1 A Look at Quantum Mechanics

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1.1 From classical to quantum worlds

Classical mechanics works very well for describing how many of the day-to-day things we encounter move and change. Classical mechanics (when it wasn't called classical mechanics) was used back in the late 1600s by physicists like Issac Newton and Johannes Kepler to describe very accurately, the motion of the planets. Theoretically, given initial conditions for some particle in a system, classical mechanics can tell you exactly what will happen to a particle in the future - where it will be and how fast it is going.

However, for very small objects, classical mechanics falls apart. When we are working with things like molecules, atoms, and down to the smallest subatomic particles, predictions from classical mechanics are very inaccurate and the big reason for this is really not intuitive: almost everything that happens with atoms and so on has uncertainty. Whereas there is zero uncertainty in how things move in classical mechanics, in quantum mechanics we can't know for sure where something is or where it is going.

So why do we use quantum mechanics? Quantum mechanics is still very powerful for predictions - it's just that they are *statistical* predictions - for example we can calculate a particles *expected* location, and we can calculate exactly *how* uncertain this prediction is. For this reason, averages, standard deviations, and probability distributions are all very important.

1.2 Wavefunctions

For simplicity, we will stick to particles which can only move in one dimension, like a point along a number line. Consider one particle, and let the quantity x represent a position along our line. In quantum mechanics, since we cannot express a particle's position exactly, we use "wavefunctions", written as $\psi(x)$, as a sort-of probability distribution for the likelihood of finding the particle at x - called "probability amplitudes". One important distinction however is that the probability of finding our particle at x is not given by $\psi(x)$, but rather it's absolute square:

$$p(x) = |\psi(x)|^2 \tag{1}$$

This is the "probability density" distribution for our particle position, which must be integrated over to find the probability that the particle is in a certian window. For eaxmple, if we want to find the probability that out particle is between two values of x, say is in the interval $[a, b]$, then we simply integrate $p(x)$ from a to b:

$$P(a \leq x \leq b) = \int_a^b p(x)\, dx = \int_a^b |\psi(x)|^2\, dx$$

As we do this, we are "counting up" all the probabilities in this window - the sum of which should be the total probability we're looking for. For this reason, it's important that when

we integrate from $-\infty$ to ∞, we get 1, since the particle should have a 100% chance of existing somewhere on the line. This is called normalization, and it's summed up in the following *requirement* for a wavefunction:

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

We introduce wavefunctions because much of the math of quantum mechanics cannot be expressed only in terms of $p(x)$, but $p(x)$ can always be easily found for any wavefunction. (The reason for this is that $p(x)$ is always a real valued function - but quantum mechanics relies heavily on the power granted by complex-valued function, which the wavefunction, in general, is.)

1.3 The Schrodinger equation

The central equation which describes location and motion for a single particle in quantum mechanics is the Schrodinger equation:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x) \tag{3}$$

Here $\psi(x)$ is the wavefunction of the particle and $V(x)$ is a function which gives the potential energy of the particle for every point x. $\hbar$ is called the reduced plank constant, m is the mass of the particle, and E is the energy of the particle. In many cases, these are all constant, and assuming $V(x) = V_0$ is also constant, then we can rewrite the Schrodinger equation in the following form, combining all these constants into one big constant, A.

$$\frac{d^2}{dx^2}\psi(x) = -A\psi(x) \tag{4}$$

where

$$A = \frac{2m(E - V_0)}{\hbar^2} \tag{5}$$

It's this form of the Schrodinger equation that we'll use to study how quantum mechanics describes a particles motion.

2 Particle in a well

The "particle in a well" problem is one of the most fundamental of all quantum physics problems - and a favorite of every quantum physics class. The system consists of a single particle trapped in an infinite potential, and we wish to describe where the particle is in the well. The following is adapted from

> A.P. French and Edwin Taylor (1978). *Introduction to Quantum Physics* (1st ed.). The M.I.T. Introductory Physics Series. ISBN 978-0393091069.

see this for a more complete description.

2.1 Statement

Suppose we have a particle with mass m sitting on our 1D number line between two "walls" which the particle cannot pass at $x = 0$ and $x = L$, i.e. our potential function is

$$V(x) = \begin{cases} 0 & 0 \le x \le L \\ +\infty & \text{else} \end{cases}$$

The particle is free to move around inside the well with $V_0 = 0$, but can never be outside it, i.e. $\psi(x < 0) = \psi(x > L) = 0$. Our job is to find the wavefunction $\psi(x)$.

