In this second of two review lectures on quantum mechanics and physics we discuss the Hamiltonian operator, solution of the Schrodinger equation, and how to make a simple atomic qubit from a particle-in-a-box model of the hydrogen atom.

1 Readings

Any elementary quantum mechanics text from the list, e.g., Griffiths, Introduction to QM, Chs. 1, 2, 3.

2 The Hamiltonian

What is the Hamiltonian operator? Classically, the Hamiltonian is the energy operator, $H = \frac{p^2}{2m} + V(x)$. Quantum mechanically, we would like to use either the position or momentum basis to represent the operator since then either x or p will be diagonal, and consequently also any corresponding functions of these operators that occur in the Hamiltonian. Thus in a position representation $V(x)$ is diagonal, while in a momentum representation $\frac{p^2}{2m}$ is diagonal. E.g.,

$$\begin{aligned}
\hat{V} &= \int dx dx' |x\rangle \langle x| V |x'\rangle \langle x'| \\
&= \int dx dx' |x\rangle V(x) \delta(x - x') \langle x| \\
&= \int dx |x\rangle V(x) \langle x|
\end{aligned}$$

We usually have a more complicated potential energy term than kinetic term, so prefer to work in the position representation - will illustrate with an example below. So, we need to express $\hat{p}^2/2m$ in the position representation. Let's start with getting $\hat{p}$. We expect that the time derivative of $\langle \hat{x} \rangle$ is related to classical velocity v and hence to classical momentum $p = mv$, which should in turn be $m \langle \hat{p} \rangle$. So

$$\frac{d}{dt} \langle x \rangle = \frac{d}{dt} \int \psi^*(\tau,t) x \psi(\tau,t) d\tau = \frac{d}{dt} \int x \rho(\tau,t) d\tau$$

where $\rho(\tau,t) = |\psi(\tau,t)|^2$ and τ is the three-dimensional coordinate in general. Now for a normalized wave function this is a probability density whose total integral has to be conserved in order to keep the particle number constant. By Gauss' theorem it has to therefore at all times satisfy the continuity equation

$$\frac{\partial \rho(\tau)}{\partial t} + \nabla \cdot j(\tau) = 0$$

where the current density $j(\tau)$ is given by

$$j(\tau) = \frac{\hbar}{2mi} \nabla \cdot [\psi^*(\tau) \nabla \psi(\tau) - (\nabla \psi^*(\tau)) \psi].$$

Now we can rewrite the time derivative of $\rho(x)$ in terms of the current density $j(\tau)$, evaluate the integral by parts, and remove the boundary terms at $x \to \infty$, to obtain

$$\begin{aligned}
\frac{d}{dt}\langle x\rangle &= \frac{d}{dt}\int x\rho(\tau,t)d\tau \\
&= -\int x\nabla\cdot j(\tau)d\tau \\
&= -\int \nabla\cdot(j(\tau)x)\,d\tau + \int j_x d\tau \\
&= \int j_x d\tau
\end{aligned}$$

Now using the definition of the current density and integrating by parts we arrive at

$$\langle p\rangle = m\frac{d}{dt}\langle x\rangle = \int \psi^*(\tau)\frac{\hbar}{i}\nabla\psi(\tau)d\tau$$

which leads to the definition of the momentum operator

$$\hat{p} = \frac{\hbar}{i}\nabla.$$

Hence the kinetic energy operator in the position representation is $\hbar^2/2m\nabla^2$.

So, what if we had used the momentum representation? Then the kinetic energy would be simple, merely the diagonal form $p^2/2m$ and we would need to evaluate x in the momentum representation. This is given by $x = i\hbar d/dp$. Now suppose we had some non-trivial potential energy, e.g., $V(x) = 1/cosh^2(x)$. This happens. Then the potential energy would be given by $V(p) = 1/cosh^2(i\hbar d/dp)$ which is really not something that you want to deal with in your partial differential equation for the wave function!

3 The Schrodinger Equation and its Solutions

What is the role of energy here? It is very intertwined with time dependence. Let's examine how...

