Particle in an Infinite Well

- Consider the following equation

$$\nabla^2 \psi(x,y) = -\alpha \psi(x,y)$$

where $\alpha > 0$. Can we solve this w/ the boundary conditions $\psi(0,y) = \psi(L,y) = \psi(x,0) = \psi(x,W) = 0$?

- Sure, let's start w/ S.o.V. & look for solutions $f(x)g(y)$:

$$g(y)\frac{\partial^2 f(x)}{\partial x^2} + f(x)\frac{\partial^2 g(y)}{\partial y^2} = -\alpha f(x) g(y)$$

$$\hookrightarrow \frac{1}{f(x)}\frac{\partial^2 f(x)}{\partial x^2} + \frac{1}{g(y)}\frac{\partial^2 g(y)}{\partial y^2} = -\alpha$$

- Now, I listed two homogeneous boundary conditions for both x <u>and</u> y, which suggests trig functions for <u>both</u> variables.

- We couldn't do this for an eqn. like $\nabla^2 u(x,y) = 0$, where trig functions in x imply exponentials in y, and vice-versa.

- But when I apply S.o.V. to $\nabla^2\psi = -\alpha\psi$ this is fine:

$$\frac{1}{f}\frac{\partial^2 f}{\partial x^2} = -k^2 \qquad \frac{1}{g}\frac{\partial^2 g}{\partial y^2} = -p^2 \qquad -k^2 - p^2 = -\alpha$$

That $-\alpha$ $(\alpha>0)$ term on the RHS means I can use a negative S.o.V. constant for both my x & y eqns.

$$\hookrightarrow f(x) = A\cos(kx) + B\sin(ky) \qquad g(y) = C\cos(py) + D\sin(py)$$

$$\text{w/ } k^2 + p^2 = \alpha^2$$

- The B.C. @ $x=0$ tells us $A=0$, and the B.C. @ $x=L$ forces $k = n\pi/L$, $n \in \mathbb{Z}$ & $n \geq 1$.

- Likewise, the B.C. @ $y=0$ & $y=W$ set $C=0$ & $p = m\pi/W$ w/ $m \in \mathbb{Z}$ & $m \geq 1$.

- So our S.o.V. solutions look like

$$f(x)\,g(y) = B \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi y}{W}\right) \qquad \text{w/} \quad \frac{n^2\pi^2}{L^2} + \frac{m^2\pi^2}{W^2} = \alpha.$$

- Now, depending on the value of α, L, & W this may or may not work! Suppose I told you $L = W = 1$ and $\alpha = 25\pi^2$. Then you'd conclude

$$\frac{n^2\cancel{\pi^2}}{1} + \frac{m^2\cancel{\pi^2}}{1} = 25\cancel{\pi^2} \Rightarrow n=3 \text{ \& } m=4 \ \underline{\text{or}} \ n=4 \text{ \& } m=3$$

So in that case there are <u>two</u> solutions.

- But what if I said $L=1$, $W=2$, and $\alpha = 17$

$$\frac{n^2\pi^2}{1} + \frac{m^2\pi^2}{4} = 17 \longleftarrow \text{No solutions w/ } n,m \in \mathbb{Z}!$$

In that case our problem has no solutions!

- Maybe a <u>better</u> question is what values of α let this problem have interesting solutions? In that case the answer is just

$$\alpha = \frac{n^2\pi^2}{L^2} + \frac{m^2\pi^2}{W^2} \qquad n,m \in \mathbb{Z} \text{ \& } \geq 1$$

which combines $k = n\pi/L$ & $p = m\pi/L$ from our boundary conditions w/ the requirement $-k^2 - p^2 = -\alpha$ to make S.o.V. work!

- What does this have to do w/ particles and wells?
- In Quantum Mechanics, a particle w/ mass M that can move in the x & y directions w/ potential energy U(x,y) is described by a <u>WAVE FUNCTION</u> $\Psi(x,y,t)$ that satisfies the Schrödinger Equation:

$$i\hbar \frac{\partial}{\partial t}\Psi(x,y,t) = \left(-\frac{\hbar^2}{2M}\nabla^2 + U(x,y)\right)\Psi(x,y,t)$$

- What if we used S.o.V. to look for sol'ns of the form $T(t)\psi(x,y)$? We'd arrive at:

$$\frac{1}{T(t)} i\hbar \frac{\partial T(t)}{\partial t} = \frac{1}{\psi(x,y)}\left(-\frac{\hbar^2}{2M}\nabla^2 + U(x,y)\right)\psi(x,y)$$

