Chapter 4

Continuous Quantum States

4.1 Continuous Quantum States

We must now expand our notion of Hilbert space, since the dimension (ie. number of basis states) runs to infinity. A continuous obserable, such as position x, must be represented by an infinite-dimensional matrix

$$\hat{x} = \begin{pmatrix} x_1 & 0 & \cdots & 0 \\ 0 & x_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_\infty \end{pmatrix}$$

where $\mathbf{x}_j$ denotes all possible positions on a line and we take the limit where j becomes a continuous variable. If the particle is sitting at a known position, x_p, then its state, $|\psi\rangle$, can be represented in the position-basis by the infinite-dimesional vector

$$|\psi\rangle = |x_p\rangle = (0, 0, \ldots, 0, 1, 0, \ldots, 0, 0),$$

where only the p^{th} position is nonzero. Of course, the particle's state might alternatively be composed of an arbitrary superposition of position states:

$$|\psi\rangle = a_0 \, |x_0\rangle + a_1 \, |x_1\rangle + \cdots$$

where $|a_0|^2 + |a_1|^2 + \cdots = 1$.

As you can imagine, the matrix/vector notation becomes extremely awkward at this point as we attempt to cope with an infinite number of infinitesimally-spaced basis states. A common "fix" for this problem is as follows: Suppose the particle's state, $|\psi\rangle$ is some arbitrary superposition of infinitesimally-spaced position eigenstates. We now ask, "What is the quantum amplitude for the particle to lie at an arbitrary position, x, represented by the position eigenstate, $|x\rangle$?" The answer is the inner product, $\langle x|\psi\rangle$. Since x is a continuous variable, this inner product is a continuous function of x. For the sake of convenience, we define this continuous function as $\psi(x) = \langle x|\psi\rangle$.

Rather than struggling to tediously write down infinite superpositions of infinitesimally-spaced basis states, we simply represent the state of a particle in a continuous basis with the compact, continuous inner-product function, $\psi(x)$. This contains all of the complex information of the infinite-dimensional superposition of states. Since $|\psi\rangle$ is a unit vector in an infinite-dimensional Hilbert space, then $\psi(x)$ must satisfy the condition,

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} \langle\psi|x\rangle \langle x|\psi\rangle \, dx = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$$

The operator that represents position, X, now operates on the inner product, $\psi(x)$, to yield the eigenvalue equation

$$X\psi(x) = x\psi(x),$$

where x is a scalar.

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 for the particle to be at position x at time t. Schrödinger's equation for this situation says:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t)$$

where H is the Hamiltonian, or energy operator for a particle that can move in one dimension. To move foraward we must determine what the Hailtonian is for a particla that can move continuously in one dimension Calssically the energy is well defined in terms of the momentum, p, and position, x, of the particle,

$$E(p,x) = \frac{p^2}{2m} + V(x)$$

Here, $p^2/2m$ is the kinetic energy of the particle and $V(x)$ is the classical potential energy of the particle when it sits at position x. The form of $V(x)$ varies depending upon what interactions the particle is subjected to. Translating the classical energy function, $E(p,x)$ in to a quantum mechanical energy operator, H, is not an obvious procedure. To do this we will rely on an axiom of quantum mechanics that we will try to justify (but *not* derive) later on.

Axiom: If the classical energy operator for a system is $E(p, x)$, then the quantum mechanical Hamiltonian can be written as $H = E(\hat{p}, \hat{x})$, where $\hat{p}$ and $\hat{x}$ are the quantum mechanical momentum and position operators, respectively. In the position basis, the $\hat{x}$ operator is simply the function x, whereas the $\hat{p}$ operator is $\hat{p} = -i\hbar\partial/\partial x$.

For a free particle with mass, m that is moving in one dimension then

$$H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}.$$

Notice that $V(x) = 0$ because the particle is free. It is then straightforward to obtain the stationary state energy enigenstates by solving the time-independent Schrödinger equation,

$$H\psi(x) = E\psi(x) \qquad \longrightarrow \qquad -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x)$$

The solutions of this equation yield the (unnormalized) free particle eigenstates,

$$\psi_k(x) = e^{ikx},$$

where $k = \sqrt{2mE}/\hbar$. In order to include time evolution in our solution then we must solve the full time-dependent Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$

To intuitively understand the form of Schrödinger's equation in this situation, the following naive discussion might be helpful. 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 $\phi(x) = \frac{\psi(x+\delta x)+\psi(x-\delta x)}{2}$ (since $\frac{\partial\Psi}{\partial t} \propto i\frac{\partial\Psi^2}{\partial x^2}$ and $\frac{\partial\Psi^2}{\partial x^2} \propto (\Psi(x) - \Phi(x)))$. 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. The wave function will not change in time unless $\Psi(x)$ exhibits actual curvature. To intuitively understand why this is a Hermitian operator, you might find it helpful to write down what this operator looks like in the discrete approximation we introduced above.