2.2 Solution

Since all possible locations of the particle, we have a constant $V_0 = 0$ potential, we can use Eqn. 4 to solve for the wavefunction. This equation is a second-order ordinary differential equation. This just means the highest order derivative in the equation is second order and our function, $\psi(x)$, is a single variable function. We can solve this differential equation for $\psi(x)$, by asking ourselves "what kind of function is equal to its own second derivative (up to a constant)?". Functions that come to mind might include e^x, $\sin x$, and $\cos x$.

While it looks like a few functions could do the trick, we have boundary conditions to apply which occur at each "wall": $\psi(x < 0) = \psi(x > L) = 0$ which happens to imply that $\psi(0) = \psi(L) = 0$ (since $\psi(x)$ must be continuous). For this reason, an exponential function cannot work since exponentials will never equal 0 at more than one point; furthermore $\cos x$ cannot work since we need our function to go to zero at 0. It happens that $\sin x$ is the correct form for our $\psi(x)$ since it satisfies the first boundary condition, $\psi(0) = 0$ where other functions fall.

So far we have the following for our wavefunction,

$$\psi(x) = C \sin(\omega x)$$

Where C, the amplitude, and ω, the angular frequency, have yet to be determined. We can determine ω by plugging $\psi(x)$ into Eqn. 4, and solving:

$$\frac{d^2}{dx^2}\psi(x) = -A\psi(x) \quad \rightarrow \quad \frac{d^2}{dx^2}(A\sin(\omega x)) = -A \cdot C\sin(\omega x)$$
$$\rightarrow \quad -\omega^2 A\sin(\omega x) = AC\sin(\omega x)$$
$$\rightarrow \quad \omega = \sqrt{A}$$

And so far
$$\psi(x) = C\sin(\sqrt{A}x)$$

but we have the other $\psi(L) = 0$ boundary condition to apply. i.e.

$$\psi(L) = C\sin(\sqrt{A}L) = 0$$

And this only occurs for $\sqrt{A}L = n\pi$ for $n = 0, 1, 2, \ldots$. So, it *must* be the case that $\sqrt{A} = \frac{n\pi}{L}$. How can be be sure this is even possible? Recall A in Eqn. 5. m, V_0, and $\hbar$ are all constants, the only "variable" in Eqn. 5 is the energy E. Indeed substituting our formula for A into the relation $\sqrt{A}L = n\pi$ give a striking *requirement* for the energy E of the particle:

$$\sqrt{A}L = n\pi \quad \rightarrow \quad \sqrt{\frac{2m(E-V_0)}{\hbar^2}}L = n\pi$$

$$\rightarrow \quad E = \frac{n^2\pi^2\hbar^2}{2mL^2} + V_0 \quad \text{for } n = 1, 2, 3, \ldots$$

The energy of the particle is *quantized* (hence "quantum mechanics"), meaning the energy can only take on discrete values determined by the integers n. This is very unlike classical mechanics. We call each of these discrete possible energies "energy levels" of our particle in the well.

Now that we know $\sqrt{A} = \frac{n\pi}{L}$ is legal, we can update our formulation for the wavefunction to be
$$\psi(x) = C\sin\left(\frac{n\pi}{L}x\right)$$

Note that for each n, we get a unique wavefunction corresponding to that energy level. All that remains it to find the constant C. We've satisfied the boundary conditions already, so the only remaining requirement is to normalize the wavefunction. This is done by calculating the integral in Eqn. 2, and finding C such that it equals 1:

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx$$
$$= \int_0^L C^2 \sin^2(\omega x) \, dx$$
$$= \frac{1}{2}C^2 L \quad \rightarrow \quad C = \sqrt{\frac{2}{L}}$$

And so we finally have a full representation for our wavefuntion *for each energy level n*, denoted as $\psi_n(x)$, and given by

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) & 0 \leq x \leq L \\ 0 & \text{else} \end{cases} \tag{6}$$

where the energy levels of the particle, denoted by E_n, are

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} + V_0 \quad \text{for } n = 1, 2, 3, \ldots \tag{7}$$

2.3 Conclusion

An important take-away from the above is that energy levels are quantized - not just in this system, but all quantum mechanical systems. And interestingly, this result comes out of pure mathematical necessity - in order to satisfy boundary conditions. Of course this has been confirmed by experiments to indeed happen in nature, but it is worth noting that it also comes mathematically from making little to no assumptions about how nature works.