First, let's consider the Schrodinger equation for a free particle, $V(x) = 0$:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}\psi(x,t) \tag{1}$$

with m the particle's mass and $\hbar = \frac{h}{2\pi}$. Recall that Planck's constant has a value of $h = 6.6\times10^{-34}J\cdot s$. This is a very small quantity with respect to ordinary macroscopic levels, and is the main reason why quantum effects are not usually noticeable.

If we take this Schrodinger equation and plug in our trial solution $\psi(x,t) = e^{i(kx-\omega(k)t)}$, we find that this trial solution works provided that $\omega(k) = \frac{\hbar k^2}{2m}$. This is known as the dispersion relation for a free particle. Now, notice that the most general solution is a linear superposition of such functions for many different k values:

$$\psi(x,t) = \int dkA_k e^{i(kx-\omega(k)t)} \tag{2}$$

This superposition solution is known as a *wave packet*. The velocity of a wave packet is $v = \frac{\partial\omega}{\partial k} = \frac{\partial}{\partial k}\left(\frac{\hbar k^2}{2m}\right) = \frac{\hbar k}{m}$. This is the "group velocity". We can also quickly rearrange this to note that $mv = \hbar k$. But what is "mv"? It's the momentum, p! Therefore we conclude that $p = \hbar k$. This is a relationship between the physical momentum of a particle and the wave-vector of a wavefunction. We can illuminate this further as follows:

$$p = \hbar k = \left(\frac{h}{2\pi}\right)\left(\frac{2\pi}{\lambda}\right) = \frac{h}{\lambda} \tag{3}$$

This is known as the DeBroglie relation, and it actually predates the Schrodinger equation.

Now we will consider how to solve the Schrodinger equation in general, when there is also a non-zero potential energy term, $V(x)$ (say, due to an electric field). If there is a potential energy in the system, then the Hamiltonian becomes:

$$\hat{H} = KE + PE = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{4}$$

To be clear about the distinction between operators and functions, we'll denote quantum mechanical operators with "hats", e.g. $\hat{H}$ or $\hat{p}$.

The Schrodinger Equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t) \tag{5}$$

defines the relationship between the energy of a system (through $\hat{H}$) and its time development. Can we understand this relationship better?

First, we note that this is a partial differential equation, which means that it is a differential equation with more than one variable (x and t in this case). We now employ a handy math trick for partial differential equations, and assume that the solution to the Schrodinger Equation can be written as the product $\psi(x,t) = \psi(x)\phi(t)$. This is called *separation of variables*. If we plug this into the Schr. Eqn. and divide both sides by $\psi(x)\phi(t)$:

$$i\hbar\psi(x)\frac{\partial}{\partial t}\phi(t) = \phi(t)\hat{H}\psi(x) \rightarrow i\hbar\frac{\frac{\partial\phi}{\partial t}}{\phi(t)} = \frac{\hat{H}\psi(x)}{\psi(x)} \tag{6}$$

The left hand side (LHS) is a function of t, and the right hand side (RHS) is a function of x. Therefore, for this solution to make sense for all possible x and t, both sides must equal a *constant*. What is that constant? Why, *energy*, of course!

So, the Schr. eqn. breaks into two equations, one in time (t) and one in space (x):

$$space : \hat{H}\psi(x) = E\psi(x) \tag{7}$$

$$time : i\hbar\frac{\partial\phi(t)}{\partial t} = E\phi(t) \tag{8}$$

This time equation is easy: $\phi(t) = e^{-iEt/\hbar} \to \phi(t) = e^{-i\omega t}$, $\omega = \frac{E}{\hbar}$, or $E = \hbar\omega$. (Planck-Einstein relation.)

The spatial equation is harder. It is called the "time-independent Schrodinger equation." However difficult to solve, this equation is a special type of equation known as an *eigenvalue* problem, where "operator $\times\psi$" = "constant $\times\psi$." Thus the Schr. eqn. reduces to an eigenvalue problem, which has a storied history in mathematics. To solve the Schr. eqn., one must find the set of wavefunctions $\{\psi_k(x)\}$ that return to themselves (times a constant) when acted on by $\hat{H}$: $\hat{H}\psi_k(x) = E_k\psi_k(x)$. Each solution ψ_k has an energy E_k associated with it. The states $\{\psi_k\}$ and only they have well-defined energies. The energies $\{E_k\}$ are the set of all physically allowed energies of the system.

