Intermediate Quantum Mechanics Lecture 6 Notes (2/9/15) Particle on a line

Particle on a line

- We have described the spin state of an electron. We'll now discuss the spatial state of a particle on a line. In order to completely describe the state of an electron, both its spin state and spatial state must be given.
- The state of a classical particle on a line is specified by giving it position and its momentum. The time evolution of the particle is then obtained by giving the position and momentum as a function of time, x(t) and p(t). This describes a trajectory in phase space. In quantum mechanics, the state of a particle on a line is very, very different.

Particle on a lattice

• We'll start by describing the state of a particle in terms of discreet positions. That is, the particle can only be at points 1, 2, etc. where the total number of points is n. We'll take the case that the particle only lives between x = -L/2 and x = L/2 on a line of length L. We can later take L to be infinity if we like.

$$|1\rangle |2\rangle |3\rangle |i\rangle |n\rangle \\ -L/2 \overleftarrow{\Delta L} X L/2$$

• We'll take as the basis vectors the *n* states $|1\rangle$, $|2\rangle$, ..., $|n\rangle$ where $|i\rangle$ is the state corresponding to the particle being at point *i*. We can then express any state $|\psi\rangle$ as a linear superposition of these states:

$$|\psi\rangle = \psi_1 |1\rangle + \psi_2 |2\rangle + \dots + \psi_n |n\rangle = \sum_i \psi_i |i\rangle$$

where the ψ_i 's are complex numbers.

• The basis vectors are orthonormal and satisfy the completeness relation.

$$\langle i \, | \, j \,
angle \; = \; \delta_{ij} \qquad \qquad \sum_i \; |i
angle \langle i | \; = \; \hat{I}$$

• The components of $|\psi\rangle$ in this basis are given by:

$$\psi_{i} = \langle i | \psi \rangle \qquad \qquad |\psi\rangle = \sum_{i} |i\rangle \langle i | \psi \rangle$$

• The norm of $|\psi\rangle$ is given by:

$$\langle \psi | \psi \rangle = \sum_{i} \langle \psi | i \rangle \langle i | \psi \rangle = \sum_{i} \psi_{i}^{*} \psi_{i} = 1$$

where $\psi_i^* \psi_i$ is the probability for the particle to be in state $|i\rangle$.

• The inner product of the two states $|\phi\rangle$ and $|\psi\rangle$ is given by:

$$\langle \phi \, | \, \psi \, \rangle \; = \; \sum_i \phi_i^* \psi_i$$

• Formally, what we have here is just a generalization of the 2-dimensional vector space of spin to an *n*-dimensional vector space. The basis state $|i\rangle$ can be represented as an *n*-component column matrix and $|\psi\rangle$ is represented in this basis by the components ψ_i .

$$|i\rangle = \begin{pmatrix} 0\\0\\\cdot\\\cdot\\\cdot\\1\\\cdot\\\cdot\\0 \end{pmatrix} \qquad |\psi\rangle = \begin{pmatrix} \psi_1\\\psi_2\\\cdot\\\cdot\\\cdot\\\cdot\\\psi_i\\\cdot\\\cdot\\\cdot\\\psi_i\\\cdot\\\cdot\\\psi_n \end{pmatrix}$$

Continuous distribution in x

- We would now like to extend this to the case in which the particle is distributed continuously in x. In order to do this, we need to change the sum over i into an integral over dx. That requires making a couple of redefinitions.
- In the discreet case, there are *n* points distributed uniformly over a line of length L. The separation between points is: $\Delta L = L/n$. We want to go to the limit where $n \to \infty$ and ΔL goes to the infinitesimal length dx. We first need to get a ΔL factor in the discreet case sums so that we can take $\Delta L \to dx$.
- First consider the expression for the norm of $|\psi\rangle$. We define:

$$\psi(x_i) \equiv \frac{\psi_i}{\sqrt{\Delta L}}$$

$$\langle \psi | \psi \rangle = \sum_{i} \psi_{i}^{*} \psi_{i} = \sum_{i} \psi^{*}(x_{i}) \psi^{*}(x_{i}) \Delta L \longrightarrow \int \psi^{*}(x') \psi^{*}(x') \, dx' = 1$$

• In the expression for $|\psi\rangle$, we define $|x_i\rangle \equiv \frac{|i\rangle}{\sqrt{\Delta L}}$.

$$|\psi\rangle = \sum_{i} \psi_{i} |i\rangle = \sum_{i} \psi(x_{i}) |x_{i}\rangle \Delta L \longrightarrow \int \psi(x') |x'\rangle dx'$$

• The completeness relation becomes:

$$\sum_{i} |i\rangle\langle i| = \sum_{i} |x_i\rangle\langle x_i|\Delta L \longrightarrow \int |x'\rangle\langle x'| \, dx' = \hat{I}$$

• The inner product of the two states $|\phi\rangle$ and $|\psi\rangle$ is given by:

$$\langle \phi | \psi \rangle = \int \phi^*(x')\psi(x') \, dx'$$

• All seems to be in order except that the base states $|x\rangle$ are not normalized:

$$\langle x_i | x_j \rangle = \frac{\delta_{ij}}{\Delta L} \longrightarrow \delta(x_i - x_j)$$

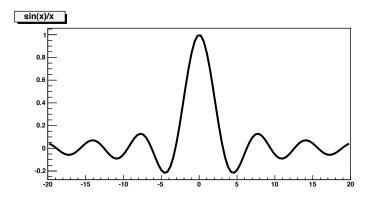
where $\delta(x_i - x_j)$, called the Dirac delta function, is zero if $x_i \neq x_j$ and is infinite (or undefined) when $x_i = x_j$. This means that the basis states $|x\rangle$ are not physically allowed states. That's alight. The basis states don't have to be physical states as long as the physical states $|\psi\rangle$, can be properly normalized, $\langle \psi | \psi \rangle = 1$.

The Dirac δ function

- Paul Dirac invented the δ -function in the 1920's while formulating quantum mechanics in terms of bra and ket vectors as we've been doing. The mathematicians, at the time, were very concerned. The δ -function was nothing like what they would consider a sensible (analytic) function and they thought that Dirac and other physicists were being inexcusably sloppy. Did Dirac and other physicists care? Probably not. As long as they were able to develop a theory that correctly described nature, they were happy. The theory could later be shown to be rigorous or maybe the mathematicians would do it for them.
- In fact in the 1930's and 1940's, motivated in large part in response to the work of Dirac, mathematicians developed distribution theory that among other things showed that the concept of the δ -function could be made rigorous. More correctly, the δ -function is a functionals or distribution. It acts on a function (vector) yielding a scalar, as shown below.
- We can think of the δ -function as the limit of a rectangular function of width ΔL and height $1/\Delta L$. As $\Delta L \to 0$, the function will become infinitesimally thin and infinitely high while the area under the function $(1/\Delta L)\Delta L$ remains equal to 1.
- More specifically, as noted in the homework, the δ -function can be written as:

$$\delta(x) = \lim_{K \to \infty} \left(\frac{\sin Kx}{\pi x} \right) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk$$

The function $\frac{\sin Kx}{x}$ has value K at x = 0 and first zero's at $x = \pm \pi/K$. So, as K becomes larger, it grows in height and becomes narrower. A plot of the function for K = 1 $\frac{\sin x}{x}$ is shown here.



• The important equations involving the δ -function are:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} \, dk \qquad \int \delta(x' - x_0) \, dx' = 1 \qquad \int f(x') \delta(x' - x_0) \, dx' = f(x_0)$$