- Both sides must equal a constant for this to work. Let's call that constant 'E'

$$i\hbar\frac{\partial T}{\partial t} = ET \Rightarrow T(t) = (\text{Const})\, e^{-i\frac{E}{\hbar}t}$$

$$-\frac{\hbar^2}{2M}\nabla^2\psi(x,y) + U(x,y)\psi(x,y) = E\psi(x,y)$$

- When E is a positive, real const. we call this a 'Stationary state,' since $\Psi^*(x,y,t)\Psi(x,y,t)$ doesn't change over time. ($\Psi^*\Psi$ is the thing we do with a W.F. to find the probability that the particle is @ position x,y @ time t!)
- This constant E is just the <u>energy</u>.
- Now imagine a potential energy U(x,y) that is zero when $0 \le x \le L$ <u>and</u> $0 \le y \le W$, & <u>infinite</u> everywhere else.

- This is called an 'infinite well' because the particle is trapped in the region $0 \leq x \leq L$ & $0 \leq y \leq W$. No amount of energy lets it 'climb out' since $U = \infty$ outside the well.

- For the wave function this means $\Psi(x,y,t) = 0$ if $x \leq 0$, $x \geq L$, $y \leq 0$, or $y \geq W$, since the particle can never be found there.

- So, inside the ∞-well, the Schrödinger eqn says a stationary state w/ energy E satisfies

$$E\,\psi(x,y) = -\frac{\hbar^2}{2M}\nabla^2\psi(x,y)$$

$$\text{w/ } \psi(0,y) = \psi(L,y) = \psi(x,0) = \psi(x,W) = 0$$

- This is the problem we just solved, with $\alpha = \frac{2ME}{\hbar^2}$!

- Since E was a constant <u>we</u> introduced via S.o.V., our question about "which α work?" now makes more sense.

- A particle of mass M in an ∞-well of length L & width W is only allowed to have certain energies. They are:

The allowed energies are labeled by a pair of integers n & m.

$$E_{n,m} = \frac{\hbar^2\pi^2}{2M} \times \left(\frac{n^2}{L^2} + \frac{m^2}{W^2}\right) \qquad n,m \in \mathbb{Z} \text{ \& } \geq 1$$

The wave function for a state w/ energy $E_{n,m}$ is:

$$\Psi(x,y,t) = (\text{Constant})\, e^{-i\frac{E_{n,m}}{\hbar}t} \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi y}{W}\right)$$

Fixed by requiring $\int_0^L dx \int_0^W dy\, |\Psi(x,y,t)|^2 = 1$

- A few notes about this. First, $\hbar$ has units of J·s, so $E_{n,m}/\hbar$ indeed has units of (angular) frequency & we often write $\omega_{n,m} = E_{n,m}/\hbar$ or

$$\omega_{n,m} = \frac{\hbar \pi^2}{2M}\left(\frac{n^2}{L^2} + \frac{m^2}{W^2}\right)$$

- The W.F. times its 'Complex Conjugate' is related to the probability of detecting the particle in the vicinity of (x,y) around time t

Here, this means Ψ w/ $i \to -i$

$$P(x,y,t) \propto \Psi(x,y,t)\,\Psi^*(x,y,t)$$

Since the particle has to be <u>somewhere</u> in the well, the probabilities have to add up to '1', and this tells us how to <u>Normalize</u> the W.F.

$$1 = \int_0^L dx \int_0^W dy\ \Psi(x,y,t)\,\Psi^*(x,y,t)$$

So if the system is in a state w/ energy $E_{n,m}$

$$1 = (\text{const})^2 \int_0^L dx \int_0^W dy\ \cancel{e^{-i\frac{E_{n,m}}{\hbar}t}} \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi y}{W}\right) \cancel{e^{+i\frac{E_{n,m}}{\hbar}t}} \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi y}{W}\right)$$

$$= (\text{const})^2 \underbrace{\int_0^L dx\ \sin^2\left(\frac{n\pi x}{L}\right)}_{L/2} \underbrace{\int_0^W dy\ \sin^2\left(\frac{m\pi y}{W}\right)}_{W/2}$$

$$\hookrightarrow (\text{const})^2 = \frac{4}{LW} \Rightarrow (\text{const}) = \frac{2}{\sqrt{LW}}$$

So the normalized W.F. for the stationary state (n,m) is

$$\Psi(x,y,t) = \frac{2}{\sqrt{LW}}\, e^{-i\frac{E_{n,m}}{\hbar}t} \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi y}{W}\right)$$

$$\text{w/ } E_{n,m} = \frac{\hbar^2\pi^2}{2M} \times \left(\frac{n^2}{L^2} + \frac{m^2}{W^2}\right)$$