The full time-dependent solution is $\psi(x,t) = \psi(x)\phi(t) = \psi_k(x)e^{-iE_kt/\hbar}$. Since these are linear equations we can add solutions, just as above for the free particle case. So, the most general solution to the Schrodinger equation is $\psi(x,t) = \sum_k A_k\psi_k(x)e^{-iE_kt/\hbar}$.

This tells us the rule for time evolution in quantum mechanics: if you want to know how a wave function evolves in time then you just break it down into energy eigenfunctions and multiply each one by a time-dependent phase factor whose frequency is proportional to its energy.

Example: Suppose at time t=0 we have $\psi(x) = A_1\psi_1(x) + A_2\psi_2(x) + A_3\psi_3(x)$ where $\hat{\psi}_i(x) = E_i\psi_i(x)$. What is $\psi(x,t)$ for $t \neq 0$?

To solve this, we can just add in the phase factors:

$$\psi(x,t\neq 0) = A_1\psi_1(x)e^{-iE_1t/\hbar} + A_2\psi_2(x)e^{-iE_2t/\hbar} + A_3\psi_3(x)e^{-iE_3t/\hbar} \tag{9}$$

Let's do another example: For a free particle $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \to \psi_k(x) = e^{ikx}, E_k = \frac{\hbar^2k^2}{2m}$. Therefore, $\psi(x,t) = e^{ikx}e^{-i\frac{\hbar k^2}{2m}t}$ as seen before.

In general $\hat{H}\psi(x) = E\psi(x)$ can be a very difficult differential equation to solve. Physicists and chemists spend a great deal of time solving this equation!

Note that we have already derived this time evolution earlier when analyzing the unitary evolution of a quantum state: $\psi(x,t\neq 0) = e^{-i\hat{H}t/\hbar}\psi(x,t=0)$, with $e^{-i\hat{H}t/\hbar}$ the time evolution operator. Recall how we approached it before:

Any $\psi(x,t=0)$ can be written $\psi(x,t=0) = \sum_k A_k\psi_k(x)$, so:

$$\psi(x,t\neq 0) = e^{-i\hat{H}t/\hbar}\left(\sum_k A_k\psi_k(x)\right) = \sum_k A_k e^{-i\hat{H}t/\hbar}\psi_k(x) = \sum_k A_k\psi_k(x)e^{-iE_kt/\hbar} \tag{10}$$

which is the same as above, since $\psi_k(x)$ is an eigenfunction of $\hat{H}$ with eigenvalue E_k.

The time-independent Schr. eqn. sets a condition that determines what the allowed energies of a system are and what the states look like that have well-defined energy ("well-defined" means you'd get the same answer if you measured the energy of all of the members of an identically prepared ensemble of systems in that state). However, we can also construct states that have well-defined values of other physical quantities, like momentum, position, and angular momentum.

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.

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 $\hat{H}\psi = E\psi$).

So let's discuss measurement. If $|\psi>= a_1|\psi_{E_1}> +a_2|\psi_{E_2}> +a_3|\psi_{E_3}> + \cdots$, what is the result of a measurement of energy? One of the postulate of QM is that the result of the measurement must be an eigenvalue of $\hat{H}$. ψ will collapse onto one of these eigenstates with some probability. What's the probability of obtaining E_3? $P_3 = |<\psi_e|\psi>|^2 = a_3^2$ And what is ψ after measurement? ψ is projected to ψ_3 upon an observation of E_3. So, measurement is a random collapse onto one of the eig. states of the observable you are measuring!

The same holds for momentum: If we are discussing momentum then it's best to work with momentum eigenstates.

$$\hat{p}\psi_p = p\psi_p \Rightarrow \{\psi_p\}, \{p\}$$

Suppose $|\psi>= b_1|\psi_{p_1}> +b_2|\psi_{p_2}> +b_3|\psi_{p_3}> + \cdots$ What is a result of a measurement of momentum? We will end up measuring an eigenvalue of momentum with some probability, and then collapse onto that eigenstate ($P_2 = |b_2|^2$).

The exact same thing happens for the observables $\hat{x}$, $\hat{L}$, etc. The eigenstates of these observables define bases, and measurement of that observable randomly collapses us onto one of those eigenstates.