One might ask, what is the velocity of a particle in quantum mechanics? Schrödinger'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 superposition 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 spread left while part might spread right. So there is not always a unique velocity we can ascribe to the particle. Part of the problem is semantics related, and depends on how one defines velocity. If velocity is defined as the time rate of change of the position expectation value, $v = \frac{d\langle x\rangle}{dt}$, then we see that it leads to nonsensical results. The simple case of a free particle moving through space with well defined momentum, $\hbar k$, where $\psi_k(x,t) = A\exp\left(i\left(kx - \omega t\right)\right)$, since there is no well defined position. On the other hand, if a partical is defined by highly localized wavepacket moving though space (such as $\psi(x,y) = A\exp\left(-\left(x - vt\right)^2\right)$), then one might reasonably speak of the particles velocity.

In quantum mechanics, we tend to sidestep this problem by focusing more on the momentum of a particle. The idea is that even if we don't know the location of a particle, and do not know it's actual trajectory, we can still know the magnitude and direction of its momentum. Momentum is thus a primary observable in quantum mechanics with a well-defined operator, $\hat{p} = -i\hbar\vec{\nabla}$, and eigenstates, $\psi(x) = \exp\left(i\vec{k}\cdot\vec{x}\right)$. The momentum of electrons is commonly measured in angle-resolved photoionization experiments that use electrostatic deflection techniques to steer electrons having particular momentum towards a detector. Even if a particle is in a state, $\psi(\vec{x},t)$, that is not a momentum eigenstate, one can still ask the question, "What is the amplitude that this particle has a momentum $\vec{k}$?". The answer here is simple the overlap of $\psi(\vec{x},t)$ with the $\vec{k}$ momentum eigenstate, $\psi_k(x) = e^{i\vec{k}\cdot\vec{x}}$. Because the momentum eigenstates are complete (they span the Hilbert space of continuous functions), it is then reasonable to define the momentum space wavefunction our state (as opposed to the position space wavefunction),

$$\tilde{\phi}(k,t) = \frac{1}{\sqrt{2\pi}}\left\langle e^{ikx}|\phi(x,t)\right\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\phi(x,t)dx$$

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 momentum of a particle. The point is that if we try to completely localize the particle's position, then its momentum is the Fourier transform of the delta function and is therefore maximally uncertain. Conversely if the particle has a definite momentum then its position is maximally uncertain. How best can we localize both position and momentum? 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 momentum occurs when both superpositions are Gaussian (the Fourier transform of a Gaussian is another Gaussian), and this gives us the uncertainty relation: $\Delta x \Delta p \geq \hbar/2$.

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

$$\Delta A = \sqrt{\langle\Psi| A^2 |\Psi\rangle - \langle\Psi| A |\Psi\rangle^2} = \sqrt{\bar{A^2} - (\bar{A})^2}. \tag{4.1}$$

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

$$\Delta A \Delta B \geq \frac{1}{2}\big|\langle\Psi| [A, B] |\Psi\rangle\big| \tag{4.2}$$

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

$$\Delta x \Delta p \geq \frac{1}{2}\hbar. \tag{4.3}$$

(Note that here the bound is independent of the state $|\Psi\rangle$, unlike in the general case ((4.2)).)

