Section 1: Intro to Quantum Mechanics

Thursday, September 16, 2021 9:52 PM

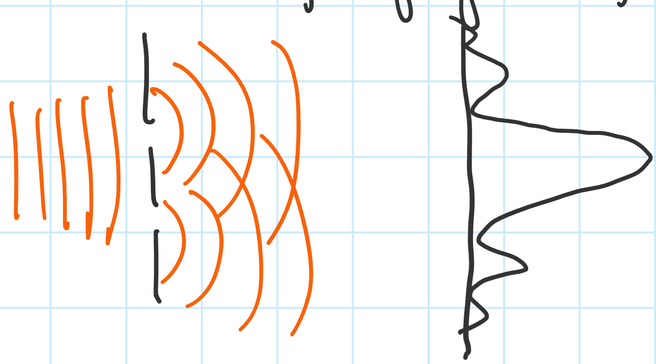
Disclaimer:

The following will include a lot of complicated math and can be overwhelming at first glance. However, for this class and in general as you continue along your careers, I would like to emphasize that typically the gory details of the derivation are not nearly as important as the final results and the physical intuition. So, for this section I will try to emphasize those points, and tell a story through the math as it were.

I The Wave Function

a) Why waves?

Consider light going through two slits



Interference pattern emerges!

This is b/c the electric fields are adding and subtracting together,

$E_1(x) + E_2(x)$

However, the measurable quantity is not E, but rather the intensity $I \propto |E|^2$

Well, we could do a similar thing w/ particles (say, an electron beam)

In this case, we get a similar looking interference pattern

$\Longrightarrow$ Wave phenomena

However, the pattern arises asymptotically, that is, any particular electron could show up anywhere (can't predict), show up anywhere (can't predict), but in the limit of a lot of electrons the distribution energies.

$\Rightarrow$ probabilistic theory

So in keeping with this train of thought we might say:

1) Wave theory
2) Measurable quantity is some probability distribution
3) The measurable quantity should be related to $|\text{wave}|^2$

b) Schrodinger Equation

$$\boxed{i\hbar \frac{\partial}{\partial t} \Psi(x,t) = H\,\Psi(x,t)}$$

$\hbar$: Reduced Planck constant, $= h/2\pi$

Ψ : wave function

H : Hamiltonian, equal to total

energy $T + V$

kinetic $\quad$ potential

This equation governs the time and spatial evolution of $\Psi(x,t)$. Physically, while wave functions can interfere w/ each other, what we find useful is $|\Psi|^2$, which is the probability density function to find the particle within some position

$$dP(x) = |\Psi(x,t_0)|^2\, dx$$

$$P(a \le x \le b) = \int_a^b |\Psi(x,t_0)|^2\, dx$$

If we want to find the expected value of particle position x,

$$\langle x \rangle = \int_{-\infty}^{\infty} x\, |\Psi(x,t_0)|^2\, dx$$

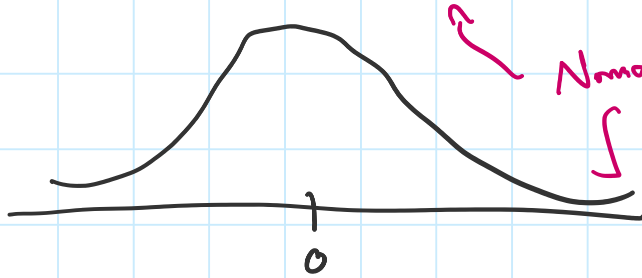
Ex: What is the expected position of a particle with wave function

$$\Psi(x,t_0) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{-x^2/4\sigma^2} \quad ?$$

$|\Psi(x,t)|^2 = \Psi^* \Psi$

$$|\Psi(x,t_0)|^2 = \Psi^* \Psi$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}$$



Normalization factor!

$$\int |\Psi|^2 dx = 1$$

We could calculate the integral

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi|^2 dx = \int_{-\infty}^{\infty} \frac{x}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}$$

but since we have an even function times an odd, $\langle x \rangle = 0$

Without proof, I will also claim that the Hamiltonian can be written as

$$H = T + V = \frac{p^2}{2m} + V(x)$$

$$= \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

Why $\frac{p^2}{2m} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$ is an interesting question, but not important for this class. Rather, I'd like to point out the potential energy term $V(x)$, which the potential energy term $V(x)$, which is what often changes and results in different (thus interesting phenomena)

c) Solving the Schrodinger Eqn

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + V(x)\Psi$$

Separation of variables:

- Guess: $\Psi(x,t) = \psi(x)\,T(t)$

$$i\hbar\,\psi(x)\frac{dT(t)}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}T(t) + V(x)\psi(x)T(t)$$

