

La función $\delta(x)$

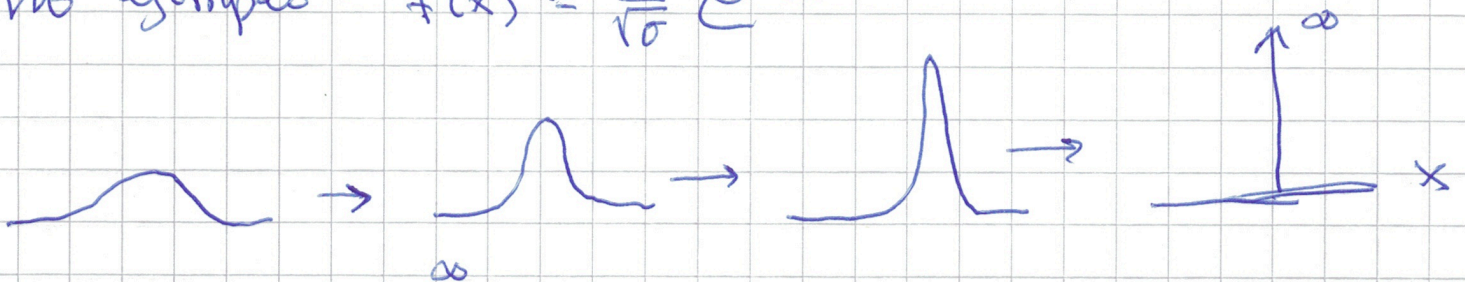
considere $f(x) = \begin{cases} 1/a & 0 < x < a \\ 0 & \text{caso contrario} \end{cases}$

tomen límite $a \rightarrow 0$



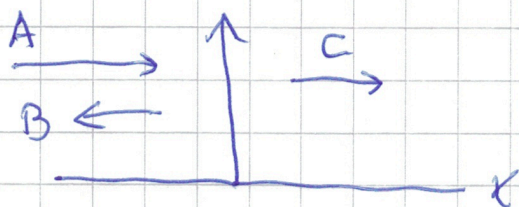
$$\lim_{a \rightarrow 0} f(x) = \delta(x), \text{ donde } \int_{-\infty}^{\infty} \delta(x) dx = 1$$

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



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

Scattering a través de una función $S(x)$



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

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

$$\text{def: } \gamma = \frac{2m\Omega}{\hbar^2} \\ k^2 = \frac{2mE}{\hbar^2}$$

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

$$\psi(x) = A e^{i k x} + B e^{-i k x}$$

$$x > 0: \psi(x) = C e^{i k x}$$

$$\text{cont. de } \psi \text{ en } x=0: A + B = C \quad (2)$$

discontinuidad de ψ en $x=0$

$$(1) \rightarrow -\psi'' + \gamma S(x) \psi = k^2 \psi \quad \Bigg| \int_{-e}^e$$
$$-\psi'(x) \Big|_{-e}^e + \gamma \int_{-e}^e S(x) \psi = k^2 \int_{-e}^e \psi dx$$

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

$$-i k C + i k (A - B) + \gamma C = 0$$

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

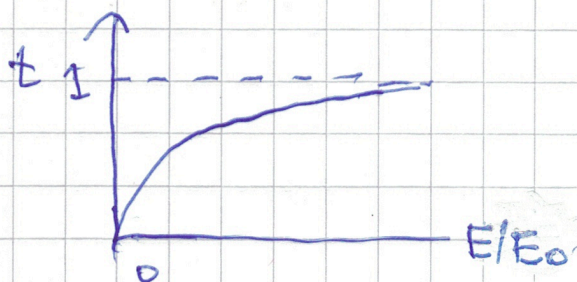
$$A-B = \frac{(ik-\gamma)C}{ik} \quad (3)$$

$$A+B = C$$

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

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

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



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

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

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

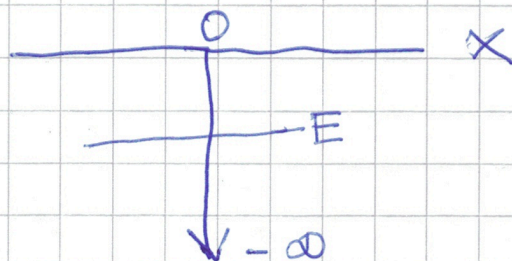
$$-\frac{\hbar^2}{2m} \psi'' - \Omega \delta(x) \psi = E \psi$$