Let us now prove the uncertainty relations ((4.2)). By direct computation it is easy to see that

$$(\Delta A)^2 = \langle\Psi|\,(A-\bar{A})^2\,|\Psi\rangle \tag{4.4}$$

Indeed,

$$\begin{aligned}\langle\Psi|\,(A-\bar{A})^2\,|\Psi\rangle &= \langle\Psi|A^2 - 2A\bar{A} + (\bar{A})^2\,|\Psi\rangle \\ &= \bar{A}^2 - 2\bar{A}\bar{A} + (\bar{A})^2 \\ &= \bar{A}^2 - (\bar{A})^2\end{aligned}$$

Hence

$$\begin{aligned}&(\Delta A)^2(\Delta B)^2 \\ &\qquad = \langle\Psi|(A-\bar{A})^2\,|\Psi\rangle\,\langle\Psi|(B-\bar{B})^2\,|\Psi\rangle \\ &\qquad = \langle(A-\bar{A})\Psi|(A-\bar{A})\Psi\rangle\langle(B-\bar{B})\Psi|(B-\bar{B})\Psi\rangle\end{aligned}$$

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

$$|\langle\Theta|\Phi\rangle|^2 \leq \langle\Theta|\Theta\rangle\langle\Phi|\Phi\rangle$$

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

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

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

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

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

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\big|\langle\Psi|\,[A-\bar{A},B-\bar{B}]_+\,|\Psi\rangle\big|^2 + \frac{1}{4}\big|\langle\Psi|\,[A,B]\,|\Psi\rangle\big|^2 \tag{4.5}$$

Note that the uncertainty relations ((4.5)) are in fact stronger than the relations ((4.2)) mentioned at the start of this section. To go from ((4.5)) to ((4.2)) we simply drop the anticommutator term. The reason why ((4.2)) are almost universally used in literature instead of ((4.5)) 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

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

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 ((4.3)). On the other hand, for a state such that

$$\Delta x \Delta p >> \frac{1}{2}\hbar \tag{4.6}$$

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 ((4.3)) plays a significant role (i.e. places constraints on what happens to the state) only in situations in which

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

Such situations are those that are very close to classical, i.e. gaussian wavepackets 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 ((4.6)) 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 ((4.2)) is zero. Indeed,

$$\langle\Psi| [A, B] |\Psi\rangle = \langle\Psi| AB - BA |\Psi\rangle =$$
$$a \langle\Psi| B |\Psi\rangle - \langle\Psi| B |\Psi\rangle a = 0 \tag{4.7}$$

. 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

$$\langle\Psi| [x, p] |\Psi\rangle = \langle\Psi| xp - pAx |\Psi\rangle =$$
$$x \langle\Psi| p |\Psi\rangle - \langle\Psi| p |\Psi\rangle x = 0. \tag{4.8}$$

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

$$\langle\Psi| [x, p] |\Psi\rangle = i\hbar \langle\Psi| |\Psi\rangle = i\hbar, \tag{4.9}$$

contradicting ((4.7)). The correct answer is ((4.9)) 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 ((4.8)). Rather we need to use normalizable states and make take the correct limits.

4.2 The Classical Limit

Introduction

If quantum mechanics is to have a chance of being a true theory of nature rather than a simple approximation valid only for microscopic particles, it must be able to describe classical physics when we perform experiments that are in the "classical regime", i.e. when dealing with macroscopic objects and when asking about their simple mechanical properties. The systems studied so far, such as qubits, although they are the simplest quantum systems, are not a good starting point for understanding the classical limit. Indeed, they are genuine quantum systems far from classical objects: there are no classical objects that have only two states - all classical systems have a continuous number of states (they can be located anywhere and have any velocity).

A good place to start enquiring about the classical limit is a free particle. For simplicity we discuss here the case of a particle in 1-dimension. The generalization to 3-d is quite straightforward.

Gaussian Wavepacket

It would be tempting to start by analyzing the movement of a free particle with a well defined momentum. However, if the momentum of a particle is perfectly well defined, i.e. $\Delta p = 0$, then its location is completely undefined, $\Delta x = \infty$. So this is not a good candidate for an approximation of a classical particle. The wave function that is the closest to the classical case is a gaussian wave packet

$$\psi(x, t = 0) = ce^{-\frac{(x-x_0)^2}{2\sigma^2}} e^{\frac{ip_0 x}{\hbar}}$$

Here c is a normalization constant.

This wave packet describes a particle that is localized around $x = x_0$ and momentum $p = p_0$. Both the position probability distribution and the momentum probability distribution are very simple: they each are described by a simple gaussiam peak.