- Group terms by variable:

$$i\hbar \frac{dT/dt}{T} = -\frac{\hbar^2}{2m}\frac{d^2\psi/dx^2}{\psi} + V(x)$$

- For these to always be equal despite depending on different variables, the must be equal to a <u>constant.</u>

$$i\hbar \frac{dT/dt}{T} = E$$

$$\rightarrow \frac{dT}{dt} = -\frac{iE}{\hbar}T$$

$$\rightarrow T(t) \propto e^{-iEt/\hbar}$$

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

$\overline{\quad}$
ψ

$$\Rightarrow \boxed{\begin{array}{c} -\dfrac{\hbar^2}{2m}\dfrac{d^2\psi}{dx^2} + V(x)\psi = E\psi \\ H\psi = E\psi \\ \text{Time-Independent Schrodinger Eqn} \end{array}}$$

This is an eigenvalue equation, where the energy E is the eigenvalue. One would typically solve for the energy eigenvalues and eigenfunctions.

(2) Potential Wells

a) Example: Infinite Square Well

$$V(x) = \begin{cases} 0 & 0 \le x \le L \\ \infty & x < 0, \\ & x > L \end{cases}$$

TISE: $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad 0 \le x \le L$$

$$\psi(x<0) = \psi(x>L) = 0$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

$$s^2 = -\frac{2mE}{\hbar^2}$$

$$s = i\sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi(x) = A\, e^{i\sqrt{\frac{2mE}{\hbar^2}}x} + B\, e^{-i\sqrt{\frac{2mE}{\hbar^2}}x}$$

$$\psi(x) = A_- e^{i\sqrt{\frac{2mE}{\hbar^2}}x} + B_- e^{-i\sqrt{\frac{2mE}{\hbar^2}}x}$$

$$= A\cos\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) + B\sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right)$$

Boundary conditions:

$$\psi(x=0) = 0$$
$$\psi(x=L) = 0$$

$$\Rightarrow \psi(0) = A = 0$$
$$\psi(L) = B\sin\left(\sqrt{\frac{2mE}{\hbar^2}}L\right) = 0$$

$$\Rightarrow \sqrt{\frac{2mE}{\hbar^2}}L = n\pi, \quad n \in \mathbb{Z}$$

Multiple possible solutions! E is the only thing that is unknown, so index by n to create a "spectrum" of energy.

$$\sqrt{\frac{2mE_n}{\hbar^2}}L = n\pi$$

$$\Rightarrow E_n = \frac{(n\pi\hbar)^2}{2mL^2}$$

For convenience, also define

$$k_n = \frac{\sqrt{2mE_n}}{\hbar}$$

In conclusion,

- $E_n = \frac{(n\pi\hbar)^2}{2mL^2}$

- $\psi_n(x) = B \sin\left(\frac{n\pi x}{L}\right)$,

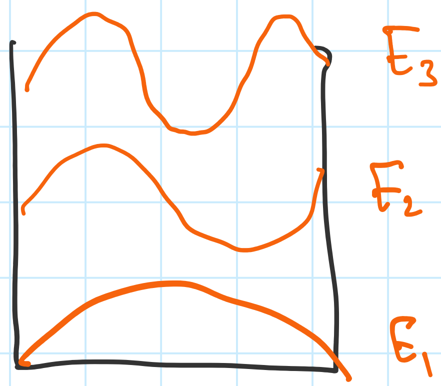
  $n = 1, 2, 3 \ldots$

  (What is B? exercise for the reader)

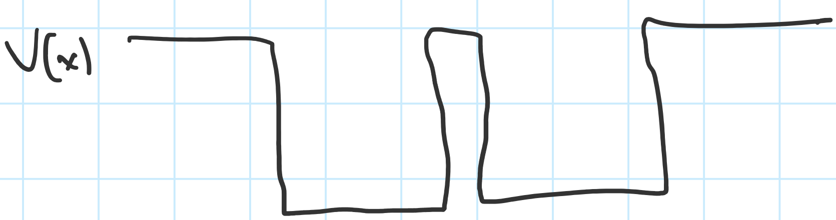
- Discrete spectrum of energies

  $\Longrightarrow$ quantization !

