Chapter 9

Continuous Quantum Systems

9.1 The wavefunction

So far, we have been talking about finite dimensional Hilbert spaces: if our system has k qubits, then our Hilbert space has 2^n dimensions, and is equivalent to $\mathbb{C}^{2^n}$. This follows because a set of qubits has a finite number of states: it is only possible to measure each qubit in the state $|1\rangle$ or $|0\rangle$. However, qubits with their finite states are not the only thing that quantum mechanics can deal with. Certainly we could try to measure the position of a quantum particle, and the possible outcomes lie on a continuum. In what follows we describe how to deal with 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 observable, 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, in 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 pth 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 $|a_0|^2 + |a_1|^2 + \cdots = 1$.

The matrix/vector notation becomes extremely awkward as we attempt to cope with an infinite number of infinitesimally-spaced basis states. To deal with this, suppose the particle's state, $|\psi\rangle$ is some arbitrary superposition of infinitesimally-spaced position eigenstates. If we now ask, "What

is the probability-density that the particle will lie at an arbitrary position, x, represented by the position eigenstate, $|x\rangle$?" Just as in the finite case, 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. This leads us to define $\psi(x) = \langle x|\psi\rangle$, and it is called the *wavefunction* of the particle with respect to position.

Now, rather than struggle to tediously write down infinite superpositions of infinitesimally-spaced basis states, we need only specify the continuous 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

$$\langle\psi|\psi\rangle = \lim_{\Delta x_j \to 0} \sum_{x_j=-\infty}^{\infty} \langle\psi|x_j\rangle \langle x_j|\psi\rangle \, \Delta x_j = \int_{-\infty}^{\infty} \langle\psi|x\rangle \langle x|\psi\rangle \, dx = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$$

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.

9.2   The Schrödinger Equation

The fundamental equation of quantum mechanics is the Schrödinger Equation, stumbled upon by physicist Erwin Schrödinger in 1925. The Schrödinger equation tells us how a quantum particle in a continuous system should behave. The equation is very difficult to solve, in fact in most real situations it is impossible to solve. For a particle free to move in one dimension, the Schrödinger equation reads

$$H\Psi(x,t) = i\hbar\frac{d}{dt}\Psi(x,t)$$

where H is the Hamiltonian, or energy operator, of a particle that can move in one dimension.

Classically the energy of a particle is simply the sum of its kinetic and potential energy. The total energy of a particle with mass m is well defined in terms of the momentum p and position x of the particle, and is given by

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

Here, $p^2/2m$ is the kinetic energy and $V(x)$ is the classical potential energy of the particle at position x. The form of $V(x)$ depends upon what interactions the particle is subjected to (e.g. an electron in a magnetic field, or a free photon). Exactly how to get from the classical energy function, $E(p,x)$ to the quantum mechanical energy operator, H, is not totally obvious. 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 $\hat{p} = -i\hbar\frac{\partial}{\partial x}$.

To really understand this, we need a few examples.

The Free Particle

Our first example will be that of a free particle in 1 dimension. Here free means that the particle is subject to no potential interactions with other particles. Schrödinger's equation says

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

Because the particle is free, its classical energy is just its kinetic energy $\frac{p^2}{2m}$; the potential energy $V(x) = 0$. Thus,

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

and

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

At first glance, this equation looks daunting and difficult to solve, it is in fact a second order partial differential equation. However, a mathematical trick called "separation of variables" makes the equation fairly easy to solve. The mathematical formalism of separation of variables is not necessary for this course, so if the following discussion is not helpful to you, feel free to skip it. The important result we derive is that the Schrödinger equation can be separated into into two parts:

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

where $\Psi(x,t) = \psi(x)\phi(t)$.

Here's how it works. Because the derivatives in the Schödinger equation are with respect to different variables, there is an easy way to solve the equation. Because the right hand side and the left hand side of the equation depend on different variables entirely, we can say that the time dependence of Ψ is independent of x dependence: $\Psi(x,t) = \Psi(x,0)\Psi(0,t)$. For if this were not true, then when we change x without changing t, the right hand side of the Shrödinger equation changes differently from the left hand side.

In equation form, this translates to:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,0)\right][\Psi(0,t)] = [\Psi(x,0)]\left[i\hbar\frac{\partial}{\partial t}\Psi(0,t)\right]$$

If we let $\psi(x) = \Psi(x,0)$ and $\phi(t) = \Psi(0,t)$, we see that changing x does not change either $\phi(t)$ or $\frac{\partial}{\partial t}\phi(t)$: these terms are constant with respect to $\psi(x)$. Thus we can separate the above equation into two parts, one that describes the time dependence, and one that describes the position dependence.

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

The first equation is called the *time-independent* Schrödinger equation, and it is fairly easy to solve. The constant E is used because the Hamiltonian on the right hand side is the energy of the particle: $H\psi = E\psi$. The solution to the time independent Schrödinger equation is

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

where $k = \sqrt{2mE}/\hbar$. If we let k run negative, then we only need to think about the first solution.

The solution to the time portion of the Schrödinger equation is

$$\phi_k(t) = e^{-i\omega t}$$

where $\omega = E/\hbar = \hbar k^2/2m$. Because the time dependent equation is not dependent upon the potential energy, this is *always* the time dependence of a system. To turn a solution of the the time independent Schrödinger euqtion into a time dependent solution, just tack on an $e^{-iE_k/\hbar}$ to each kth energy eigenstate.

