

# bración y Rotación en Mecánica Cuántica

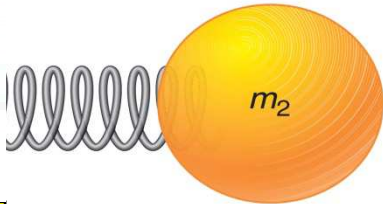


armónico unidimensional  
gido  
ción del momento angular  
s propias y valores propios de los operadores de momento  
...  
nicos esféricos

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# El oscilador armónico clásico unidimensional

$$-kx \quad (\text{Ley de Hooke})$$



$$F = \mu a = \mu \frac{d^2x}{dt^2} \rightarrow \mu \frac{d^2x}{dt^2} + kx = 0$$

Soluciones de la ecuación diferencial

$$x(t) = c_1 e^{+i\sqrt{(k/\mu)}t} + c_2 e^{-i\sqrt{(k/\mu)}t}$$

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$$x(t) = b_1 \cos \sqrt{\frac{k}{\mu}}t + b_2 \sin \sqrt{\frac{k}{\mu}}t$$

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Frecuencia de vibración  $\nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$

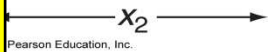
Frecuencia angular  $\omega = 2\pi\nu$

$$x(t) = A \sin(\omega t + \alpha)$$

Ecuación de movimiento

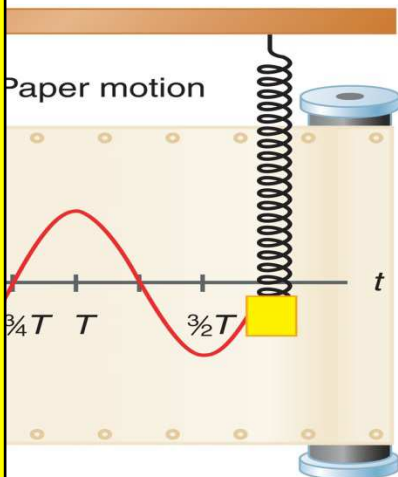
$$E_{potential} = \frac{1}{2} kx^2 \quad \text{and} \quad E_{kinetic} = \frac{1}{2} \mu v^2$$

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$$\frac{x_1 + m_2 x_2}{m_1 + m_2}$$

$$\frac{m_1 m_2}{m_1 + m_2}$$



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# El oscilador armónico cuántico unidimensional

Energía potencial :  $V(x) = \frac{1}{2}kx^2$

$$-\frac{\hbar^2}{2\mu} \frac{d^2\psi_n(x)}{dx^2} + \frac{kx^2}{2} \psi_n(x) = E_n \psi_n(x)$$

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$$\psi_n(x) = A_n H_n(\alpha^{1/2} x) e^{-\alpha x^2/2}, \text{ for } n = 0, 1, 2, \dots$$

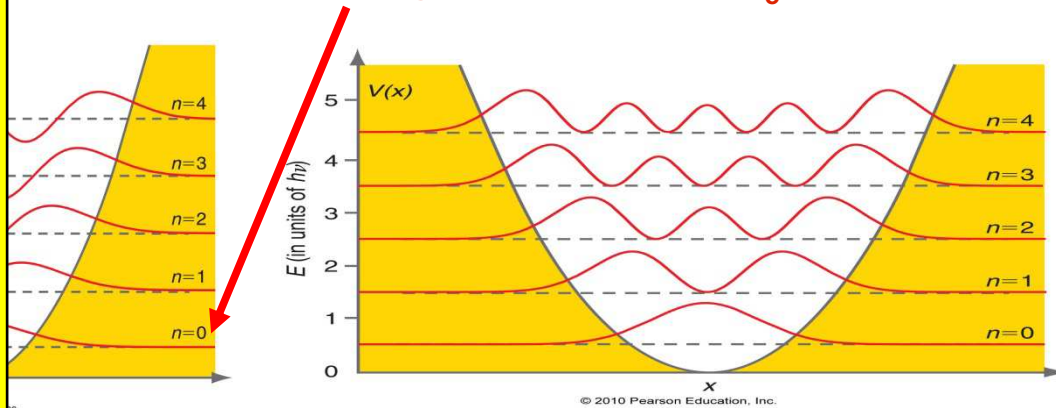
$(\alpha = (k\mu)^{1/2}/\hbar)$

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$$E_n = \hbar \sqrt{\frac{k}{\mu}} \left( n + \frac{1}{2} \right) = hv \left( n + \frac{1}{2} \right) \text{ with } n = 0, 1, 2, 3, \dots$$

