1 Recap

The Schroedinger equation is a PDE that describes an electron (or other particle) moving in a specific potential $V(\vec{r})$.

$$i\hbar\frac{\partial\psi}{\partial t} = \underbrace{-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)}_{\text{kinetic energy}} + \underbrace{V(x,y,z)\psi}_{\text{potential energy}} \tag{1}$$

PH 425	Quantum fundamentals
PH 426	Central forces
PH 427	Periodic systems
PH 451	Quantum capstone

Figure 1: OSU Physics classes that cover quantum mechanics in more detail.

When we change the potential energy, we change the PDE, and with a different PDE we expect to find a different set of standing waves. Historically, only four potential energies are taught in QM classes, because these are (almost) the only four that can be solved by hand.

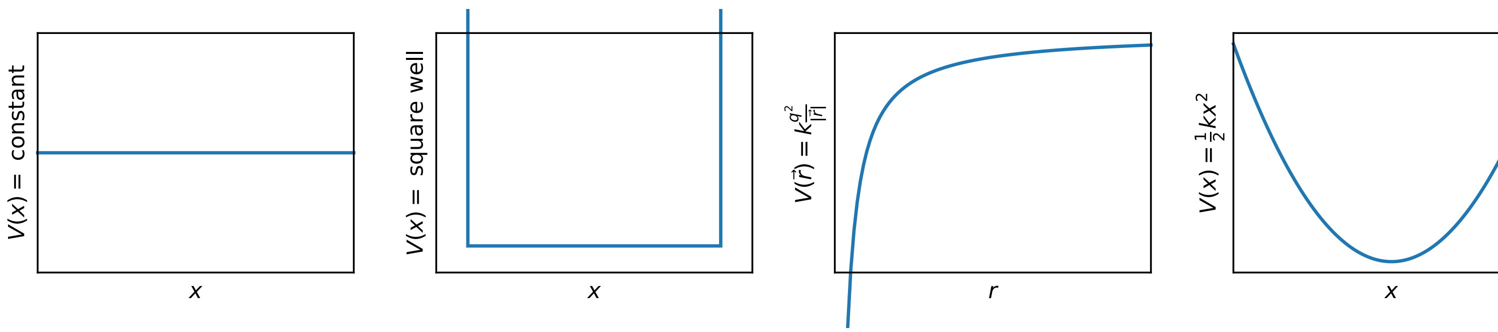

Figure 2: **Exactly solvable systems:** constant potential (PH 426), square well potentials (PH 425 and PH 427), $1/r$ potential in 3D (PH 426), and parabolic potentials (also known as harmonic oscillator) (PH 451).

2 Example: harmonic oscillator

Note: this section is for your edification, but will involve math that I don't expect you to be able to solve yet by yourselves. Let's start with the example I animated last time, which was 1D a harmonic oscillator. We need to start by writing down the PDE, which just involves replacing $V(x,y,z)$ with $\frac{1}{2}kx^2$ and removing the y and z derivatives:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2\psi \tag{2}$$

Now this is a differential equation, so to solve it we need to guess at a form for the solution. I'll start by assuming it's a standing wave which means that

$$\psi(x,t) = \psi(x,t=0)e^{-i\omega t} \tag{3}$$

This causes the time dependence to just rotate in the complex plane while the probability density doesn't change. ω is the angular frequency, and we don't yet know what its value is. So now we just need to guess a function for $\psi(x, t = 0)$. Since the particle is bound by the spring, we want a function that approaches zero as $|x| \to \infty$. **Spend 5 minutes coming up with one or more guess functions of x that are continuous, differential, and go to zero as $x \to \pm\infty$.**

3 Summary: How to solve quantum mechanics

(This is seriously oversimplified!)

1. Write down the PDE with the desired $V(x, y, z)$.
2. Solve (or look up) the standing waves $\psi_n(x, y, z, t)$.
3. List the frequencies ω_n associated with each ψ_n.
4. $\hbar\omega_n \to$ energy level diagram.
5. Energy differences gives optical emmission or absorption spectra.

Different potential energies give different energy level diagrams. There are also different rules (called *selection rules*) for which energy levels can have transitions that involve emitting or absorbing light.

