

1 Schrodinger equation (continued)

1.1 Energy eigenstates

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

This is not something that can really be derived. This is a postulate. It's a starting point. We can try to justify it and show that it makes sense and is reasonable, but we can't derive it. Perhaps the strongest justification is that it explains experiments. It correctly explains the world around us. In a regular physics class we'd spend a lot of time talking about all those experiments, and how they're explained by QM.

But this is not a regular physics class. This class is called "Qubits, QM, and Computers," so the most important point for us here is that this equation describes the behavior of qubits, the elements that carry quantum information. Understanding this equation will help us to manipulate qubits and create quantum gates.

The first thing to note is that there is a special relationship in QM between the energy of a system and its time development. *A Trick:* 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*. 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 $\{E_k\}$. It's an eigenfunction equation. (Time dependence is easy: $\psi(x,t) = \psi(x)\phi(t) = \psi_k(x)e^{-iEt/\hbar}$.)

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 $\hat{H}\psi_1 = E_1\psi_1$ 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)

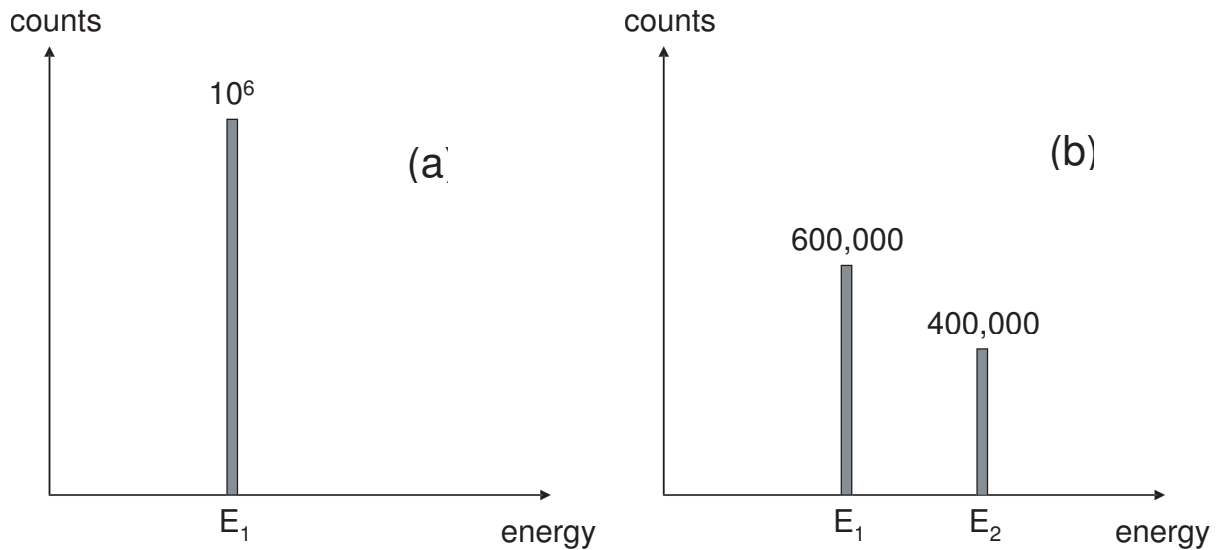


Figure 1: Histograms of particle energy measurements.

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) $\times(\psi')$? 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.

1.2 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 $\psi(x, t \neq 0)$?

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

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?

$$\psi(x, t) = \sqrt{\frac{3}{5}}\psi_1 e^{-iE_1 t/\hbar} + \sqrt{\frac{2}{5}}\psi_2 e^{-iE_2 t/\hbar}$$

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 $f(x) = a_1\psi_1(x) + a_2\psi_2(x) + a_3\psi_3(x) + \dots$, a linear superposition of the energy eigenstates $\{\psi_k\}$. Note that you must find the overlap: $a_i = \langle \psi_k | f \rangle$ for this to be meaningful. In position space, this is accomplished by the integral:

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

The time dependence is then given by

$$\psi(x, t) = a_1\psi_1(x)e^{-iE_1 t/\hbar} + a_2\psi_2(x)e^{-iE_2 t/\hbar} + a_3\psi_3(x)e^{-iE_3 t/\hbar} + \dots$$

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 $\psi(x, t) = \psi_i(x)e^{-iE_i t/\hbar}$. The probability density $P(x, t)$ is then given by

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

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

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 points where the potential energy $V \rightarrow \infty$. This has the effect of *disallowing* any ψ to be nonzero in this region. 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 not normalized over all space $x \in \{-\infty, \infty\}$ but instead 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.