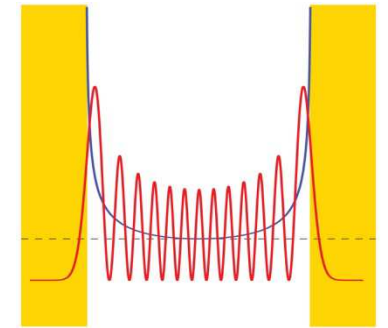
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**Energía de punto cero  $E_0 = \frac{1}{2} hv$**



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Densidades de probabilidad de los primeros estados cuánticos del oscilador armónico unidimensional



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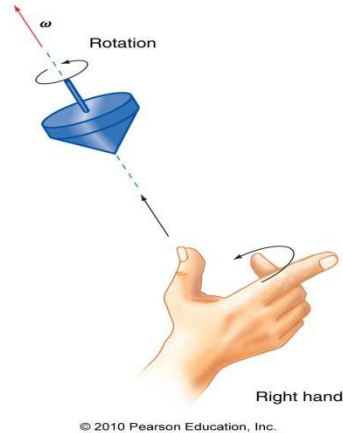
Densidades de probabilidad del duodécimo estados cuántico del oscilador armónico unidimensional

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# El rotor rígido clásico



$$|\boldsymbol{\omega}| = \frac{d\theta}{dt}$$

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velocidad angular

$$\boldsymbol{\alpha} = \frac{d|\boldsymbol{\omega}|}{dt} = \frac{d^2\theta}{dt^2}$$

aceleración angular

$$\mathbf{v} = \frac{\Delta \mathbf{s}}{\Delta t} = \frac{\mathbf{r}\Delta\theta}{\Delta t} \quad \text{in the limit as } \Delta t \rightarrow 0, \quad \mathbf{v} = \frac{r d\theta}{dt} = r\boldsymbol{\omega}$$

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$$E_{kinetic} = \frac{1}{2}\mu v^2 = \frac{1}{2}\underbrace{\mu r^2}_{\text{momento de inercia}}\omega^2 = \frac{1}{2}I\omega^2$$

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momento angular  $\mathbf{l} = \mathbf{r} \times \mathbf{p}$

Para un movimiento circular  $\mathbf{r}$  y  $\mathbf{p}$  son perpendiculares

$$l = r \cdot p \cdot \text{sen } \theta = r \cdot p$$

$$E = \frac{p^2}{2\mu} = \frac{l^2}{2\mu r^2} = \frac{l^2}{2I}$$

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$m_2$

$r_2$

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miltoniano para una molécula con N átomos  
cluyendo los grados de libertad electrónicos

$$\hat{H}_{trans}(r_{cm}) + \hat{H}_{vib}(\tau_{internal}) + \hat{H}_{rot}(\theta_{cm}, \phi_{cm})$$

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$$\psi_{trans}(r_{cm}) \psi_{vib}(\tau_{internal}) \psi_{rot}(\theta_{cm}, \phi_{cm})$$

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$$E_{total} = E_{trans} + E_{vib} + E_{rot}$$

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# El rotor rígido bidimensional cuántico

$$\left. \frac{\partial^2 \psi(x, y)}{\partial y^2} \right)_{r=r_0} = E\psi(x, y) \xrightarrow{x^2+y^2=r_0^2} -\frac{\hbar^2}{2\mu r_0^2} \frac{d^2 \Phi(\phi)}{d\phi^2} = E\Phi(\phi)$$

$$\Phi_+(\phi) = A_{+\phi} e^{im_l \phi} \quad \text{and} \quad \Phi_-(\phi) = A_{-\phi} e^{-im_l \phi}$$

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$$\text{si } \Phi(\phi+2\pi) = \Phi(\phi)$$

$$\cos 2\pi m_l + i \sin 2\pi m_l = 1 \quad \longrightarrow \quad m_l = 0, \pm 1, \pm 2, \pm 3, \dots$$

