Solución Ecuación Schrödinger para un potencial central

$$\Downarrow$$

$$V(\vec{r}) = V(r) \quad \text{(En coord. esféricos)}$$

$$\boxed{-\frac{\hbar^2}{2M}\nabla^2\psi_E(\vec{r}) + V(\vec{r})\psi_E(\vec{r}) = E\,\psi_E(\vec{r})} \qquad (*)$$

$E = \text{cte} =$ Energía del sistema

En coord. esféricos se tiene que:

$$\nabla^2 = \frac{1}{r^2}\hat{D}_r + \frac{1}{r^2}\hat{D}_{\theta,\varphi}$$

siendo los operadores:

$$\hat{D}_r = \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)$$

$$\hat{D}_{\theta,\varphi} = \frac{1}{\operatorname{sen}\theta}\frac{\partial}{\partial\theta}\left(\operatorname{sen}\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\operatorname{sen}^2\theta}\frac{\partial^2}{\partial\varphi^2} = -\frac{\hat{L}^2}{\hbar^2}$$

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reemplazando en la Ec. (*)

$$-\frac{\hbar^2}{2Mr^2}\hat{D}_r\psi_E(\vec{r}) - \frac{\hbar^2}{2Mr^2}\hat{D}_{\theta,\varphi}\psi_E(\vec{r}) + V(\vec{r})\psi_E(\vec{r}) = E\,\psi_E(\vec{r}) \qquad (**)$$

Luego

$$\psi_E(\vec{r}) = \psi_E(r,\theta,\varphi)$$
$$V(\vec{r}) = V(r)$$

Sea $\psi_E(r,\theta,\varphi) = R(r)\,T(\theta)\,\Phi(\varphi) = RT\Phi$

Obs.
$$\hat{D}_r \psi_E(\vec{r}) = T\Phi\left(\hat{D}_r R\right)$$
$$\hat{D}_{\theta,\varphi} \psi_E(\vec{r}) = R\left(\hat{D}_{\theta,\varphi} T\Phi\right)$$

Luego en (**)

$$\frac{-\hbar^2}{2Mr^2}\, T\Phi\left(\hat{D}_r R\right) - \frac{\hbar^2}{2Mr^2}\, R\left(\hat{D}_{\theta,\varphi} T\Phi\right) + \left(V(r) - E\right)RT\Phi = 0$$

Multiplicamos la ec. anterior por : $\left(-\frac{2Mr^2}{\hbar^2\, RT\Phi}\right)$

$$\Downarrow$$

$$\frac{1}{R}\left(\hat{D}_r R\right) + \frac{1}{T\Phi}\left(\hat{D}_{\theta,\varphi} T\Phi\right) + \frac{2Mr^2}{\hbar^2}\left(E - V(r)\right) = 0$$

$$\Downarrow$$

$$\underbrace{\frac{1}{R}\left(\hat{D}_r R\right) + \frac{2Mr^2}{\hbar^2}\left(E - V(r)\right)}_{\text{Solo depende de } r} = \underbrace{-\frac{1}{T\Phi}\left(\hat{D}_{\theta,\varphi} T\Phi\right)}_{\text{solo depende de } \theta \text{ y } \varphi} = \eta_\ell$$

constante de separación

$$\Downarrow$$

Ecuación radial

$$\frac{1}{R}\left(\hat{D}_r R\right)+\frac{2Mr^2}{\hbar^2}\left(E-V(r)\right)=\eta_\ell \quad (\ell = \text{constante por determinar})$$

$$\Downarrow$$

$R = R(r) = R_{E\ell}(r)$ (R depende de r, ℓ y E)

$$\therefore \quad \frac{d}{dr}\left(r^2\frac{dR_{E\ell}(r)}{dr}\right)+\frac{2Mr^2}{\hbar^2}\left(E-V(r)\right)R_{E\ell}(r)=\eta_\ell R_{E\ell}(r)$$

$$\Downarrow$$

$$-\frac{\hbar^2}{2Mr^2}\frac{d}{dr}\left(r^2\frac{d}{dr}R_{E\ell}(r)\right)+\left(V(r)-E+\frac{\eta_\ell\hbar^2}{2Mr^2}\right)R_{E\ell}(r)=0$$