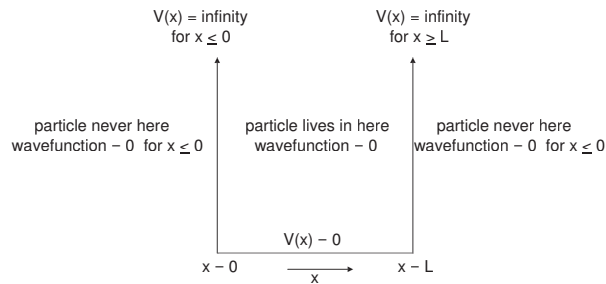


Figure 2: Particle in a box

The first thing to note is that we've done this problem before! For a free particle we know that we have solutions $\psi_E(x) = Ae^{ikx} + Be^{-ikx}$ with energies $E_k = \frac{\hbar^2 k^2}{2m}$. 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

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

with eigenfunctions

$$\psi_n(x) = C \sin \frac{n\pi}{l} x$$

Are we done? No, because we must normalize.

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

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:

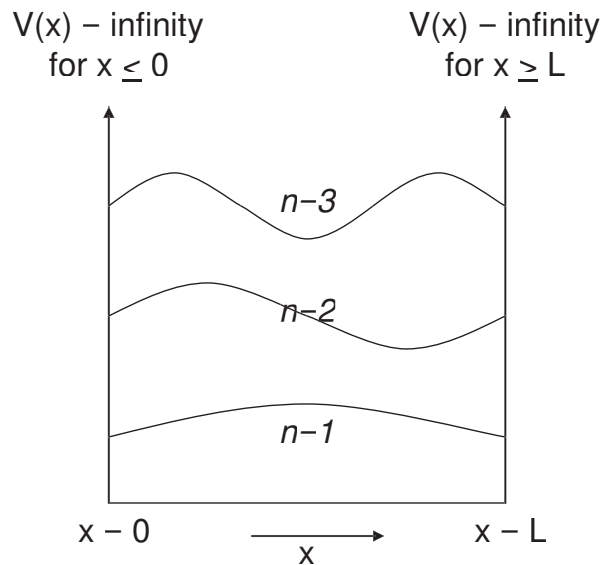


Figure 3: The first three eigenfunctions of the particle in a box system.

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 $|0\rangle$ and $|1\rangle$ by just restricting our state space to the bottom two eigenstates:

$$|0\rangle = \sqrt{\frac{2}{l}} \sin \left(\frac{\pi}{l} x \right), E_0 = \frac{\hbar^2 \pi^2}{2ml^2}$$

$$|1\rangle = \sqrt{\frac{2}{l}} \sin \left(\frac{2\pi}{l} x \right), E_1 = \frac{4\hbar^2 \pi^2}{2ml^2}$$

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_k for $k \geq 2$.

Suppose, as we have in the past, that the state of the electron qubit is $|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$. What is the state at $t \neq 0$?

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{2}{l}} \sin\left(\frac{\pi}{l}x\right) \right) e^{-iE_0t/\hbar} + \frac{1}{\sqrt{2}} \left(\sqrt{\frac{2}{l}} \sin\left(\frac{2\pi}{l}x\right) \right) e^{-iE_1t/\hbar}$$

2 Other eigenbases

Now, the previous discussion was carried out in the "energy" basis, by which we mean we sought the eigenstates of the Hamiltonian and expressed our quantum states in that eigenbasis. This is, of course, very convenient for describing the time development of the state. But sometimes you might want to write a qubit state in terms of the eigenstates of a different physical quantity.