- Like normal modes of a string

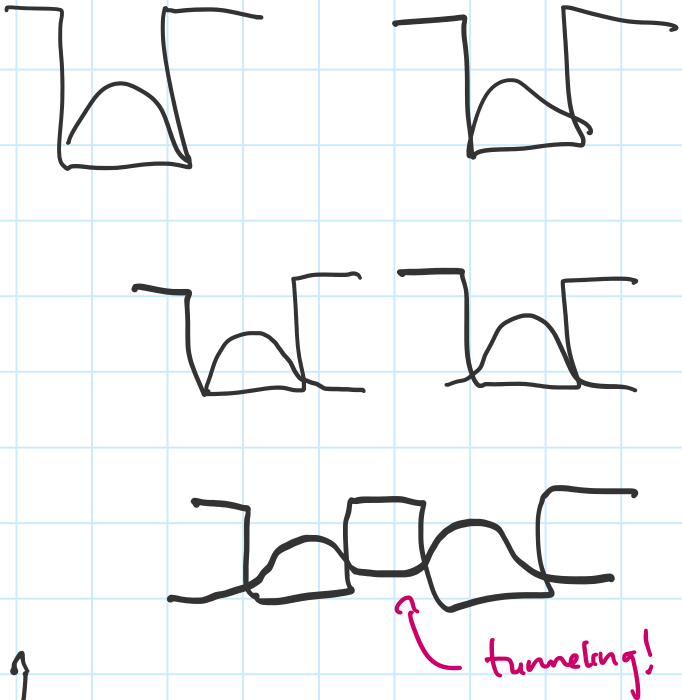


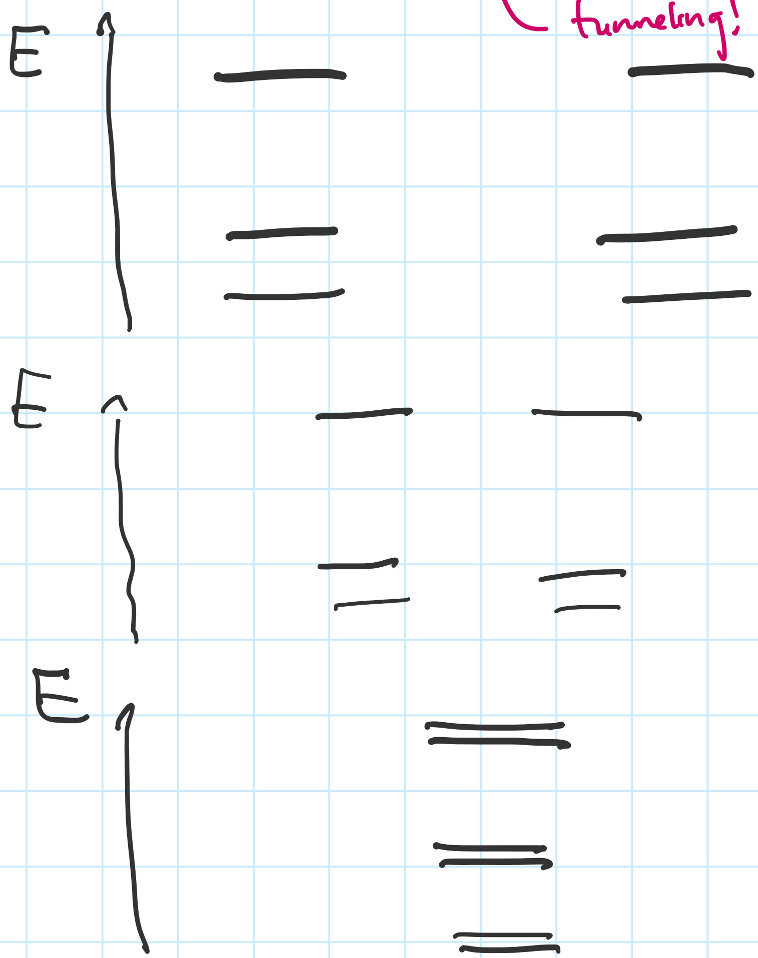
b) Coupled Potential Wells



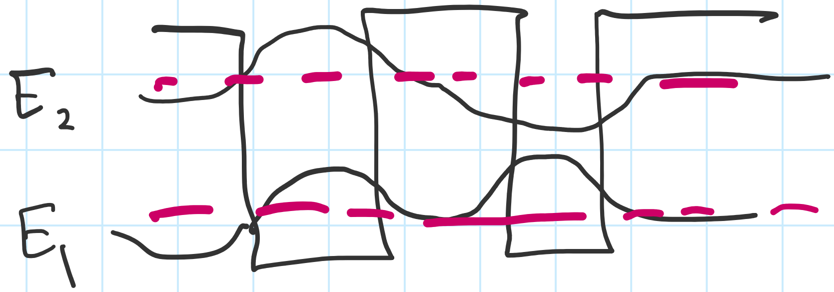
What do you think will happen?