Question: What if we take an ensemble of identically prepared states and measure the same physical quantity for each? How do we determine (theoretically) the average value of the measurements? This will lead us to the definition of an *expectation value*.

Example: ENERGY. Suppose we know states $\{\psi_E\}$, $\{E\}$. If an ensemble is prepared in $|\psi>=|\psi_E>$ then the situation is simple: $<E>= E_0$. But what if we prepare an ensemble in a state $|\psi>$ in a superposition state which is not an eigenstate of $\hat{H}$, e.g. $|\psi>= a_1|\psi_{E_1}> +a_2|\psi_{E_2}> +a_3|\psi_{E_3}> + \cdots$? What is $<E>$ then?

$$<E>= E_1 Prob[E_1] + E_2 Prob[E_1] + E_3 Prob[E_3] + \cdots$$

where $Prob[E_i]$ is just

$$Prob[E_i] = |<\psi_{E_i}|\psi>|^2 = |a_i|^2$$

This yields:

$$<E>= |a_1|^2 E_1 + |a_2|^2 E_2 + |a_3|^2 E_3 + \cdots$$

Our shorthand for this is given by:

$$< E >=< \psi|\hat{H}|\psi >$$

which is known as the expectation value of the Hamiltonian (or equivalently of the energy). You can readily show that this $< E >=< \psi|\hat{H}|\psi >$ yields the proper expression.

We can do this for *any* observable! Consider arbitrary observable $\hat{A}$. The average value of this quantity for ensemble of systems prepared in $|\psi >$ is $< A >=< \psi|\hat{A}|\psi >$.

It should be noted that it is sometimes hard to evaluate the expectation value. Take the continuous basis for example ($|x >$). Suppose $\psi(x) =< x|\psi >= Ae^{-x^2}$. What is the average value of measured momentum for an ensemble of systems?

$$< \hat{p} >=< \psi|\hat{p}|\psi >= \int_{-\infty}^{\infty} \psi^*(x)\hat{p}\psi(x)dx = \int_{-\infty}^{\infty} \left(A^* e^{-x^2}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left(Ae^{-x^2}\right)dx = 0$$

So, in this instance the expectation value is zero. It is left as an exercise to evaluate $< p^2 >$ (symmetry analysis will immediately tell you if it zero or not).

4 Particle-in-a-box model for atomic qubit

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.

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

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

with eigenfunctions

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

Are we done? No, because we must normalize.

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

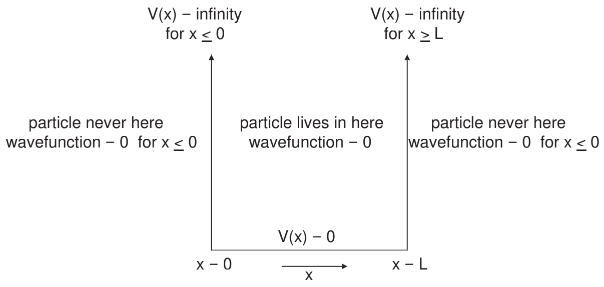

Figure 1: Particle in a box

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:

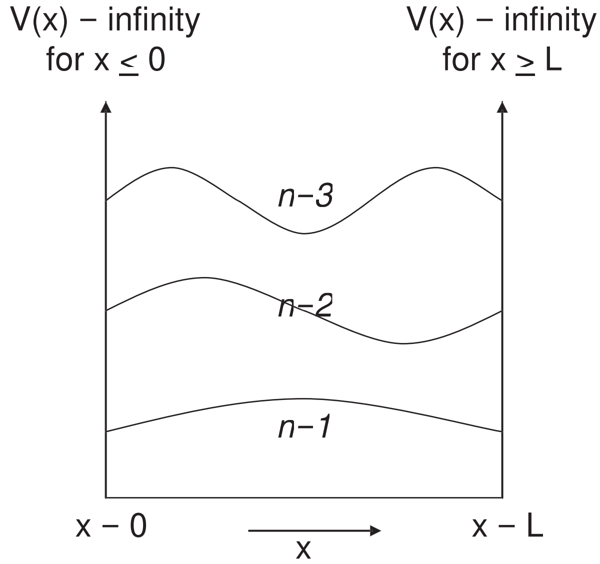

Figure 2: The first three eigenfunctions of the particle in a box system.

