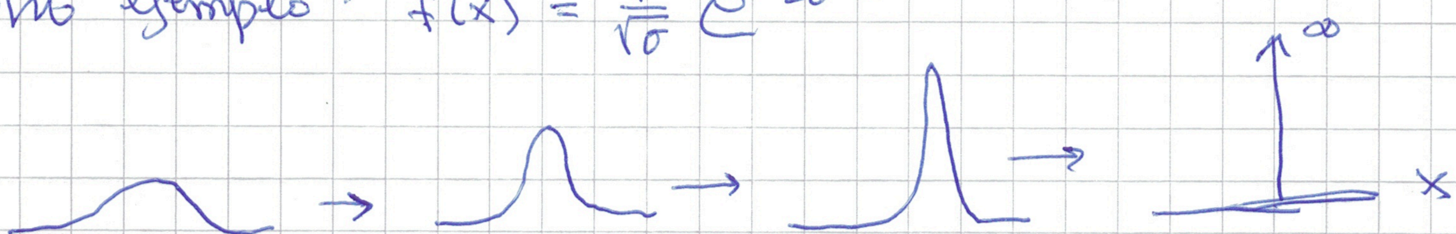
La función $\delta(x)$

considere $f(x) = \begin{cases} 1/a & 0 < x < a \\ 0 & \text{caso contrario} \end{cases}$

toman límite $a \to 0$

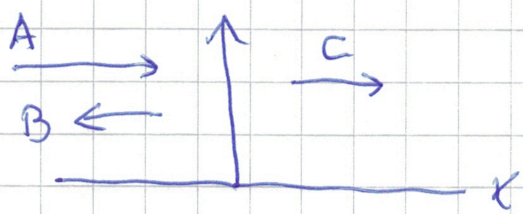
$$\lim_{a \to 0} f(x) = \delta(x) \text{ , donde } \int_{-\infty}^{\infty} \delta(x)\,dx = 1$$

otro ejemplo: $f(x) = \frac{1}{\sqrt{\sigma}} e^{-\frac{x^2}{2\sigma^2}}$



se cumple: $\int_{-\infty}^{\infty} f(x)\,\delta(x-b)\,dx = f(b)$

Scattering a través de una función $\delta(x)$



$$-\frac{\hbar^2}{2m}\psi'' + \Omega\,\delta(x)\,\psi(x) = E\psi$$

(1) $$-\psi'' + \left(\frac{2m\Omega}{\hbar^2}\right)\delta(x)\psi = \frac{2mE}{\hbar^2}\psi$$

def: $\gamma = \dfrac{2m\Omega}{\hbar^2}$

$k^2 = \dfrac{2mE}{\hbar^2}$

$x<0$: $-\psi'' = k^2\psi \Rightarrow \psi = \{e^{\pm ik}\}$

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

$x>0$: $\psi(x) = Ce^{ikx}$

cont. de ψ en $x=0$: $A+B=C$ (2)

discontinuidad de ψ en $x=0$

(1) $\rightarrow$ $-\psi'' + \gamma\,\delta(x)\psi = k^2\psi \quad \Big/ \int_{-\epsilon}^{\epsilon}$

$$-\psi'(x)\Big|_{-\epsilon}^{\epsilon} + \gamma\int_{-\epsilon}^{\epsilon}\delta(x)\psi = k^2\int_{-\epsilon}^{\epsilon}\psi\,dx$$

$$-\psi'(+\epsilon) + \psi'(-\epsilon) + \gamma\psi(0) = 0$$

$$-ikC + ik(A-B) + \gamma C = 0$$

$$ik(A-B) = (ik-\gamma)C$$

$$A-B = \frac{(ik-\gamma)}{ik}C \qquad (3)$$

$$A+B = C$$

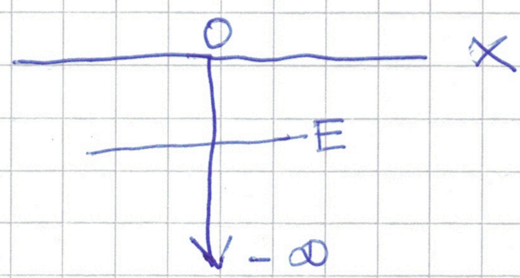
$$2A = C\left\{1+\frac{(ik-\gamma)}{ik}\right\} = \left(\frac{2ik-\gamma}{ik}\right)C$$