Isolated wells:

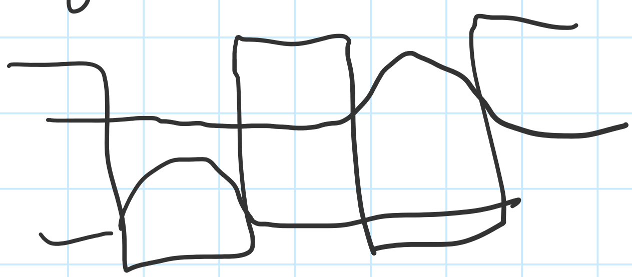




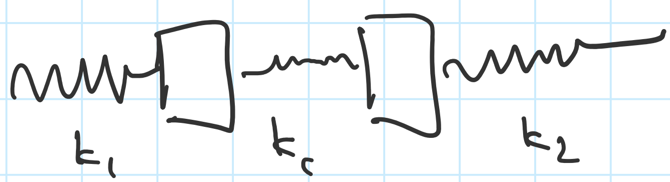
Specifically, our energy eigenstates become "coupled", forming symmetric / antisymmetric modes



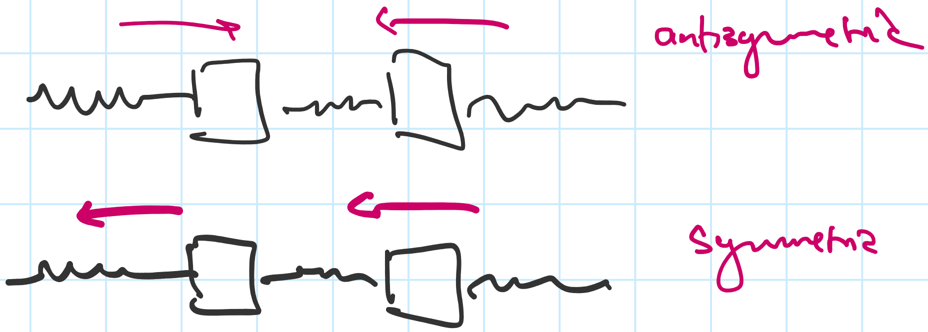
Why does this happen? Why not prefer these eigenstates?



Consider coupled oscillators:



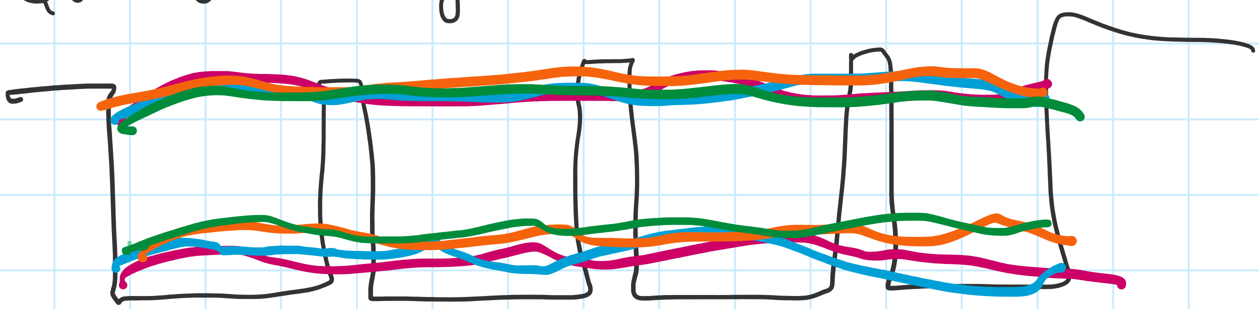
At a certain point, doesn't make sense to think of exciting just one spring → have to excite both.



Returning to the wells, it makes more sense to think of the particle having sense to think of the particle having equal probability of being located in either well — its wave function is "split" between the two because of the coupling (via QM tunneling).

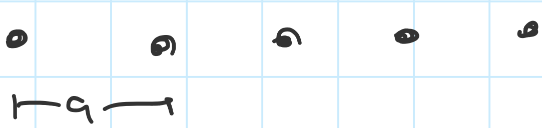
c) Multiple Quantum Wells

QW Java Widget here?



"Bands" form!