For example, you might want to describe the wavefunction of your qubit in terms of basis states that have well-defined position, or momentum, or angular momentum. Each of these bases can be found by solving a corresponding eigenvalue problem. In order to get these "well-defined" states you just have to know the operators and solve the eigenvalue problem.

HOWEVER: While you can always construct an eigenstate of *one* physical quantity, you might not be able to construct a state that is a simultaneous eigenstate of two physical quantities; i.e. a state that has well-defined values for two observables.

Question: Is it possible to construct a state $\psi_{x,p}$ such that $\hat{x}\psi_{x,p}(x) = x_0\psi_{x,p}(x)$ AND $\hat{p}\psi_{x,p}(x) = p\psi_{x,p}(x)$? Such a state would have simultaneously well-defined position (x_0) and momentum (p).

3 Commutators

A relevant theorem to help answer the question:

Theorem: Consider two operators \hat{A} and \hat{B} (representing two physical quantities). It is possible to construct a simultaneous eigenstate, ψ_{ab} , of both \hat{A} and \hat{B} iff $[\hat{A}, \hat{B}] = 0$ where $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator between \hat{A} and \hat{B} .

Proof (kind of): One can easily show that if $[\hat{A}, \hat{B}] = 0$ then simultaneous eigenstates exist. Suppose $\{\phi_a\}$ is a set of non-degenerate eigenstates of $\hat{A} \Rightarrow \hat{A}\phi_a = a\phi_a$. Now consider $\hat{B}(\hat{A}\phi_a) = a(\hat{B}\phi_a)$. But, $\hat{B}\hat{A} = \hat{A}\hat{B}$ from the commutator, so $\hat{A}(\hat{B}\phi_a) = a(\hat{B}\phi_a)$. So we conclude that $(\hat{B}\phi_a)$ is an eigenstate of \hat{A} with eigenvalue "a". So, $\hat{B}\phi_a \propto \phi_a$ which means that $\hat{B}\phi_a = b\phi_a$. Therefore ϕ_a is a simultaneous eigenstate of \hat{A} and \hat{B} .

So, to answer the question of whether we can construct a state of well-defined position AND momentum, then we must see if $[\hat{x}, \hat{p}] = 0$ or not.

First, what is \hat{p} ?? We know from before that

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Rightarrow \hat{p}^2 = -\hbar^2 \frac{\partial^2}{\partial x^2} \Rightarrow \hat{p} = \text{sqrt}(-\hbar^2 \frac{\partial^2}{\partial x^2}) = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

Let's test this operator $\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ on an test state:

$$\psi_k(x) = \frac{\hbar}{i} \frac{\partial}{\partial x} (e^{ikx}) = \hbar k e^{ikx} = p \psi_k(x)$$

Since we are working in the continuous basis $|x\rangle$ where $\hat{x} = x$ (meaning the position operator is just *the function x*), we can check the commutator in this basis:

$$\left[x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right] = ?$$

Notice the commutator is itself an operator, in this case one that is begging to operate on some function. Let's apply it to a test function $f(x)$ and see what happens:

$$\left[x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right] f(x) = \frac{\hbar}{i} \left(x \frac{\partial}{\partial x} - \frac{\partial}{\partial x} x \right) f(x) = \frac{\hbar}{i} \left(x \frac{\partial f}{\partial x} - \frac{\partial}{\partial x} (x f(x)) \right) = \frac{\hbar}{i} \left(x \frac{\partial f}{\partial x} - f(x) - x \frac{\partial f}{\partial x} \right) = i \hbar f(x)$$

We see the test function $f(x)$ is irrelevant and we can state that

$$[\hat{x}, \hat{p}] = i \hbar \neq 0$$

Therefore we can conclude that you cannot simultaneously know the position and momentum of a quantum state with certainty. This is a restatement of the Heisenberg Uncertainty Principle using a different language.