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$$E_{m_l} = \frac{\hbar^2 m_l^2}{2\mu r_0^2} = \frac{\hbar^2 m_l^2}{2I} \quad \text{for } m_l = 0, \pm 1, \pm 2, \pm 3, \dots$$

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**El momento angular también está cuantizado**

$$\hat{l}_z \Phi_+(\phi) = \frac{-i\hbar}{\sqrt{2\pi}} \frac{d e^{im_l \phi}}{d\phi} = \frac{m_l \hbar}{\sqrt{2\pi}} e^{im_l \phi} = m_l \hbar \Phi_+(\phi)$$

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$$|l_z| = \pm m_l \hbar$$

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# El rotor rígido tridimensional cuántico

$$-\frac{\hbar^2}{2\mu r_0^2} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} \right] = E Y(\theta, \phi)$$

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$$\sin \theta \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + [\beta \sin^2 \theta] Y(\theta, \phi) = -\frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2}$$

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función de ondas

$$= \Theta(\theta) \Phi(\phi)$$

$$\left( \frac{1}{\Theta(\theta)} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta(\theta)}{d\theta} \right) + \beta \sin^2 \theta \right) \Phi(\phi) = -\frac{1}{\Phi(\phi)} \frac{d^2 \Phi(\phi)}{d\phi^2}$$

$$\left\{ \begin{array}{l} \frac{1}{\Theta(\theta)} \sin \theta \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta(\theta)}{d\theta} \right) + \beta \sin^2 \theta = m_l^2 \\ \frac{1}{\Phi(\phi)} \frac{d^2 \Phi(\phi)}{d\phi^2} = -m_l^2 \end{array} \right.$$

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$$\beta = l(l+1), \text{ for } l = 0, 1, 2, 3, \dots \text{ and}$$

$$m_l = -l, -(l-1), -(l-2), \dots, 0, \dots, (l-2), (l-1), l$$

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$$\beta = \frac{2\mu r_0^2 E}{\hbar^2}$$

$$E_l = \frac{\hbar^2}{2I} l(l+1), \text{ for } l = 0, 1, 2, 3, \dots$$

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cos Esféricos

$$Y(\theta, \phi) = \Theta_l^{m_l}(\theta) \Phi_{m_l}(\phi)$$

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Si

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$$\psi(\theta, \phi) = \frac{\hbar^2}{2I} l(l + 1) Y_l^{m_l}(\theta, \phi), \quad \text{for } l = 0, 1, 2, 3, \dots$$

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En: hay  $2l+1$  valores distintos de  $m_l$  que generan armónicos esféricos de misma energía

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# La cuantización del momento angular

$$L^2 Y_l^{m_l}(\theta, \phi) = \hbar^2 l(l+1) Y_l^{m_l}(\theta, \phi)$$

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$$\hat{L}_x = -i\hbar \left( -\sin\phi \frac{\partial}{\partial\theta} - \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right)$$

$$\hat{L}_y = -i\hbar \left( \cos\phi \frac{\partial}{\partial\theta} - \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right)$$

$$\hat{L}_z = -i\hbar \left( \frac{\partial}{\partial\phi} \right)$$

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Regla de la cadena

Los armónicos esféricos son funciones propias de la componente z del momento angular

$$\hat{L}_z(Y_l^{m_l}(\theta, \phi)) = \Theta(\theta) \left[ -i\hbar \frac{\partial}{\partial\phi} \left( \frac{1}{\sqrt{2\pi}} e^{\pm im_l \phi} \right) \right] = \pm m_l \hbar \Theta(\theta) \Phi(\phi),$$

for  $m_l = 0, \pm 1, \pm 2, \pm 3, \dots, \pm l$

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$$\begin{aligned} & -z \frac{\partial}{\partial y} \\ & -x \frac{\partial}{\partial z} \\ & \dots \\ & -y \frac{\partial}{\partial x} \end{aligned}$$