The position probability distribution is:

$$Prob(x, t = 0) = |\psi(x, 0)|^2 = |c|^2 e^{-\frac{(x-x_0)^2}{\sigma^2}}$$

To find the momentum distribution, first recall that the momentum eigenstate wavefunction corresponding to p is $e^{\frac{ipx}{\hbar}}$. Indeed, we may readily check that:

$$\hat{p} e^{\frac{ipx}{\hbar}} = -i\hbar \frac{\partial e^{\frac{ipx}{\hbar}}}{\partial x} = p e^{\frac{ipx}{\hbar}}$$

To find the momentum distribution, we have to write $\psi(x, t)$ in the momentum eigenstates basis:

$$\phi(p, 0) = \int_{-\infty}^{\infty} \psi(x, 0) e^{\frac{ipx}{\hbar}} dx$$

The wavefunction in the momentum eigenstates basis is clearly the fourier transform of $\psi(x, 0)$. It is easy to see that

$$\phi(p, 0) = ce^{-\frac{(p-p_0)^2\sigma^2}{2\hbar^2}} e^{\frac{ix_0 p}{\hbar}}$$

Therefore the momentum probability distribution is:

$$Prob(p, t = 0) = |\phi(p, 0)|^2 = |c|^2 e^{-\frac{(p-p_0)^2\sigma^2}{\hbar^2}}$$

In fact, the gaussian wave-packet is the only wavefunction that reaches the minimal uncertainty $(\Delta x)(\Delta p) = \hbar$.

Time Evolution of the Gaussian wavepacket

The gaussian wavepacket represents a particle initially situated around x_0 and with momentum approximately p_0, hence speed $v_0 = \frac{p_0}{m}$, where m is the mass of the particle. We expect that for a macroscopic particle (i.e. large m) the particle should move with speed v_0 and at time t to arrive at $x_t = x_0 + v_0 t$. In other words, we expect to find the position distribution peaked around $x = x_0 + v_0 t$, and the distribution of momentum still peaked around $p = p_0$. Furthermore, since the initial momentum (and hence speed) is not perfectly defined, we also expect the uncertainty in position to increase. In fact, the uncertainty in speed is

$$(\Delta v) = \frac{(\Delta p)}{m} = \frac{\hbar}{m\sigma}$$

So in time t we expect the uncertainty of x to increase from σ to $\sqrt{\sigma^2 + (\Delta v)^2 t^2} = \sqrt{\sigma^2 + \frac{\hbar^2 t^2}{m^2\sigma^2}}$.

Let us now compute the time evolution. We know how the momentum eigenstates evolve in time. Indeed, momentum p corresponds to energy $E = \frac{p^2}{2m}$. Hence the time evolution is

$$e^{\frac{ipx}{\hbar}} \longrightarrow e^{\frac{ipx}{\hbar}} e^{\frac{-i}{\hbar}\frac{p^2}{2m}t}$$

Hence we can find the time evolution of $\psi(x,t)$ by using its momentum representation and applying the above equation:

$$\psi(x,t) = \int_{-\infty}^{\infty} c e^{-\frac{(p-p_0)^2\sigma^2}{2\hbar}} e^{\frac{ix_0 p}{\hbar}} e^{\frac{ixp}{\hbar}} e^{\frac{-i}{\hbar}\frac{p^2}{2m}t}$$

All we have to do is to compute the integral and see that the wave packet indeed proagates and spreads as predicted above. i.e. the initial spread of the wave packet is σ and it evolves in time to $\sqrt{\sigma^2 + \frac{\hbar^2 t^2}{m^2\sigma^2}}$. The form of this equation is in fact very instructive. It shows that when the mass increases, the spreading of the wavefunction is very slow. Planck's constant gives the scale of the spreading with time.

Consider a particle with mass 1 gram, and initial spread $\sigma = 10^{-10}$ meters, i.e. the size of an atom. Given that Planck's constant is $\hbar \approx 10^{-34} m^2 kg/s$, the time for the spread of the wave-packet to double is approximately $t = 10^{11}$ seconds, which is about 3000 years!

For a mass of 1 gram and $\sigma = 10^{-6}$ meters (1 micron) the time to double the spread is 10^{19} seconds.

4.3 Particle in a Box

Review of Schrodinger equation

Last time we saw that the Schr. Equation determines how the wave function of a particle develops in time:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$

This can be rewritten as:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t)$$

where $\hat{H}$ is an energy operator $\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$.

We saw before that there is a special relationship in QM between the energy of a system and its time development. The Sch. equation can be broken into two pieces if we write ψ as a product: $\psi(x,t) = \psi(x)\phi(t)$. This is called *separation of variables.* Where this gives us:

$$\hat{H}\psi(x) = E\psi(x)$$

and

$$\phi(t) = e^{-iEt/\hbar}$$

$\hat{H}\psi_k(x) = E_k\psi_k(x)$ is a condition that must be satisfied to find the states $\{\psi_k\}$ that well-defined energy $\{E_k\}$.