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

$$|0> = \psi_1(x) = \sqrt{\frac{2}{l}} sin\left(\frac{\pi}{l}x\right), E_{n=0} = \frac{\hbar^2 \pi^2}{2ml^2}$$

$$|1> = \psi_2(x) = \sqrt{\frac{2}{l}} sin\left(\frac{2\pi}{l}x\right), E_{n=1} = \frac{4\hbar^2 \pi^2}{2ml^2}$$

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_n for $n \geq 2$.

What about the energies of qubit states? Suppose I take 10^6 qubits prepared in state $|0\rangle = \psi_1$ 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 superposition state $\psi' = \sqrt{\frac{3}{5}}|0\rangle + \sqrt{\frac{2}{5}}|1\rangle$, 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)$\times(\psi')$? 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. However it is a perfectly valid superposition state of the qubit.

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 dont 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 electrons 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

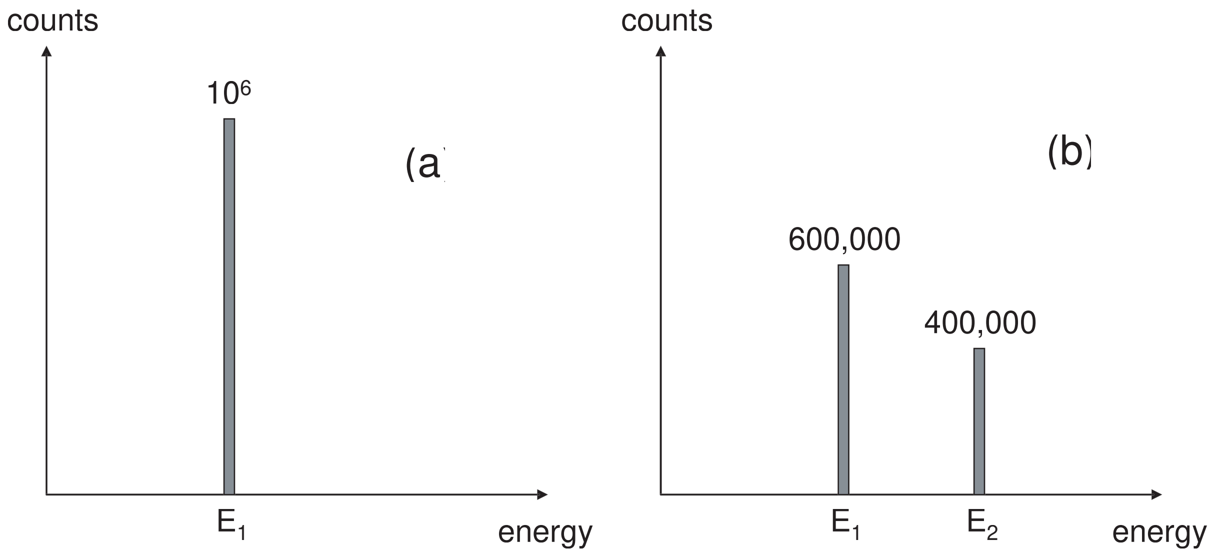

Figure 3: Histograms of particle energy measurements.

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 $l = \sqrt{\frac{3\hbar^2\pi^2}{2ml^2}}$. 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! Thats 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 107 and 117 (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:

$$|\psi(t)\rangle = \alpha|0\rangle e^{-1E_1 t/\hbar} + \beta|1\rangle e^{-iE_2 t/\hbar}$$

This can be rearranged to become:

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

One more round of rearrangement gives:

$$|\psi(t)\rangle = e^{-1E_1 t/\hbar}\left(\alpha\sqrt{\frac{2}{l}}\sin\frac{\pi x}{l} + \beta\sqrt{\frac{2}{l}}\sin\frac{2\pi x}{l}|1\rangle e^{-i(E_2-E_1)t/\hbar}\right)$$

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.

5 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 $\hat{x}\psi_{x,p}(x) = x_o\psi_{x,p}(x)$ AND $\hat{p}\psi_{x,p}(x) = p\psi_{x,p}(x)$? Such a state would have simultaneously well-defined position (x_o) and momentum (p). we will answer this in the next lecture.