Ecuaciones angulares

$$\Downarrow$$

$$\left(\hat{D}_{\theta,\varphi}\, T\Phi\right) = -\eta_{\ell}\, T\Phi$$

$$\Downarrow$$

$$\left[\frac{1}{\operatorname{sen}\theta}\frac{\partial}{\partial\theta}\left(\operatorname{sen}\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\operatorname{sen}^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] T\Phi = -\eta_{\ell}\, T\Phi$$

Obs.

$$\frac{\partial}{\partial\theta}(T\Phi) = \Phi\frac{\partial T}{\partial\theta}$$

$$\frac{\partial^2}{\partial\varphi^2}(T\Phi) = T\frac{\partial^2\Phi}{\partial\varphi^2}$$

$\therefore$

$$\Phi\frac{1}{\operatorname{sen}\theta}\frac{\partial}{\partial\theta}\left(\operatorname{sen}\frac{\partial T}{\partial\theta}\right) + T\frac{1}{\operatorname{sen}^2\theta}\frac{\partial^2\Phi}{\partial\varphi^2} = -\eta_{\ell}\, T\Phi$$

luego multiplicamos por: $\left(\dfrac{\operatorname{sen}^2\theta}{T\Phi}\right)$

$$\Downarrow$$

$$\frac{1}{T}\operatorname{sen}\theta\frac{\partial}{\partial\theta}\left(\operatorname{sen}\theta\frac{\partial T}{\partial\theta}\right) + \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2} = -\eta_{\ell}\operatorname{sen}^2\theta$$

$\Downarrow$ Reescribiendo la ecuación:

$$\underbrace{\frac{1}{T}\,\text{sen}\theta\,\frac{\partial}{\partial\theta}\left(\text{sen}\theta\,\frac{\partial T}{\partial\theta}\right)+\text{sen}^2\theta\,\eta_{\ell}}_{\text{función solo de }\theta}=\underbrace{-\frac{1}{\Phi}\,\frac{\partial^2\Phi}{\partial\varphi^2}}_{\text{función solo de }\varphi}=m^2$$

cte. de separación

Ec. para $T(\theta)$ $\left(T(\theta)=T_{\ell m}(\theta)\right)$

$$\text{sen}\theta\,\frac{d}{d\theta}\left(\text{sen}\theta\,\frac{dT_{\ell m}(\theta)}{d\theta}\right)+\text{sen}^2\theta\,\eta_{\ell}\,T_{\ell m}(\theta)=m^2\,T_{\ell m}(\theta)$$

Ecuación para $\Phi(\varphi)$ $\left(\Phi(\varphi)=\Phi_m(\varphi)\right)$

$$\frac{d^2\Phi_m(\varphi)}{\partial\varphi^2}+m^2\Phi_m(\varphi)=0$$

$\Downarrow$

solución $\Phi_m=c\,e^{im\varphi}$ $(c=\text{cte})$

Condición de contorno: $\Phi_m(\varphi)=\Phi_m(\varphi+2\pi)$

$\Downarrow$

$m=0,\pm1,\pm2,\ldots$

se conocía que $\eta_\ell = \ell(\ell+1)$. $(\ell = 0, 1, 2, \ldots)$

Finalmente

$$\psi_E(\vec{r}) = R_{E\ell}(r)\, T_{\ell m}(\theta)\, \Phi_m(\varphi) = \psi_{E\ell m}(r,\theta,\varphi)$$

<u>Obs.</u> $T_{\ell m}(\theta)\, \Phi_m(\varphi) = Y_\ell^m(\theta,\varphi)$

armónicos esféricos