$$\langle \phi(t) \,|\, \psi(t) \,\rangle \;=\; \langle \phi(0) \,|\, \psi(0) \,\rangle$$
This means that if two systems are in orthogonal states, then they are always in orthogonal states:
$$\langle \phi(0) \,|\, \psi(0) \,\rangle \;=\; 0 \qquad \Rightarrow \qquad \langle \phi(t) \,|\, \psi(t) \,\rangle \;=\; 0$$
and if a system is in a state normalized to one it is always in a state normalized to one.
$$\langle \psi(0) \,|\, \psi(0) \,\rangle \;=\; 1 \qquad \Rightarrow \qquad \langle \psi(t) \,|\, \psi(t) \,\rangle \;=\; 1$$
- This means that, just as in classical physics, if two systems are in distinct states they will always be in distinct states.

Unitary operators

- The state of a system at time t is given by the time translation operator, $\hat{U}(t)$, that translates the system from a state $|\psi(0)\rangle$ at time $t = 0$ to the state $|\psi(t)\rangle$ at time t.
$$|\psi(t)\rangle \;=\; \hat{U}(t)\,|\psi(0)\rangle$$

- The bra state $\langle\psi(t)|$ is then given by:

$$\langle\psi(t)| \;=\; \langle\psi(0)|\hat{U}^\dagger(t)$$

- Using the postulate that the inner product remain constant, we have:

$$\langle\phi(t)\,|\,\psi(t)\,\rangle \;=\; \langle\phi(0)|\hat{U}^\dagger(t)\hat{U}(t)\,|\psi(0)\rangle \;=\; \langle\phi(0)\,|\,\psi(0)\,\rangle$$

This requires that:

$$\hat{U}^\dagger(t)\hat{U}(t) \;=\; \hat{I} \qquad \text{or} \qquad \hat{U}^\dagger(t) \;=\; \hat{U}^{-1}(t)$$

- An operator with this property is called a **unitary** operator. Note that it is not Hermitian.

The time dependent Schrodinger Equation

- Another postulate of quantum mechanics is that $\hat{U}(t)$ is a linear operator. All attempts to formulate quantum mechanics with non-linear operators have failed completely.
- We must have that if $t = 0$ the time translation does nothing: $\hat{U}(0) = \hat{I}$
- We also have that, since $\hat{U}(t)$ is linear, for an infinitesimal time $t = \epsilon$, the lowest order term is proportional to ϵ. This gives to lowest order in ϵ:

$$\hat{U}(\epsilon) \;=\; \hat{I} - \frac{i\epsilon}{\hbar}\,\hat{H}$$

where we have intentionally taken the factor of $-i/\hbar$ out of the operator $\hat{H}$ for reasons that you will soon see.

- The operator $\hat{H}$ is Hermitian.

$$\hat{I} \;=\; \hat{U}^\dagger(\epsilon)\hat{U}(\epsilon) \;=\; \left(\hat{I} + \frac{i\epsilon}{\hbar}\,\hat{H}^\dagger\right)\left(\hat{I} - \frac{i\epsilon}{\hbar}\,\hat{H}\right) \;=\; \hat{I} + \frac{i}{\hbar}\,(\hat{H}^\dagger - \hat{H})$$

$$\Rightarrow \qquad \hat{H}^\dagger - \hat{H} \;=\; 0 \qquad \Rightarrow \qquad \hat{H}^\dagger \;=\; \hat{H}$$

- The Hermitian operator $\hat{H}$ is said to be the **generator** of time translations. We'll see later other examples of this. The position operator is the generator of space translations and the angular momentum operator is the generator of angular translations (rotations).
- We can now derive the Schrodinger equation, the equation that gives the dynamics and plays the role in quantum mechanics that Newton's Law, $F = ma$, plays in classical physics.

$$|\psi(t+\epsilon)\rangle \;=\; \left(\hat{I} - \frac{i\epsilon}{\hbar}\,\hat{H}\right)|\psi(t)\rangle \;=\; |\psi(t)\rangle \;-\; \frac{i\epsilon}{\hbar}\,\hat{H}\,|\psi(t)\rangle$$

$$|\psi(t+\epsilon)\rangle - |\psi(t)\rangle \;=\; -\frac{i\epsilon}{\hbar}\,\hat{H}\,|\psi(t)\rangle \qquad \Rightarrow \qquad \frac{|\psi(t+\epsilon)\rangle \;-\; |\psi(t)\rangle}{\epsilon} \;=\; -\frac{i}{\hbar}\,\hat{H}\,|\psi(t)\rangle$$

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

- Previously, I told you that the above Schrodinger equation was one of the postulates of quantum mechanics. Actually, I lied a bit. The postulates are that the inner product is conserved $\langle\phi(t)\,|\,\psi(t)\,\rangle \;=\; \langle\phi(0)\,|\,\psi(0)\,\rangle$ and that $\hat{U}(t)$ is a linear operator. The Schrodinger equation then follows from these two postulates.