$$\Rightarrow \frac{C}{A} = \frac{2ik}{2ik-\gamma} \Rightarrow t = \left|\frac{C}{A}\right|^2 = \frac{1}{1+(\gamma/2k)^2}$$

$$\therefore \quad t = \frac{1}{1+(E_0/E)}, \quad \text{donde } E_0 = \frac{m\Omega^2}{2\hbar^2}$$

Nota: t es el mismo si $\Omega \to -\Omega$

Estado ligado de $V(x) = -\Omega\delta(x)$



$$V(x) = -\Omega\delta(x)$$

$$-\frac{\hbar^2}{2m}\psi'' - \Omega\delta(x)\psi = E\psi$$

$$-\psi'' - \gamma\delta(x)\psi = -k^2\psi$$

donde $\gamma = \frac{2m\Omega}{\hbar^2}$ y $k^2 = -\frac{2mE}{\hbar^2}$ $\quad (E<0)$

entonces, $\psi'' + \gamma\delta(x)\psi = k^2\psi$ (4)

Si $x \neq 0$, $\psi'' = k^2\psi \Rightarrow \psi = \{e^{\pm kx}\}$

$\psi(x) = A e^{-k|x|}$ cont. de ψ en $x=0$ ✓

Discont. de ψ' en $x=0$:

$+ \quad \psi'(\epsilon) - \psi'(-\epsilon) + \gamma\psi(0) = 0$

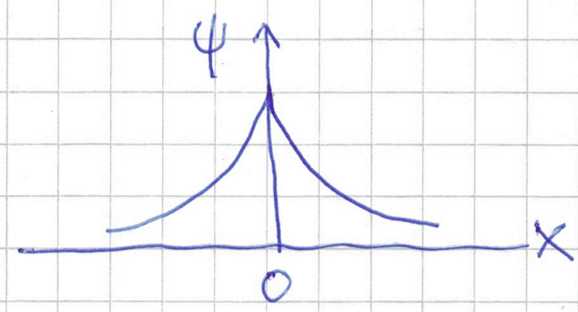
$-Ak - Ak + \gamma A \Rightarrow +2\cancel{A}k = \gamma\cancel{A} \Rightarrow \gamma = 2k$ (5)

$\gamma^2 = 4k^2 = 4\left(-\frac{2mE}{\hbar^2}\right)$

$\left(\frac{2m\Omega}{\hbar^2}\right)^2 = \frac{8m|E|}{\hbar^2} \Rightarrow \boxed{|E| = \frac{m\Omega^2}{2\hbar^2}}$ (6)

Normalización $\quad 1 = \int_{-\infty}^{\infty} |\psi|^2 dx = \int_{-\infty}^{\infty} A^2 e^{-k|x|}$

$\Rightarrow A = \sqrt{\frac{m\Omega}{2\hbar^2}}$



$\psi(x) = \sqrt{\frac{m\Omega}{2\hbar^2}}\, e^{-\left(\frac{m\Omega}{\hbar^2}\right)|x|}$