But what does "well-defined" energy mean? It means two things: (1) A state ψ has well-defined energy if $\hat{H}\psi = C\psi$ where "C" = energy of state. (2) A state ψ has well defined energy if an ensemble (read, many copies) of systems all prepared in the state ψ give the same answer if you measure energy (i.e. E = "C" if $\hat{H}\psi = E\psi$).

Consider, for example, two states ψ_1 and ψ_2 such that $\hat{H}\psi_1 = E_1\psi_2$ and $\hat{H}\psi_2 = E_2\psi_2$. We also required that $E_1 \neq E_2$, which in quantum mechanical language means that the *eigenvalues are non-degenerate.* Suppose I take 10^6 qubits prepared in state ψ_1 and measure their energy and make a histogram. What does the histogram look like? See Figure 1(a).

Now suppose that I prepare 10^6 qubits in the state $\psi' = \sqrt{\frac{3}{5}}\psi_1 + \sqrt{\frac{2}{5}}\psi_2$, measure *their* energies, and make a histogram. How does it look? See Figure 1(b)

Ask yourself, is ψ' a state with well-defined energy? *NO*. Why not? ψ' is not an eigenstate of the Hamiltonian operator. Let's check this:

$$\hat{H}\psi' = \hat{H}\left(\sqrt{\frac{3}{5}}\psi_1 + \sqrt{\frac{2}{5}}\psi_2\right) = \sqrt{\frac{3}{5}}E_1\psi_1 + \sqrt{\frac{2}{5}}E_2\psi_2$$

Does this equal (constant)×(ψ')? No, because as stated E_1 and E_2 are not equal. Therefore ψ' is not an eigenstate of the energy operator and has no well-defined energy.

Time dependence

So how do these states change in time? Suppose $\psi(x, t = 0) = \psi_1(x)$ where $\hat{H}\psi_1 = E_1\psi_1(x)$. What is $\psi(x, t \neq 0)$?

$$\psi(x, t) = \psi_1(x)e^{-iE_1t/\hbar}$$

But what if $\psi(x, t = 0) = \psi' = \sqrt{\frac{3}{5}}\psi_1 + \sqrt{\frac{2}{5}}\psi_2$? What's $\psi(x, t \neq 0)$ in this case?

$$\psi(x, t) = \sqrt{\frac{3}{5}}\psi_1 e^{-iE_1t/\hbar} + \sqrt{\frac{2}{5}}\psi_2 e^{-iE_2t/\hbar}$$

Each piece of the wavefunction with well-defined energy dances to its own little drummer. *It spins at frequency $\propto$ its energy.*

But what if I give you $\psi(x, t = 0) = f(x)$ where $f(x)$ is an arbitrary function? What is $\psi(x, t \neq 0)$ in this case? This strategy is the same. You must solve $\hat{H}\psi_k(x) = E_k\psi_k(x)$ to get the eigenstates $\{\psi_k\}$ and their associated energies $\{E_k\}$. Then, you express $f(x)$ as $f(x) = a_1\psi_1(x)+a_2\psi_2(x)+a_3\psi_3(x)+\cdots$, a linear superposition of the energy eigenstates $\{\psi_k\}$. Note that you must find the overlap: $a_i =< \psi_x|f >$ for this to be meaningful. In position space, this is accomplished by the integral:

$$< \psi_i|f >= \int_{-\infty}^{\infty} \psi_i^*(x)f(x)dx$$

The time dependence is then given by

$$\psi(x, t) = a_1\psi_1(x)e^{-iE_1t/\hbar} + a_2\psi_2(x)e^{-iE_2t/\hbar} + a_3\psi_3(x)e^{-iE_3t/\hbar} + \cdots$$

So time dependence in QM is easy if you know the $\{\psi_k\}$'s. The set $\{\psi_k\}$ forms a special basis. If you write ψ in this base then time dependence is easy!

This is often called the basis of stationary states. Why? Because if $\psi = \psi_i(x)$ where $\hat{H}\psi_i = E_i\psi_i$ then $\psi(x,t) = \psi_i(x)e^{-iE_it/\hbar}$. The probability density $P(x,t)$ is then given by

$$P(x,t) = |\psi(x,t)|^2 = \left(\psi_i(x)e^{-iE_it/\hbar}\right)^* \left(\psi_i(x)e^{-iE_it/\hbar}\right) = |\psi_i(x)|^2$$

Therefore the time dependence for the probability density dropped out and does not change in time.