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

$$\text{donde } \gamma = \frac{2m\Omega}{\hbar^2}$$

$$\text{y } k^2 = -\frac{2mE}{\hbar^2}$$

$$(E < 0)$$



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

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

$\psi(x) = A e^{-k|x|}$

cont. de ψ en $x=0$ ✓

discont. de ψ' en $x=0$:

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

$-Ak - Ak + \gamma A \Rightarrow +2Ak = \gamma A \Rightarrow \gamma = 2K$ (5)

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

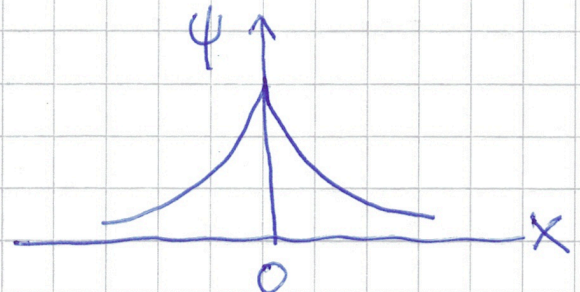
$\left(\frac{2m\Omega}{\hbar^2}\right)^2 = \frac{8m|E|}{\hbar^2} \Rightarrow |E| = \frac{m\Omega^2}{2\hbar^2}$ (6)

Normalización

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

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

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



CLASE. INTERRUPTIDA AT. THIS. POINT

Ec. Schrödinger en 2D: caso fácil

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

$$\text{Sea } H(x,y) = H_x(x) + H_y(y)$$

$$\text{entonces } \Psi(x,y) = X(x) Y(y) \quad (\text{separación variable})$$

$$\text{con } H_x(x) X(x) = E_x X$$

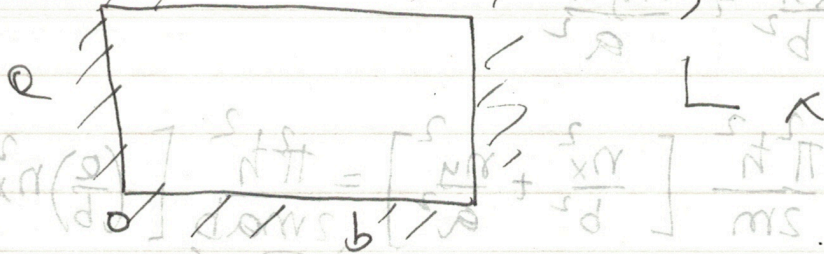
$$H_y(y) Y(y) = E_y Y$$

$$\begin{aligned} \Rightarrow (H_x + H_y) X Y &= (H_x X) Y + X (H_y Y) = E_x X Y + E_y X Y \\ &= (E_x + E_y) X Y \end{aligned}$$

$\therefore$

$$\begin{aligned} E &= E_x + E_y \\ \Psi(x,y) &= X(x) Y(y) \end{aligned}$$

Schrödinger Eq. in 2-D



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

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

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

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

$$\Rightarrow -\frac{X''}{X} + \frac{Y''}{Y} = -k^2$$

$\underbrace{\quad}_{k_x^2} \quad \underbrace{\quad}_{k_y^2}$

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

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

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

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

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

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

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

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

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

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	$\rightarrow E_1$
1	2	17/4	$\rightarrow E_3$
2	1	2	$\rightarrow E_2$
2	2	5	$\rightarrow E_4$

Si $b = 10a$

n_x	n_y	E/E_0	
1	1	10.1	dimension 1 congelade
2	1	10.4	
3	1	10.9	
4	1	11.6	
...	...	...	
17	2	38.9	
1	2	40.1	

Ec. de Schrödinger en 3D

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

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

$$\begin{aligned} \check{p}^2 &= \check{p}_x^2 + \check{p}_y^2 + \check{p}_z^2 = (-i\hbar \frac{\partial}{\partial x})^2 + (-i\hbar \frac{\partial}{\partial y})^2 + (-i\hbar \frac{\partial}{\partial z})^2 \\ &= -\hbar^2 \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] = -\hbar^2 \nabla^2 \end{aligned} \quad (3)$$

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

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

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

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

↙
autofunción

↘
autoenergía ($\in \mathbb{R}$)