3 Periodic Potential



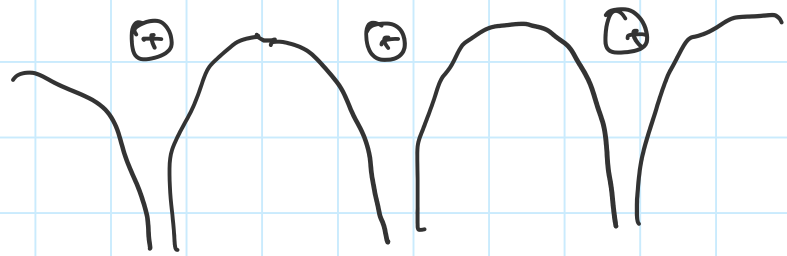
Crystal lattice has periodicity

$\Rightarrow$ expect potential to be periodic

$$V(x+a) = V(x)$$

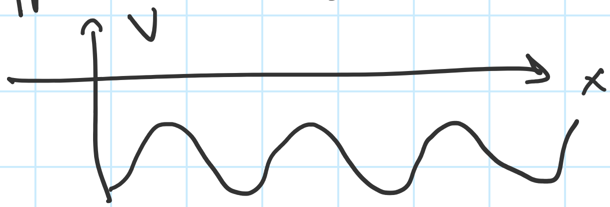
Physically Coulomb potential

Physically, Coulomb potential



(from positively charged nucleus)

Approximation: $V(x) = V_0 + V_1 \cos\left(\frac{2\pi x}{a}\right)$



Free particle:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

de Broglie wavelength

$$\Rightarrow \psi(x) \propto e^{\pm ikx}$$

$$\text{where } k = \frac{\sqrt{2mE}}{\hbar} = \frac{2\pi}{\lambda}$$

Traveling waves!

$$\Psi(x,t) = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}$$

+x dir   −x dir

Consider $k = \frac{\pi}{a}$ $(\lambda = 2a)$:

Bragg interference: $n\lambda = 2a\sin\theta$

$\Rightarrow n=1, \ \theta = 90^\circ$

$\Rightarrow \lambda = 2a$

(Point 3, strong interference occurs when $\lambda \sim a$, i.e. same order $\longrightarrow$ "sees" more of the potential)

$\xrightarrow{\quad Ae^{ikx} \quad}$ electron going this way...

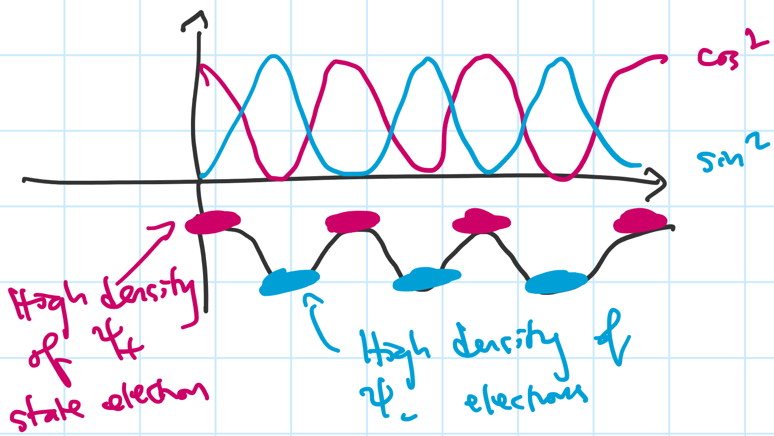
$\xleftarrow{\quad Be^{-ikx} \quad}$ ... gets reflected back

Those parts interfere to form standing waves, like on a string.

$$\psi_\pm \propto \left[e^{ikx} \pm e^{-ikx} \right] e^{-i\omega t}$$

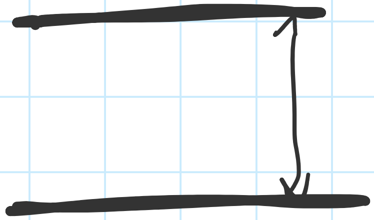
$$\propto \cos(kx) e^{-i\omega t}$$

$$\text{or } \sin(kx) e^{-i\omega t}$$



ψ_-: lots of electrons at minimum of potential $\longrightarrow$ low energy

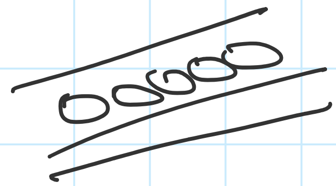
ψ_+: lots of electrons at maximum of potential $\longrightarrow$ high energy



split energy levels
$\Rightarrow$ bandgap!

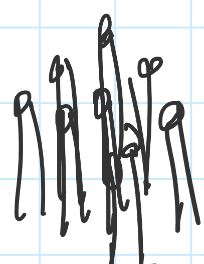
Bottom line: a periodic potential creates a bandgap for waves.

See: • photonic crystals



$\Rightarrow$ periodic index of refraction n

• phononic crystals



"Órgano", Eusebio Sempere
Nature 378, 241 (1995)

$\Rightarrow$ periodic Young's modulus Y