Particle in a Box

Let's do an example now! Let's consider a situation where we want to use the electrons inside atoms as qubits. How do we describe the physical details of these qubits? What are their allowed energies? How do they change in time? *What do we do???* We solve the Schr. equation, that's what.

As is the case in most QM problems, we must find the Hamiltonian $\hat{H}$. $\hat{H}$ in this case is the energy operator for an electron in an atom. To know this then we must make some assumptions about how electrons behave in an atom.

Let's assume that atoms are very tiny ($\approx 10^{-10}$ meter) 1-D boxes with very hard walls. The walls are located at position $x = 0$ and $x = l$. This model works surprisingly well. Inside the box $\hat{H}$ is given by the free particle Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$. Outside the box we model the very hard walls as regions where the potential energy V $\rightarrow \infty$. This has the effect of *disallowing* any ψ to be nonzero outside the box. If it did exist in this region its energy (obtained, as always, by applying the Hamiltonian) would also go to infinity. That's too much energy for our little electrons, so we can say that we will restrict our wavefunctions $\psi(x)$ to functions which vanish at $x \leq 0$ and $x \geq l$.

$$\psi(x = 0) = \psi(x = l) = 0$$

Strictly speaking, we mean that $\psi(x \leq 0) = \psi(x \geq l) = 0$. We will see that this will allow us to construct wavefunctions which are normalized over our restricted box space $x \in \{0, l\}$. The system as we've described it can be sketched is sketched in Figure 2.

Guessing that $\psi(x) = e^{ikx}$ is an eigenstate of the equation $H\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = E\psi(x)$, we get that the energy $E = \frac{\hbar^2k^2}{2m}$. It follows that we have solutions $\psi_E(x) = Ae^{ikx} + Be^{-ikx}$ with energies $E_k = \frac{\hbar^2k^2}{2m}$. Are we done? No, because we need to impose our *boundary condition* that $\psi(x =$

$0) = \psi(x = l) = 0$ since those walls are hard and do not allow particles to exist outside of the free particle box we've constructed.

Our previous solution $\psi_E(x) = Ae^{ikx} + Be^{-ikx}$ is fine, but we can also write another general solution as follows:

$$\psi_E(x) = C\sin(kx) + D\cos(kx)$$

As we will see, this is a convenient choice. If we know impose our first boundary conditions:

$$\psi_E(x = 0) = 0 = C\sin[k(x = 0)] + D\cos[k(x = 0)] = C(0) + D(1) = D$$

So $D = 0$ and we can forget about the cosine solution. The second boundary condition tells us:

$$\psi_E(x = l) = 0 = C\sin(kl) = 0$$

This is satisfied for all $kl = n\pi$, where n is an integer. Therefore, we have $k_n = \frac{n\pi}{l}$ which gives us our *quantized* eigenfunction set. The energy eigenvalues are

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2m}$$

with eigenfunctions

$$\psi_n(x) = Csin\left(\frac{n\pi}{l}x\right)$$

Are we done? No, because we must normalize.

$$<\psi_n|\psi_n> = \int_0^l |\psi_n(x)|^2 dx = 1 \Rightarrow \int_0^l C^2 sin^2\left(\frac{n\pi}{l}x\right)dx = 1 \Rightarrow C = \sqrt{\frac{2}{l}}$$

So normalization has given us our proper set of energy eigenfunctions and eigenvalues:

$$\psi_n(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{n\pi}{l}x\right), E_n = \frac{\hbar^2 n^2 \pi^2}{2ml^2}$$

Higher energy states have more nodes. Some of the wavefunctions can be sketched as follows:

What does this have to do with the discrete quantum state picture as described in the context of qubits? To obtain a qubit from this system, we can construct our standard basis $|0>$ and $|1>$ by just restricting our state space to the bottom two eigenstates:

$$|0>=\sqrt{\frac{2}{l}}\sin\left(\frac{\pi}{l}x\right), E_{n=1}=\frac{\hbar^2\pi^2}{2ml^2}$$

$$|1>=\sqrt{\frac{2}{l}}\sin\left(\frac{2\pi}{l}x\right), E_{n=2}=\frac{4\hbar^2\pi^2}{2ml^2}$$

Physically this would mean forcing the total energy of the system to be less than E_2, meaning that the particle could never have any overlap with ψ_n for $n \geq 2$.

