Continuous quantum states, Particle on a line and Uncertainty relations

So far we have considered k-level (discrete) quantum systems. Now we turn our attention to continuous quantum systems, such as a particle on a line, which can be in any of an infinite number of classical states. The quantum state of this system is a superposition over all possible positions of the particle. Let us denote by $\psi(x)$ the amplitude with which the particle is at point x. We want ψ to represent a unit vector, now in an infinite dimensional Hilbert space. This is expressed by the condition $\int |\psi(x)|^2 dx = 1$. The operator that measures the position of the particle is denoted by X, and operates on $\psi(x)$ by $X\psi(x) = x\psi(x)$. We now turn to the dynamics of a free particle on a line. i.e. we wish to study how $\psi(x)$ evolves as a function of time t. Let us denote by $\psi(x,t)$ the amplitude with which the particle is at position x at time t. Schrödinger's equation for this situation says:

$$i\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}.$$

Let us try to intuitively understand the form of Schrodinger's equation in this case. Intuitively, Schrodinger's equation says that the change in amplitude at each point x is proportional to the difference between the amplitude $\psi(x)$ at x, and the average amplitude in its infitesimal local neighborhood $\phi(x) = \frac{\psi(x+\delta x)+\psi(x-\delta x)}{2}$. Thus each point may be thought of as locally looking right and left and comparing its amplitude to the average amplitude in its infinitesimal neighborhood. To maintain unitary evolution, the change is orthogonal to the current amplitude — this is reflected in the appearance of $i = \sqrt{-1}$ in Schrodinger's equation. But wait a minute, why is the change proportional to the second derivative with respect to x, rather than the first derivative. After all each point x is comparing its value to the average of its neighbors. Make sure that you understand why this corresponds to the second derivative.

the Hamiltonian operator $H = \partial^2/\partial x^2$, so Schrodinger's equation reads

Now let us try to understand what the velocity of this particle is? Schrodinger's equation tells us given the current superposition of locations for the particle, what the new superposition is after δt time. How do we determine the velocity of the particle? The difficulty is that the superpoition at time t only determines the probability distribution specifying the location of the particle, and as the superposition evolves, it specifies a new probability distribution at time $t+\delta t$. The difficulty is that part of the distribution might seem to spread left while part might seem to spread right. So there does not seem to be a unique velocity we can ascribe to the particle. Here is a way out of this difficulty:

Suppose we were to consider $\psi(x) = e^{ikx}$, then applying Schrodinger's equation to this just makes every point rotate in phase. This is just like rotating a slinky - which makes it seem to translate with a definite velocity. In this case the velocity would be $\sim k$. It follows that the amplitude with which an arbitrary state ϕ has velosity k is given by

$$\langle \psi | \phi \rangle = \langle e^{ikx} | \phi \rangle = \int_{-\infty}^{\infty} e^{ikx}\phi(x,t)dx.$$

This is similar to the Fourier transform of the wavefunction, that is, we can describe another wavefunction in velocity space as the F.T. of the position wave function:

$$\hat{\phi}(k,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\phi(x,t)dx.$$

1 Uncertainty Relations

The position-momementum uncertainty relation for a particle in 1-dimension is a consequence of this fourier transform relationship between the position and velocity of the particle. The point is that if we try to completely localize the particle's position, then its velocity is the Fourier transform of the delta function and is therefore maximally uncertain. Conversely if the particle has a definite velocity then its position is maximally uncertain. How best can we localize both position and velocity? This depends upon our measure of spread. One convenient measure is the standard deviation. For this measure, one can show that the product of the standard deviations of position and velocity occurs when both superpositions are Gaussian (the Fourier transform of a Gaussian is another Gaussian), and this gives us the uncertainty relation: $\Delta x \Delta v \geq \hbar/2$.

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2 Heisenberg uncertainty relations

As we discussed in previous sections, when two observables do not commute, in general we cannot know the value of both of them simultaneously. For example, if A and B do not commute, there are states $|\Psi\rangle$ that are eigenstates of A (and therefore A is known with certainty), but are not eigenstates of B (hence B is not known with certainty). Of course, the most detailed description of how much we know about A and B in an arbitrary state $|\Psi\rangle$ is to give the probability distributions $P(A = a)$ for a measurement of A to yield the eigenvalue a and $P(B = b)$ for a measurement of B to yield the eigenvalue b when the quantum system is in the state $|\Psi\rangle$. Many times however, such detailed information is not necessary, and is difficult to manipulate; one would rather use some simpler indicators. The most famous such indicators are the so called *uncertainty relations* that describe constraints on the simultaneous *spread* of the values of two observables.