Now, because $\Psi(x,t) = \psi(x)\phi(t)$, the final

$$\boxed{\Psi_k(x,t) = e^{i(kx - \omega t)}}$$

We see that for each k (or E) there is a solution, which gives us a continuous set of solutions to the Schrödinger equation. We can think of the set Ψ_k as a basis for the possible states of our particle, since linear combinations of solutions to a linear differential equation are also solutions to the same equation.

Particle in a Box

Another classic example where Schrödinger's equation is actually solvable is the particle in a box, also known as the infinite square well. In this problem, the particle is free move however it likes within a single line segment (this is its box), but is not allowed to leave.

While this situation is unrealistic and does not occur in nature, it is a half decent way to approximate an atom. You can think of an electron in a hydrogen atom, for example, as being trapped in a box. The potential near the central proton is much lower than far from it. It might be a stretch to say that the this is the same as our particle in a box, but they certainly are similar.

The way to describe the particle in a box is to say that the potential inside the box is 0, while the potential outside is infinite: it would take infinite energy for the particle to exist outside of its little line segment, thus it cannot exist outside of the box.

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < a \\ \infty & \text{otherwise} \end{cases}$$

Inside the box, the Hamiltonian is $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$. Outside the box we simply mandate that $\Psi(x,t) = 0$.

Furthermore, to make sure that the Schrödinger equation makes sense, we will require that $\Psi(x, t)$ is continuous. Because $\psi(x) = 0$ outside of the box, we require that:

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

We first solve the time-independent Schrödinger equation without worrying about the above restriction:

$$\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

We already solved this, and our solution was $\psi_k(x) = Ae^{ikx} + Be^{-ikx}$. But before we can call this done we need to impose our *boundary condition*, i.e. the restriction that $\psi(0) = \psi(a) = 0$.

To get rid of the complex exponentials and make life a little easier, we recall that for some C and D,[1]

$$Ae^{ikx} + Be^{-ikx} = C\sin(kx) + D\cos(kx)$$

So $\psi_k(x) = C\sin(kx) + D\cos(kx)$ for some C and D. To find the conditions on C and D, we impose our boundary conditions:

$$\psi_k(0) = C\sin(0) + D\cos(0) = D$$

But $\psi_k(0) = 0$ so $D = 0$, and we can forget about the cosine solution. The second boundary condition tells us:

$$\psi_k(a) = C\sin(ka) = 0$$

This can only be satisfied when $ka = n\pi$, where n is an integer. And because $k = \sqrt{2mE}/\hbar$, the only allowed energies are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$. Thus, our (almost final) set of solutions is, for each integer n,

$$\psi_n(x) = C\sin\left(\frac{n\pi x}{a}\right) \text{with energy} E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Notice how the *quantization* of energy levels, the fact that there is a discreet set of energy eigenvalues, and quantization of basis states simply falls out of the math. This kind of phenomenon is what gives quantum mechanics its name.

There is one last step before we can call it a day. We need to make sure that $\langle psi_n|\psi_n\rangle = 1$ for all n. This is called *normalizing* the wavefunctions.

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

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[1]If you have never seen this before, it is not too bad of an exercise to find C and D with the identity $e^{ikx} = \cos(kx) + i\sin(kx)$.

so that $C = \sqrt{2/a}$.

With everything normalized and all boundary conditions accounted for, we finally have our proper set of energy eigenfunctions and eigenvalues:

$$\psi_n(x) = C \sin\left(\frac{n\pi x}{a}\right) \text{with energy} E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Qubits

While it is important to have this background in quantum mechanics to better understand quantum information science, there is a direct connection between the solution to the particle in a box problem and qubits. We have discussed several examples of qubits in previous lectures, one of which used the ground state and first excited state of an atom as the two states of a qubit. Because the particle in a box is a simple model for a hydrogen atom, we will discuss hydrogen atom qubits in the context of the square well.

To obtain a qubit from particle in a box system, we can construct our standard basis $|0\rangle$ and $|1\rangle$ by restricting our state space to the bottom two eigenstates:

$$|0\rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right), \qquad E_1 = \frac{\hbar^2 \pi^2}{2ma^2}$$

$$|1\rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right), \qquad E_2 = \frac{4\hbar^2 \pi^2}{2ma^2}$$

Physically this would mean demanding that the energy in the box be less than or equal to E_2, meaning that the particle could never have any overlap with ψ_n for $n > 2$. This can be done in the lab by cooling the atom to very low temperatures (perhaps laser cooling).

In fact, given the right length a of the box, the lowest two states of the hydrogen atom are approximated very well by the infinite square well. Because of this, we can do some calculations to take a look at what a hydrogen atom qubit looks like. An arbitrary qubit superposition of the electron state can be written as

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle = \alpha \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) + \beta \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$$

The time evolution of this state at some later time t can be tacked on by multiply each eigenstate by $e^{-iE_n/\hbar}$, as noted in the free particle problem:

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

This can be rearranged to become:

$$|\psi(t)\rangle = e^{-iE_1t/\hbar}\left(\alpha\,|0\rangle + \beta\,|1\rangle\,e^{-i(E_2-E_1)t/\hbar}\right)$$

or

$$\boxed{|\psi(t)\rangle = e^{-iE_1t/\hbar}\left(\alpha\,|0\rangle + \beta\,|1\rangle\,e^{-i(\Delta E)t/\hbar}\right)}$$

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