This extremely simple model of a confined particle is actually very useful physically, and pops up in many real-world applications. In fact, the particle-in-a-box model provides one of the simplest meaningful descriptions of an atom. In an atom the "confined" particle is an electron and "the box" is created by the Coulomb attraction between the negatively charged electron and the positively charged nucleus. Most atoms have a lot of electrons, but all atoms behave (at some level) in a manner that is very similar to the simplest atom which is hydrogen. Hydrogen has just one electron that circles around one proton. Solving the exact Schroedinger equation for the motion of an electron around a proton involves some complexities that we don't want to worry about right now, but suffice to say that the energy is determined most strongly by the radial motion of electron. (i.e. the electron's radial distance from the proton). The "radial Schroedinger Equation" of the electron then looks very much like the simple "particle-in-a-box" model that we have just solved. The ground state and quantized excited states of hydrogen look like standing waves in much the same way as the particle-in-a-box wave-functions. Higher energy states of hydrogen have more nodes just like the particle-in-a-box states.

We can even make the analogy somewhat quantitative. The actual energy difference between the ground state and first excited state of hydrogen is known to be $\Delta E_H \approx 10$ eV and the diameter of a hydrogen atom is know to be $L_H \approx 1$ Angstrom $\approx 10^{-10}$ meters $= 1/10$ nm. (i.e. the width of the hydrogen ground state wave function). In the particle-in-a-box model that we just solved, the energy difference between the ground state (n=1) and first excited state (n=2) is $\Delta E_{P.I.B.} = E_2 - E_1 = \frac{3\hbar^2\pi^2}{2ml^2}$. We can then ask ourselves what is the size of a 1-d box that yields an energy difference between ground state and first excited state that is the same as the corresponding energy difference in hydrogen. This is easy to calculate by setting $\Delta E_{P.I.B.} = \Delta E_H$.

Then we have $\frac{3\hbar^2\pi^2}{2ml^2} = \Delta E_H$ and $l = \sqrt{\frac{3\hbar^2\pi^2}{2m\Delta E_H}}$. If we plug in $\Delta E_H = 10$ eV, m=mass of electron, and the value for h, then we find that l=3.4 Angstroms (do this calculation yourself). This is only a factor of 3 different from the width of an actual hydrogen atom! That's pretty good. So, if we were to trap an electron in a little 1-d box of a length of l = 3.4 Angstroms then the energy difference between the N=1 and N=2 states would be exactly the same as the energy difference between the first two states of hydrogen. We could then identify those two states as qubit states $|0\rangle$ and $|1\rangle$ (like we did before). An arbitrary qubit superposition of the electron state could then be written as

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle = \alpha\sqrt{\frac{2}{l}}\sin\frac{\pi x}{l} + \beta\sqrt{\frac{2}{l}}\sin\frac{2\pi x}{l}$$

The time evolution of this state at some later time t can be written by adding the energy dependent phase factors:

$$|\psi(t)\rangle = \alpha\,|0\rangle\, e^{-iE_1 t/\hbar} + \beta\,|1\rangle\, e^{-iE_2 t/\hbar}$$

This can be rearranged to become:

$$|\psi(t)\rangle = e^{-iE_1 t/\hbar}\left(\alpha\,|0\rangle + \beta\,|1\rangle\, e^{-i(E_2-E_1)t/\hbar}\right)$$

One more round of rearrangement gives:

$$|\psi(t)\rangle = e^{-iE_1 t/\hbar}\left(\alpha\sqrt{\frac{2}{l}}\sin\frac{\pi x}{l} + \beta\sqrt{\frac{2}{l}}\sin\frac{2\pi x}{l}\,|1\rangle\, e^{-i(\Delta E_H)t/\hbar}\right)$$

The important point to notice here is that as time passes then the phase difference between the two qubit states differs by a rate that is proportional to ΔE_H, the energy difference between them. For atomic systems this is a pretty fast rate, since $\Delta E_H = 10$ eV corresponds to a frequency of $\nu = \frac{\Delta E_H}{h} = 2.5 \times 10^{15}$ Hz. This is very close to the frequency of optical light, and that is why atomic qubits are controlled optically via interaction with light pulses.