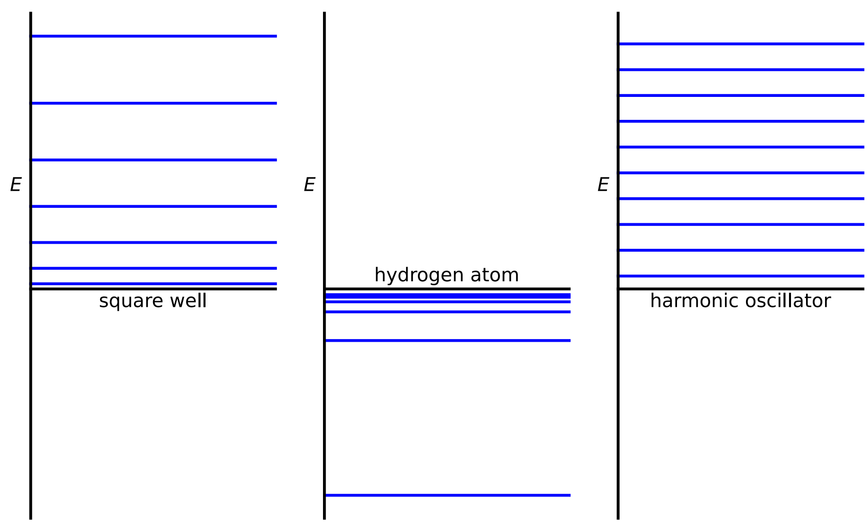

Figure 3: Energy level diagrams for the three exactly solvable bound systems shown above.

4 Example: hydrogen molecular ion

Example: Write down V for the electron in an H_2^+ ion.

Let's consider a simple physical system that we *can't* solve analytically, but it would be good to at least figure out how to write down the potential energy. In this case, we will treat the two nuclei (protons) as stationary. This is called the Born-Oppenheimer Approximation, and can be justified because the mass of the proton is far greater than the mass of the electron. We define the positions of the protons as $\vec{R_1}$ and $\vec{R_2}$, and that of the electron as $\vec{r}$.

$$V(\vec{r}) = -k\frac{e^2}{|\vec{r} - \vec{R_1}|} - k\frac{e^2}{|\vec{r} - \vec{R_2}|} \tag{4}$$

where e is the charge of an electron, and k is Coulomb's constant (which is 1 in sane sets of units, and is $\frac{1}{4\pi\epsilon_0}$ in SI units).

5 Example: free particle (and de Broglie wavelength)

We can next consider an even simpler case (but less like the general case), which is a free particle, with potential $V = 0$ moving in just one dimension. This is a much simpler differential equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \tag{5}$$

So once again we need to look for a solution. Since we have already established that we want to find a "standing wave" or energy eigenstate solution, we know the time dependence (in terms of an unknown ω) and can skip a couple of steps to find that

$$\hbar\omega\psi(x, t = 0) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \tag{6}$$

so we are looking for a function of x that if we take two derivatives gives us the same function back again. **Do you have any guesses? There are actually several correct answers.**

$$\psi(x, t = 0) = e^{\kappa x} \tag{7}$$
$$\psi(x, t = 0) = e^{ikx} \tag{8}$$
$$\psi(x, t = 0) = \cos(kx) \tag{9}$$
$$\psi(x, t = 0) = \sin(kx) \tag{10}$$

Any of these waves will work fine, although the first one will end up giving us an imaginary κ. Physicists tend to prefer the second one.

$$\psi(x, t) = \psi(x, t = 0)e^{-i\omega t} \tag{11}$$
$$= e^{ikx}e^{-i\omega t} \tag{12}$$
$$= e^{i(kx-\omega t)} \tag{13}$$

You can now see a patter quite similar to the travelling waves on a string we looked at earlier.

$$\psi(x, t = 0) = e^{\kappa x} \qquad \frac{\partial\psi}{\partial x} = \kappa\psi \qquad \frac{\partial^2\psi}{\partial x^2} = \kappa^2\psi \tag{14}$$
$$\psi(x, t = 0) = e^{ikx} \qquad \frac{\partial\psi}{\partial x} = ik\psi \qquad \frac{\partial^2\psi}{\partial x^2} = -k^2\psi \tag{15}$$
$$\psi(x, t = 0) = \cos(kx) \qquad \frac{\partial\psi}{\partial x} = -k\sin(kx) \qquad \frac{\partial^2\psi}{\partial x^2} = -k^2\psi \tag{16}$$
$$\psi(x, t = 0) = \sin(kx) \qquad \frac{\partial\psi}{\partial x} = k\cos(kx) \qquad \frac{\partial^2\psi}{\partial x^2} = -k^2\psi \tag{17}$$

Putting any of the three guesses with k in them into our PDE gives us

$$-\hbar\omega\psi = \frac{\hbar^2 k^2}{2m}\psi \tag{18}$$

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \tag{19}$$

$$KE = \frac{\hbar^2 k^2}{2m} \tag{20}$$

$$\frac{\not{1}}{\not{2}}mv^2 = \frac{\hbar^2 k^2}{\not{2}m} \tag{21}$$

$$mv = \hbar k \tag{22}$$

So we can see that $\hbar k$ is the momentum, just as $\hbar\omega$ is the energy. (The latter I haven't proven to you.) This relationship is why we like k so much, it's the momentum in "quantum units". Since $\psi \propto \sin kx$ we can also write down that

$$k = \frac{2\pi}{\lambda} \tag{23}$$

$$\lambda = \frac{2\pi}{k} \tag{24}$$

$$= \frac{2\pi\hbar}{p} \tag{25}$$

This is the de Boglie wavelenth expression, which just falls out of the wave equation.