For every observable A the spread ΔA in the state $|\Psi\rangle$ is defined as

$$\Delta A = \sqrt{\langle\Psi|A^2|\Psi\rangle - \langle\Psi|A|\Psi\rangle^2} = \sqrt{\bar{A^2} - (\bar{A})^2}. \tag{1}$$

The uncertainty relations tell that in any state $|\Psi\rangle$ the spreads of two observables A and B are constrained such that

$$\Delta A \Delta B \geq \frac{1}{2}\left|\langle\Psi|[A,B]|\Psi\rangle\right| \tag{2}$$

where $[A,B] = AB - BA$ is the commutator of A and B.

The most well-known and widely used of the uncertainty relations, the Heisenberg's uncertainty relations refer to position and momentum. Since the commutator of x and p is a just a constant, $[x, p] = i\hbar$, the uncertainty relation is

$$\Delta x \Delta p \geq \frac{1}{2}\hbar. \tag{3}$$

(Note that here the bound is independent of the state $|\Psi\rangle$, unlike in the general case (2).)

Let us now prove the uncertainty relations (2). By direct computation it is easy to see that

$$(\Delta A)^2 = \langle\Psi|(A - \bar{A})^2|\Psi\rangle \tag{4}$$

Indeed,

$$\langle\Psi|(A - \bar{A})^2|\Psi\rangle = \langle\Psi|A^2 - 2A\bar{A} + (\bar{A})^2|\Psi\rangle \tag{5}$$

$$= \bar{A^2} - 2\bar{A}\bar{A} + (\bar{A})^2 = \bar{A^2} - (\bar{A})^2 \tag{6}$$

Hence

$$(\Delta A)^2(\Delta B)^2 = \langle\Psi|(A-\bar{A})^2|\Psi\rangle\langle\Psi|(B-\bar{B})^2|\Psi\rangle = \tag{7}$$

$$\langle(A-\bar{A})\Psi|(A-\bar{A})\Psi\rangle\langle(B-\bar{B})\Psi|(B-\bar{B})\Psi\rangle \tag{8}$$

Now, the Schwartz inequality states that for any two (not necessarily normalized) states $|\Phi\rangle$ and $|\Theta\rangle$,

$$|\langle\Theta|\Phi\rangle|^2 \leq \langle\Theta|\Theta\rangle\langle\Phi|\Phi\rangle \tag{9}$$

Choosing $|\Theta\rangle = |(A-\bar{A})\Psi\rangle$ and $|\Phi\rangle = |(B-\bar{B})\Psi\rangle$ we obtain

$$(\Delta A)^2(\Delta B)^2 \geq |\langle(A-\bar{A})\Psi|(B-\bar{B})\Psi\rangle|^2 = \tag{10}$$

$$|\langle\Psi(A-\bar{A})(B-\bar{B})|\Psi\rangle|^2 \tag{11}$$

Writing $AB = \frac{1}{2}(AB+BA)+(AB-BA)$ and noting that for Hermitian matrices the anticommutator $[A,B]_+ = AB+BA$ has real eigenvalues and the commutator $[A,B] = AB-BA$ has purely imaginary eigenvalues, we obtain

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\left|\langle\Psi|[A-\bar{A},B-\bar{B}]_+|\Psi\rangle\right|^2 + \tag{12}$$

$$\frac{1}{4}\left|\langle\Psi|[A-\bar{A},B-\bar{B}]|\Psi\rangle\right|^2 \tag{13}$$

Finally, since $[A-\bar{A},B-\bar{B}] = [A,B]$ we obtain the uncertainty relations

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\left|\langle\Psi|[A-\bar{A},B-\bar{B}]_+|\Psi\rangle\right|^2 + \frac{1}{4}\left|\langle\Psi|[A,B]|\Psi\rangle\right|^2 \tag{14}$$

Note that the uncertainty relations (14) are in fact stronger than the relations (2) mentioned at the start of this section. To go from (14) to (2) we simply drop the anticommutator term. The reason why (2) are almost universally used in literature instead of (14) is that they are simpler and easier to interpret. The anticommutator has however important physical significance related to correlations between A and B, but we will not address this issue here.

Now that we proved the uncertainty relations, we should try an understand their significance. The main message of Heisenberg's uncertainty relations is that there is no quantum state in which both the position and the momentum are perfectly well defined, i.e. no state is such that if we measure the position we obtain with certainty some value x_0 and if instead we measure the momentum we obtain with certainty some value p_0. This is one of the most fundamental differences between classical and quantum physics.

Another consequence of Heisenberg's uncertainty relations is that measurements of position will, in general, disturb the momentum and vice-versa. Indeed, consider an arbitrary state $|\Psi\rangle$ which has a finite spread of momentum, $\Delta p = \Delta < \infty$. Suppose now that we measure the position with a precision δ. Following this measurement the state of the particle will change to $|\Psi'\rangle$ which is such that the spread of position is $\Delta' x = \delta$

- we simply know now the position with precision δ. But suppose that we make the position measurement with high enough precision so that $\delta\Delta < \frac{1}{2}\hbar$. In that case the momentum of the particle must have been changed by the measurement of position. Indeed, had the momentum not changed, its spread would still be $\Delta' p = \Delta p = \Delta$ and the new state would violate Heisenberg's uncertainty relations.