Ec. Schrödinger en 2D: caso fácil

$$H(x,y)\,\Psi(x,y) = E\,\Psi(x,y)$$

Sea $H(x,y) = H_x(x) + H_y(y)$

entonces $\psi(x,y) = X(x)\,Y(y)$ (separación variables)

con $H_x(x)X(x) = E_x X$

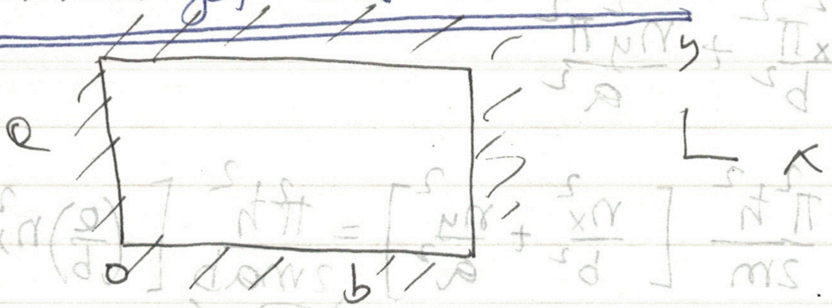
$H_y(y)Y(y) = E_y Y$

$$\Rightarrow (H_x + H_y)XY = (H_x X)Y + X(H_y Y) = E_x XY + E_y XY$$

$$= (E_x + E_y)XY$$

$$\therefore \boxed{\begin{array}{c} E = E_x + E_y \\ \psi(x,y) = X(x)Y(y) \end{array}}$$

Schrödinger Eq. in 2-D



$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y) = E\,\psi(x,y)$$

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y) = k^2\,\psi(x,y)$$

$$\psi(x,y) = X(x)\,Y(y)$$

$$\Rightarrow -X''Y - XY'' = k^2 XY$$

$$\Rightarrow \underbrace{-\frac{X''}{X}}_{k_x^2} + \underbrace{-\frac{Y''}{Y}}_{k_y^2} = k^2$$

$$\Rightarrow X'' = -k_x^2 X \Rightarrow X(x) = A\cos(k_x x) + B\sin(k_x x)$$

$$Y'' = -k_y^2 Y \Rightarrow Y(y) = C\cos(k_y y) + D\sin(k_y y)$$

$$X(0) = X(b) = 0 \Rightarrow X(x) = B\sin\left(\frac{n_x\pi}{b}x\right)$$

$$Y(0) = Y(a) = 0 \Rightarrow Y(y) = D\sin\left(\frac{n_y\pi}{a}y\right)$$

$$\Rightarrow \psi(x,y) = \tilde{A}\sin\left(\frac{n_x\pi}{b}x\right)\sin\left(\frac{n_y\pi}{a}y\right)$$

$$\boxed{\psi(x,y) = \frac{2}{\sqrt{ab}}\sin\left(\frac{n_x\pi}{b}x\right)\sin\left(\frac{n_y\pi}{a}y\right)}$$

$n_x, n_y = 1, 2, \ldots$

$\longrightarrow$

$$\frac{2mE}{\hbar^2} = \frac{n_x^2\pi^2}{b^2} + \frac{n_y^2\pi^2}{a^2}$$

$$\Rightarrow E_{n_x,n_y} = \frac{\pi^2\hbar^2}{2m}\left[\frac{n_x^2}{b^2} + \frac{n_y^2}{a^2}\right] = \underbrace{\frac{\pi^2\hbar^2}{2mab}}_{E_0}\left[\left(\frac{a}{b}\right)n_x^2 + \left(\frac{b}{a}\right)n_y^2\right]$$

si $b = 2a$

$$E_{n_x,n_y} = \frac{\pi^2\hbar^2}{2ma^2}\left[\frac{n_x^2}{4} + n_y^2\right] = E_0\left[\left(\frac{n_x}{2}\right)^2 + n_y^2\right]$$

n_x	n_y	E/E_0	
1	1	5/4	$\longrightarrow E_1$
1	2	17/4	$\longrightarrow E_3$
2	1	2	$\longrightarrow E_2$
2	2	5	$\longrightarrow E_4$

si $\boxed{b = 10a}$

n_x	n_y	E/E_0
1	1	10.1
2	1	10.4
3	1	10.9
4	1	11.6
⋮	⋮	
17	1	38.9
1	2	40.1
(18)	(1)	(42.4)

dimension Y "congelada"

