Some QM notes

1 Classical vs. Quantum Mechanics

We'll do both of these saying that we are only interested in the x spatial direction, generally you can do x, y, z but it is messier.

Classical Mechanics:

- Start with potential $U(\mathbf{r})$
- Use the potential in Newton's equation $F = ma$. That is, force in the $\mathbf{x}$ direction depends upon the potential:

$$F_x = -\frac{\partial U(\mathbf{r})}{\partial x} = \frac{dp_x}{dt} = (nonrelativistic) m \frac{d^2 x}{dt^2} \tag{1}$$

- Solve for $x(t)$ using initial conditions and equation above.
- Use $x(t)$ to calculate not only where the particle is, but its momentum (e.g. $m\frac{dx}{dt}$ nonrelativistically), energy, etc.

Quantum Mechanics:

- Start with potential $U(\mathbf{r}) \to U(x)$ (for this case we want $U(x)$).
- Put into Schroedinger's equation. Just considering x dependence, we have

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)]\Psi(x,t) = i\hbar\frac{\partial \Psi(x,t)}{\partial t} \tag{2}$$

which in many cases of interest, when we are interested in something which has a known energy and thus no time dependence, can be solved with

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} \tag{3}$$

(see Giancoli sec 39-6 for more discussion of this). In this case we instead can use a simpler equation for just $\psi(x)$,

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)]\psi(x) = E\psi(x) \tag{4}$$

- Solve for $\Psi(x,t)$ or $\psi(x)$ and E.

- Normalize the solution, i.e. make sure that

$$\int \Psi * (x,t)\Psi(x,t)dx = \int |\Psi(x,t)|^2 = 1 \tag{5}$$

which you can almost always do since if Ψ solves the equation above, Ψ times any constant also solves the equation (linear equation), so you multiply it by whatever constant is needed. It won't work for the free particle of fixed energy, and instead you need to use a wavepacket, so that the particle is "somewhere" in particular, rather than everywhere at once.

- Use $\Psi(x,t)$ to calculate things you are interested in: where the particle might be, the average value of various quantities you'd find if you measured many systems with the identical Ψ to start with, etc.

2 What you can measure with Ψ

In class and in the book, the infinite square well is done in detail, and the finite square well is done briefly. We also considered the harmonic oscillator wavefunctions and their general shape and properties, which are discussed in detail off of the Key ideas web page (hyperphysics link).

The one thing we did in class which wasn't in the book in great detail was expectation values (this has been taught in previous 7c courses so we covered it as well).

We started with the average value of x that you might measure. That is, you take a system with a wavefunction $\Psi(x,t)$ (still in 1 d, can go to 3 dimensions by solving 3d equation) and measure x. Say you do it in several systems all with the same starting value of $\Psi(x,t)$. Then you would find

$$x_1, x_2, x_3, x_4, x_5, \ldots, x_N \tag{6}$$

after say N times. The average value would be

$$< x >= \frac{x_1 + x_2 + x_3 + \ldots + x_N}{N} \tag{7}$$

and the wavefunction can predict what this will be exactly for you. (For a small number of measurements it might not get it quite right, just like tossing a coin only 6 times might not get 3 heads and 3 tails, but eventually will be 50-50.) In particular, using the wavefunction you would calculate:

$$< x >= \int_{-\infty}^{\infty} \Psi^*(x,t) x \Psi(x,t) dx \tag{8}$$

which we did for the square well. We took a particle in a fixed energy state (i.e. time independent), i.e.

$$\Psi = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} e^{-iE_n t/\hbar} \ , 0 \le x \le L, \quad E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \tag{9}$$

note that given a particular ψ there is one E that goes with it. Then we plugged in

$$\begin{aligned} < x > &= \int_0^L \Psi^*(x,t) x \Psi(x,t) dx \\ &= \int_0^L \sqrt{\tfrac{2}{L}} \sin \tfrac{n\pi x}{L} x \sqrt{\tfrac{2}{L}} \sin \tfrac{n\pi x}{L} dx \\ &= \tfrac{2}{L} \int_0^L x \sin^2 \tfrac{n\pi x}{L} dx \\ &= \tfrac{2}{L} \int_0^L x \tfrac{1}{2}(1 - \cos \tfrac{2n\pi x}{L}) dx \\ &= \tfrac{1}{L} \int_0^L x dx - \tfrac{1}{L} \int_0^L \cos \tfrac{2n\pi x}{L}) dx \\ &= \tfrac{1}{L} \tfrac{L^2}{2} - \tfrac{1}{L} \int_0^L \tfrac{L}{2n\pi} \sin \tfrac{2n\pi x}{L}) dx \\ &= \tfrac{L}{2} - 0 \end{aligned} \tag{10}$$

for the square well.

Similarly we calculated $< x^2 >$ and also $< p >$. For the wavefunction $\Psi(x,t)$, p is written

$$< p_x > = < -i\hbar \frac{\partial}{\partial x} > \tag{11}$$

and in this case the ordering is crucial,

$$< p > = \int_{-\infty}^{\infty} \Psi^*(x,t)(-i\hbar \frac{\partial}{\partial x}) \Psi(x,t) dx \tag{12}$$

and for the square well this becomes

$$< p > = \int_0^L \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} (-i\hbar \frac{\partial}{\partial x}) \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} dx = 0 \tag{13}$$

That is, it turns out the average momentum is zero, basically becasue the particle is equally likely to be going in both directions, so it cancels out. You will find that $p^2 \neq 0$, in fact that $p^2 = 2mE$ for this particle.

In general, to calculate any quantity, you calculate

$$< quant > = \int_{-\infty}^{\infty} \Psi^*(x,t)(quant) \Psi(x,t) dx \tag{14}$$

(where we are still considering only one dimension). For the quantity is a function of x you just write it out in terms of x, if it is a function of p you need to write p in terms of x, i.e. write $p = -i\hbar \partial / \partial x$.

One last point, say we are measuring something that is intrinsically quantized, like the energy, and we consider a state that doesn't have definite energy,e.g.,

$$\Psi(x,t) = \frac{1}{2}\psi_1(x)e^{-iE_1 t/\hbar} + \frac{\sqrt{3}}{2}\psi_2(x)e^{-iE_2 t/\hbar} \tag{15}$$

where e.g. E_1 and E_2 are two different energies above, corresponding to two different $\phi(x)$. Energy depends on momentum, so to find the energy of the state you use the derviative expression for it coming from its definition in terms of p. Then you can measure the average value of

$$E = \frac{p^2}{2m} + u = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U \tag{16}$$

in this state and you'll find

$$< E >= \frac{1}{4}E_1 + \frac{3}{4}E_2 \tag{17}$$

but any time you measure E in this state it will be either E_1 or E_2. The average measurement can be anything depending on the mix of ψ_1 and ψ_2 but the individual measurements for this case have to be either E_1 or E_2.