Caso sencillo: el oscilador armónico en 3D

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

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

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

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

$$\Rightarrow -X''YZ + XY''Z + XYZ'' + (V_x X)YZ + X(V_y Y)Z + XY(V_z Z) = +K^2 XYZ \quad (3)$$

$$\text{donde } K^2 \equiv 2mE/\hbar^2 \quad (4)$$

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

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

$$i) -\frac{\hbar^2}{2m} \frac{d^2 X}{dx^2} + V_x(x) = E_x$$

$$ii) -\frac{\hbar^2}{2m} \frac{d^2 Y}{dy^2} + V_y(y) = E_y$$

$$iii) -\frac{\hbar^2}{2m} \frac{d^2 Z}{dz^2} + V_z(z) = E_z$$

$$E_x + E_y + E_z = E$$

$$\frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} + \frac{\hbar^2 k_z^2}{2m} = E$$

$$X(x)'' - (m\omega/\hbar)^2 x^2 X(x) = -K_x^2 X(x)$$

$$Y(y)'' - (m\omega/\hbar)^2 y^2 Y(y) = -K_y^2 Y(y)$$

$$Z(z)'' - (m\omega/\hbar)^2 z^2 Z(z) = -K_z^2 Z(z)$$

por los resultados de los 1D schemes que

$$E_x = (n_x + \frac{1}{2}) \hbar \omega$$

$$E_y = (n_y + \frac{1}{2}) \hbar \omega$$

$$E_z = (n_z + \frac{1}{2}) \hbar \omega$$

$$n_x = 0, 1, 2, \dots$$

$$n_y = 0, 1, 2, \dots$$

$$n_z = 0, 1, 2, \dots$$

$$0 \text{ sea } E = (n_x + n_y + n_z + \frac{3}{2}) \hbar \omega$$

$$\psi_{n_x n_y n_z}(x, y, z, t) = e^{-\frac{i}{\hbar} E t} \left[\left(\frac{d}{dx} - \alpha x \right)^{n_x} e^{-\frac{\alpha x^2}{2}} \right] \left[\left(\frac{d}{dy} - \alpha y \right)^{n_y} e^{-\frac{\alpha y^2}{2}} \right] \left[\left(\frac{d}{dz} - \alpha z \right)^{n_z} e^{-\frac{\alpha z^2}{2}} \right]$$

sin normalizar

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

$$1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\psi_{n_x n_y n_z}(x, y, z)|^2 dx dy dz = \int_{-\infty}^{\infty} |x_{n_x}|^2 dx \int_{-\infty}^{\infty} |y_{n_y}|^2 dy \int_{-\infty}^{\infty} |z_{n_z}|^2 dz$$

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

n_x	n_y	n_z	N	F_N	Paridad	Deg
0	0	0	0	$\frac{3}{2}hw$	+	1
1	0	0	1	$\frac{5}{2}hw$	-	3
0	1	0	1		-	
0	0	1	1		-	
2	0	0	2	$\frac{7}{2}hw$	+	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	$\frac{9}{2}hw$	-	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?

Degeneration

$$E_N = \hbar \omega (N + \frac{3}{2})$$

$$\text{Don't } N = n_x + n_y + n_z$$

$$\text{See } N = n_x + n_y + n_z$$

$$\text{For } N \text{ fixed, } 0 \leq n_x \leq N$$

$$\text{y fixed code } 0 \leq n_x \leq N, \text{ then}$$

$$N - n_x = n_y + n_z$$

$$N' = n_y + n_z \quad \text{y } 0 \leq n_y \leq N'$$

$$\text{y fixed code } 0 \leq n_y \leq N', \quad n_z \text{ is fixed}$$

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

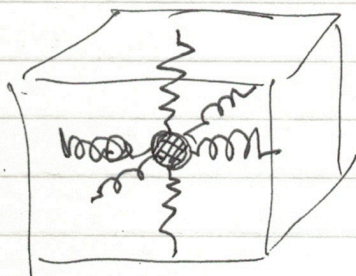
otro caso fácil: EL oscilador 3D
anisotrópico

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

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

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

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



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

$$\Rightarrow E = \hbar \omega_x [n_x + 2n_y + 3n_z + 6] \quad n_x, n_y, n_z = 0, 1, 2, \dots$$

ej. Listar los primeros 10 energías con sus degeneraciones (if any).