Ec. de schrödinger en 3D

$$\check{T} + \check{V} = \check{H} \quad (1)$$

$$\check{H} = \frac{\check{p}^2}{2m} + \check{V} \quad (2)$$

$$\check{p}^2 = \check{p}_x^2 + \check{p}_y^2 + \check{p}_z^2 = \left(-i\hbar\frac{\partial}{\partial x}\right)^2 + \left(-i\hbar\frac{\partial}{\partial y}\right)^2 + \left(-i\hbar\frac{\partial}{\partial z}\right)^2$$

$$= -\hbar^2\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right] = -\hbar^2\nabla^2 \quad (3)$$

$$\Rightarrow \check{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)$$

$$-i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t) \quad (4)$$

Estado estacionario: $\psi(\vec{r},t) = e^{-\frac{i t}{\hbar}E}\,\psi(\vec{r})$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r}) \quad (5)$$

autofunción

autoenergía ($\in \mathbb{R}$)

Caso sencillo: el oscilador harmónico en 3D

Partícula de masa m, moviéndose en 3D bajo el efecto del potencial:

$$V(\vec{r}) = \frac{1}{2} m\omega^2 r^2 \qquad (1)$$

$$= \frac{1}{2} m\omega^2 (x^2+y^2+z^2) = V_x(x) + V_y(y) + V_z(z)$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right] + V_x(x)+V_y(y)+V_z(z)\right]\psi(x,y,z) = E\,\psi(x,y,z)$$

separación de variables. $\psi(x,y,z) = X(x)Y(y)Z(z)$ (2)

$$\Rightarrow -X''YZ - XY''Z - XYZ'' + (V_xX)YZ + X(V_yY)Z + XY(V_zZ) = +K^2 XYZ \qquad (3)$$

donde $K^2 \equiv 2mE/\hbar^2$ (4)

$$\Rightarrow -\frac{X''}{X} - \frac{Y''}{Y} - \frac{Z''}{Z} + V_x + V_y + V_z = +K^2$$

$$\underbrace{\left[-\frac{X''}{X} + V_x\right]}_{\text{sólo dep. de } x} + \underbrace{\left[-\frac{Y''}{Y} + V_y\right]}_{\text{sólo dep. de } y} + \underbrace{\left[-\frac{Z''}{Z} + V_z\right]}_{\text{sólo dep. de } z} = +K^2$$

$$\left.\begin{array}{ll} \text{i)} & -\dfrac{X''}{X} + V_x(x) = k_x^2 \\ \text{ii)} & -\dfrac{Y''}{Y} + V_y(y) = k_y^2 \\ \text{iii)} & -\dfrac{Z''}{Z} + V_z(z) = k_z^2 \end{array}\right\}$$

$$k_x^2 + k_y^2 + k_z^2 = K^2$$

$$\underbrace{\frac{\hbar^2 k_x^2}{2m}}_{E_x} + \underbrace{\frac{\hbar^2 k_y^2}{2m}}_{E_y} + \underbrace{\frac{\hbar^2 k_z^2}{2m}}_{E_z} = E$$

$$\begin{aligned} X(x)'' - (m\omega/\hbar)^2 x^2 X(x) &= -K_x^2 \\ Y(y)'' - (m\omega/\hbar)^2 y^2 Y(y) &= -K_y^2 \\ Z(z)'' - (m\omega/\hbar)^2 z^2 Z(z) &= -K_z^2 \end{aligned}$$

por los resultados de 1D sabemos que

$$E_x = (n_x + \tfrac{1}{2})\hbar\omega \qquad n_x = 0,1,2,\ldots$$
$$E_y = (n_y + \tfrac{1}{2})\hbar\omega \qquad n_y = 0,1,2,\ldots$$
$$E_z = (n_z + \tfrac{1}{2})\hbar\omega \qquad n_z = 0,1,2\ldots$$