Heisenberg's uncertainty relations are very useful and have been used extensively to obtain insight into various physical processes. It is very important however to note that while these uncertainty relations are obviously extremely important, their implications are in a certain sense, quite limited.

A common mistake is to think that what H's uncertainty relations say is that if we measure position (and thus reduce Δx, then we necessarily must disturb the momentum and increase Δp. This is not the case in general. Obviously, when the state is such that

$$\Delta x \Delta p = \frac{1}{2}\hbar \tag{15}$$

then any perturbation of the state that diminishes the spread in position must be accompanied by an increase of the spread in momentum, otherwise the new state will violate Heisenberg's uncertainty relation (3). On the other hand, for a state such that

$$\Delta x \Delta p >> \frac{1}{2}\hbar \tag{16}$$

it is possible to perturb the state and decrease *both* the spread in position and the spread in momentum.

More generally, Heisenberg's uncertainty relation (3) plays a significant role (i.e. places constraints on what happens to the state) only in situations in which

$$\Delta x \Delta p \gtrapprox \frac{1}{2}\hbar. \tag{17}$$

Such situations are those that are very close to classical, i.e. gaussian wave-packets in which we try to define both the position and the momentum as well as possible. Then H's uncertainty relation simply says that there is a limit on how close to classical a quantum situation can be.

There are many interesting situations in which H's uncertainties give a quick, intuitive understanding of what is happening. A very important example is understanding the finite size of atoms (see Feynman). Consider the hydrogen atom. Classically the electron would just fall onto the proton because this leads to minimal energy. Quantum mechanically however if the electron gets closer to the proton to minimize the potential energy, it will have larger kinetic energy because as the spread in position becomes smaller the spread in momentum increases. Therefore there is some optimum size for which the sum of kinetic and potential energy is minimal. (***add more quantitative results here***)

On a more general note, we observe that the uncertainty relations involve the spreads ΔA and ΔB. It is therefore clear that they can be significant only in situations in which the probability distributions $P(A = a)$ and $P(B = b)$ are strongly peaked, (such as gaussian distributions). Only in such simple situations averages and spreads are good ways to characterize the distributions. On the other hand, in the real interesting quantum situations, meaning in situations which are far from classical, the probability distributions are not so simple. For example, consider the two slits experiment which arguably encapsulates the essence of quantum behavior. When the particle just passed the screen with the two slits, the wavefunction $\Psi(x)$ has two peaks, one for each slit. In this case the spreads of both x and p are large (16) and the inequality doesn't effectively play any role. In such situations, to try to get an understanding by looking at these inequalities is, in the best case useless and in the worst case misleading. We will discuss the connection between the two slits experiment and Heisenberg's uncertainty relations in section (?).

Finally, we note some interesting differences between observables related to systems with Hilbert spaces of finite dimension, such as qubits, and *unbounded* observables related systems with infinite dimesional Hil;bert spaces, such as the position and momentum. It is a small mathematical "paradox". Consider first a finite dimensional system. Suppose that the state $|\Psi\rangle$ is an eigenstate of A corresponding to the eigenvalue a, that is, $A|\Psi\rangle = a\Psi\rangle$. In that case, the average value of the commutator of A and B, (the right hand side of the uncertainty relation (2) is zero. Indeed,

$$\langle\Psi|[A,B]|\Psi\rangle = \langle\Psi|AB - BA|\Psi\rangle =$$

$$a\langle\Psi|B|\Psi\rangle - \langle\Psi|B|\Psi\rangle a = 0 \tag{18}$$

. Hence in this case the uncertainty relation useless. On the other hand, consider an eigenstate of x. Applying the same argument as above, we could conclude that

$$\langle\Psi|[x,p]|\Psi\rangle = \langle\Psi|xp - pAx|\Psi\rangle =$$

$$x\langle\Psi|p|\Psi\rangle - \langle\Psi|p|\Psi\rangle x = 0. \tag{19}$$

But the commutator $[x,p] = i\hbar$ so we could also conclude that

$$\langle\Psi|[x,p]|\Psi\rangle = i\hbar\langle\Psi||\Psi\rangle = i\hbar, \tag{20}$$

contradicting (18). The correct answer is (20) as it can be seen by using the explicit representations of the position and momentum representation, for example their x-representation x and $-i\frac{d}{dx}$. Of course, the point is that teh eigestates corresponding to unbounded observables such as x and p are non-normalizable states, as described in detail in section (?), so we cannot naively use them, such as in (19). Rather we need to use normalizable states and make take the correct limits.