momento  
entre sí

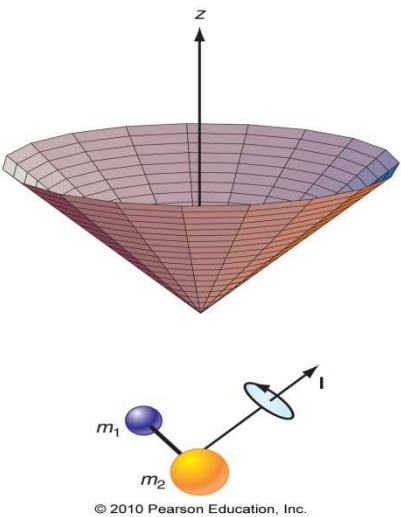
$$i\hbar \hat{L}_z$$

$$i\hbar \hat{L}_x$$

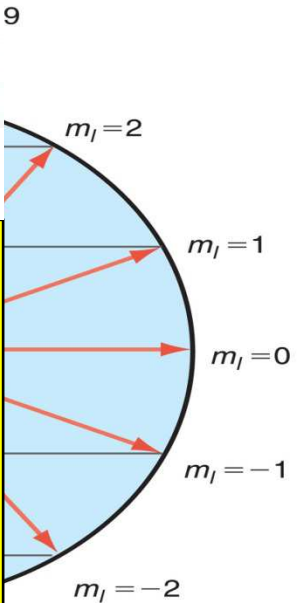
$$i\hbar \hat{L}_y$$

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# Cuantización Espacial



Orientación del vector momento angular para  $l=2$  y  $m_l=+2$



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Orientación del vector momento angular para  $l=2$

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# Los Armónicos Esféricos

$$p_x = \frac{1}{\sqrt{2}}(Y_1^1 + Y_1^{-1}) = \sqrt{\frac{3}{4\pi}} \sin \theta \cos \phi$$

$$p_y = \frac{1}{\sqrt{2}i}(Y_1^1 - Y_1^{-1}) = \sqrt{\frac{3}{4\pi}} \sin \theta \sin \phi$$

$$p_z = Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos \theta$$

$$d_{z^2} = Y_2^0 = \sqrt{\frac{5}{16\pi}}(3 \cos^2 \theta - 1)$$

$$d_{xz} = \frac{1}{\sqrt{2}}(Y_2^1 + Y_2^{-1}) = \sqrt{\frac{15}{4\pi}} \sin \theta \cos \theta \cos \phi$$

$$d_{yz} = \frac{1}{\sqrt{2}i}(Y_2^1 - Y_2^{-1}) = \sqrt{\frac{15}{4\pi}} \sin \theta \cos \theta \sin \phi$$

$$d_{x^2-y^2} = \frac{1}{\sqrt{2}}(Y_2^2 + Y_2^{-2}) = \sqrt{\frac{15}{16\pi}} \sin^2 \theta \cos 2\phi$$

$$d_{xy} = \frac{1}{\sqrt{2}i}(Y_2^2 - Y_2^{-2}) = \sqrt{\frac{15}{16\pi}} \sin^2 \theta \sin 2\phi$$

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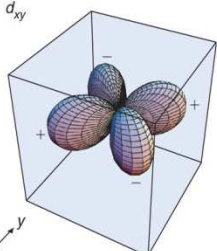
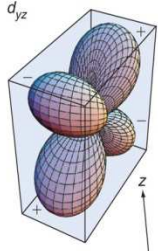
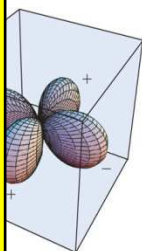
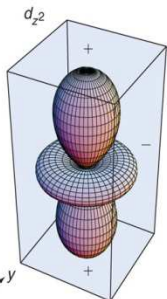
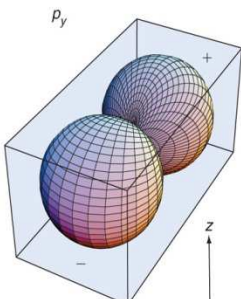
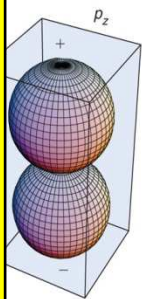
$\cos \theta$

$\sin \theta e^{\pm i\phi}$

$(3 \cos^2 \theta - 1)$

$\sin \theta \cos \theta e^{\pm i\phi}$

$\sin^2 \theta e^{\pm 2i\phi}$



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