We were also able to apply many problem solving ideas core to many physics problems: solving a differential equation, applying boundary conditions, and calculating a normalization factor. And we did this to successfully calculate the wavefunction for a quantum system!

3 Extensions and further reading

I recommend looking at the following texts if you're interested in learning more.

A.P. French and Edwin Taylor (1978). *Introduction to Quantum Physics* (1st ed.). The M.I.T. Introductory Physics Series. ISBN 978-0393091069.

David Griffiths (2004). *Introduction to Quantum Mechanics* (2nd ed.). Prentice Hall. ISBN 978-0-13-111892-8.

Here are some big ideas which we weren't able to discuss...

So far we've explored the beginnings of 1-dimensional quantum mechanics. Of course, our world is not one-dimensional, we also want a complete description of two-dimensional, three-dimensional, and in general, n-dimensional systems. The things were familiar live in 3-dimensional and 4-dimensional worlds, and when we consider systems with more than one particle, the number of dimensions is unbounded. Wavefunctions, the Schrodinger equation, and everything else we've discussed extend very nicely to multiple dimensions, it's just that we need to make the jump from single variable to multivariable calculus to do the math.

One topic we also bypassed was how exactly the uncertainty of measurements (of location and momentum) cannot be exactly zero. The "uncertainty principle" governs this principle and actually gives a relationship between the uncertainty in location measurements and the uncertainty in momentum measurements.

We also want to express systems in the real world with quantum mechanics - while the particle in the well serves as quite a good approximation to some physical system, there are much more complex and interesting problems to solve. One of the main ones, and an important triumph of quantum mechanics, is giving a full description of the hydrogen atom. We can find its wavefunctions, energy levels, orbitals, how it behaves in different electric and magnatic fields, etc.

Much more advanced topics include quantum field theory and quantum electrodynamics. Both of these fields address shortcomings of quantum mechanics including relativistic effects, high energy particles, and systems where interactions, production, and annihilation of particles takes place. If you are interested in these, have a look at

Richard Feynman (1988). *QED: The Strange Theory of Light and Matter.* Princeton University Press. ISBN 978-0691024172.

for a short and more qualitative picture of QED.

Worksheet

1. [easier] The "particle in a well" system is defined to have the potential energy function

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ +\infty & \text{else} \end{cases}$$

where $L > 0$. Graph the function $V(x)$ and find what potential energies the particle would have at $x = \frac{L}{2}, L, L+1$.

2. [easier] If a particle is in the "particle in a well" system (with $V_0 = 0$ and $L = 1$), and is in the first energy state, then the particle has the energy

$$E_1 = \frac{\pi^2 \hbar^2}{2m}$$

Suppose out particle is an electron with mass $m_e = 9.1 \times 10^{-31}$ kg and $\hbar = 1.05 \times 10^{-34}$ m^{2}kg/s. Using a calculator, find E_1 for our electron.

3. [easier – medium] Consider the "particle in a well" system at the three lowest energy levels: $n = 1, 2, 3$. Sketch the function $p(x)$ (defined in Eq. 1) for each of these values of n.

4. Consider the "particle in a well" system.

   (a) [medium – has integration] Suppose our particle is measured to be in the first energy level, $n = 1$. What is the probability that our particle is in the "left" half of the well given by $[0, L/2]$. Explain why this probability makes sense.

   (b) [medium] For the particle in part (b), what is the probability it is in the right half of the well $[L/2, L]$? Explain why the probabilities from part (a) and (b) make sense.

   (c) [tricky – integration] Suppose there are now two particles in the well incapable of interaction, one in the $n = 1$ energy level, and the other in the $n = 3$ energy level. (It's important they are incapable of interaction so they can't change energy levels after observation). What is the probability that the particles will both be in the region $[L/4, L/2]$ simultaneously?

5. [medium - can be done without knowing much about differential equations] A central idea of quantum mechanics stems from the mathematical fact that scalar multiples of a solution to the Schrodinger equation gives other solutions. If we have a wavefunctions $\psi(x)$ which is a solution to the Schrodinger Equation - Eqn. 3, then the wavefunction

$$\Psi(x) = \alpha \psi(x)$$

is also a solution for all real constants α. Show, by plugging into Eqn. 3, that if $\psi(x)$ satisfies the Schrodinger equation then $\Psi(x)$ also satisfies the Schrodinger equation as claimed above.