o sea $E = (n_x + n_y + n_z + \tfrac{3}{2})\hbar\omega$

$$\Psi_{n_x n_y n_z}(x,y,z,t) = e^{-\frac{i}{\hbar}Et}\left[\left(\frac{d}{dx} - ax\right)^{n_x} e^{-\frac{ax^2}{2}}\right]\left[\left(\frac{d}{dy} - ay\right)^{n_y} e^{-\frac{ay^2}{2}}\right]\left[\left(\frac{d}{dz} - az\right)^{n_z} e^{-\frac{az^2}{2}}\right]$$

sin normalizar

$(a \equiv m\omega^2/\hbar^2)$

$$1 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\Psi(x,y,z)|^2\, dx\,dy\,dz = \int_{-\infty}^{\infty}|X_{n_x}(x)|^2 dx \int_{-\infty}^{\infty}|Y_{n_y}(y)|^2 dy \int_{-\infty}^{\infty}|Z_{n_z}(z)|^2 dz$$

Paridad: $(-1)^{n_x+n_y+n_z}$

n_x	n_y	n_z	N	E_N	Paridad	Deg
0	0	0	0	$\frac{3}{2}\hbar\omega$	+	1
1	0	0	1	$\frac{5}{2}\hbar\omega$	−	3
0	1	0	1		−	
0	0	1	1		−	
2	0	0	2	$\frac{7}{2}\hbar\omega$	+	6
0	2	0	2		+	
0	0	2	2		+	
1	1	0	2		+	
1	0	1	2		+	
0	1	1	2		+	
3	0	0	3	$\frac{9}{2}\hbar\omega$	−	10
0	3	0	3		−	
0	0	3	3		−	
2	1	0	3		−	
2	0	1	3		−	
0	2	1	3		−	
1	2	0	3		−	
1	0	2	3		−	
0	1	2	3		−	
1	1	1	3		−	

Formula general?

Degeneración

$E_N = \hbar\omega(N + \frac{3}{2})$ donde $N = n_x + n_y + n_z$

Sea $N = n_x + n_y + n_z$

para N fijo, $0 \leq n_x \leq N$

y para cada $0 \leq n_x \leq N$, tenemos

$\underbrace{N - n_x}_{N'} = n_y + n_z$

$N' = n_y + n_z$ y $0 \leq n_y \leq N'$

y para cada $0 \leq n_y \leq N'$, n_z está FIJO

$$\# = \sum_{n_x=0}^{N} \sum_{n_y=0}^{N-n_x} 1 = \sum_{n_x=0}^{N} (N - n_x + 1) = \frac{(N+1)(N+2)}{2} \quad //$$

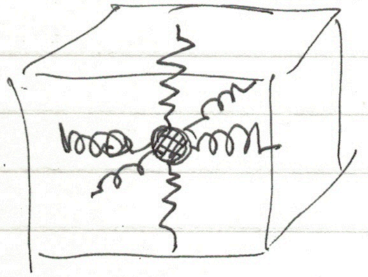
otro caso fácil: El oscilador 3D anisotrópico

$$V(x,y,z) = \frac{1}{2}m\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right)$$

con $\omega_x^2 \neq \omega_y^2 \neq \omega_z^2$.

El potencial es aún separable $V = V_x(x) + V_y(y) + V_z(z)$

$$\Rightarrow E = E_x + E_y + E_z = (n_x + \tfrac{1}{2})\hbar\omega_x + (n_y + \tfrac{1}{2})\hbar\omega_y + (n_z + \tfrac{1}{2})\hbar\omega_z$$



P. ejemplo si $\omega_y = 2\omega_x$ y $\omega_z = 3\omega_x$

$$\Rightarrow E = \hbar\omega_x\left[n_x + 2n_y + 3n_z + 6\right] \qquad n_x, n_y, n_z = 0, 1, 2, \ldots$$

Ej.: Listar las primeras 10 energías con sus degeneraciones (if any).