Esféricos Harmônicos

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Mecânica Quântica I

O Problema

- Queremos encontrar a relação entre os harmônicos esféricos:

$$Y_l^m(\theta,\varphi) \qquad\qquad Y_l^{-m}(\theta,\varphi)$$

- Vamos provar:

$$Y_l^{-m}(\theta,\varphi) = (-1)^m\left(Y_l^m(\theta,\varphi)\right)^*$$

Plano

- Vamos usar os operadores "elevação" e "redução":

$$L_{\pm} = L_x \pm iL_y$$

- Os operadores alteram o índice m e mantêm l

Usar aplicações sucessivas dos operadores para obter duas expressões equivalentes para Y_l^m

$$Y_l^l \longrightarrow Y_l^m$$

$$Y_l^{-l} \longrightarrow Y_l^m$$

1°: Obtendo $Y_l^m(\theta, \varphi)$ a partir de $Y_l^l(\theta, \varphi)$

$$Y_l^l \xrightarrow{\text{Aplicar } L_- \ (l - m) \text{ vezes}} Y_l^m$$

- Usando:

$$L_- \, Y_l^m(\theta, \varphi) = \hbar\sqrt{l(l+1) - m(m-1)} \, Y_l^{m-1}(\theta, \varphi)$$

$$= \hbar\sqrt{(l+m)(l-m+1)} \, Y_l^{m-1}(\theta, \varphi)$$

1°: Obtendo $Y_l^m(\theta,\varphi)$ a partir de $Y_l^l(\theta,\varphi)$

$$L_-\,Y_l^l(\theta,\varphi) = \hbar\sqrt{(l+l)(l-l+1)}\,Y_l^{l-1}(\theta,\varphi)$$

$2l$ 1

$$L_-\,Y_l^{l-1}(\theta,\varphi) = \hbar\sqrt{(l+(l-1))(l-(l-1)+1)}\,Y_l^{l-2}(\theta,\varphi)$$

$2l-1$ 2

⋮   ⋮

$$L_-\,Y_l^{m+1}(\theta,\varphi) = \hbar\sqrt{(l+(m+1))(l-(m+1)+1)}\,\boxed{Y_l^m(\theta,\varphi)}$$

$l+m+1$ $l-m$

↓   ↓

$\dfrac{(2l)!}{(l+m)!}$ $(l-m)!$

1°: Obtendo $Y_l^m(\theta,\varphi)$ a partir de $Y_l^l(\theta,\varphi)$

$$Y_l^m(\theta,\varphi) = \sqrt{\frac{(l+m)!}{(2l)!\,(l-m)!}}\left(\frac{L_-}{\hbar}\right)^{l-m} Y_l^l(\theta,\varphi)$$

- Usando:
  - $Y_l^l(\theta,\varphi) = \frac{(-1)^l}{2^l\, l!}\sqrt{\frac{(2l+1)!}{4\pi}}(\operatorname{sen}\theta)^l e^{il\varphi}$
  - $(L_\pm)^p\left[e^{in\varphi}F(\theta)\right] = (\mp\hbar)^p e^{i(n\pm p)\varphi}(\operatorname{sen}\theta)^{p\pm n}\frac{d^p}{d(\cos\theta)^p}\left[(\operatorname{sen}\theta)^{\mp n}F(\theta)\right]$

Com $\begin{cases} n = l \\ p = l - m \end{cases}$

- Encontramos:

$$Y_l^m(\theta,\varphi) = \frac{(-1)^l}{2^l\, l!}\sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}}\, e^{im\varphi}(\operatorname{sen}\theta)^{-m}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\operatorname{sen}\theta)^{2l}$$

2°: Obtendo $Y_l^m(\theta,\varphi)$ a partir de $Y_l^{-l}(\theta,\varphi)$

$$Y_l^{-l} \xrightarrow{\text{Aplicar } L_+ \ (l+m) \text{ vezes}} Y_l^m$$

- Usando:

$$L_+ Y_l^m(\theta,\varphi) = \hbar\sqrt{l(l+1) - m(m+1)}\, Y_l^{m+1}(\theta,\varphi)$$

$$= \hbar\sqrt{(l-m)(l+m+1)}\, Y_l^{m+1}(\theta,\varphi)$$

2°: Obtendo $Y_l^m(\theta,\varphi)$ a partir de $Y_l^{-l}(\theta,\varphi)$

$$L_+ Y_l^{-l}(\theta,\varphi) = \hbar\sqrt{(l+l)(l-l+1)}Y_l^{l+1}(\theta,\varphi)$$

$\boxed{2l}$ $\boxed{1}$

$$L_+ Y_l^{-l+1}(\theta,\varphi) = \hbar\sqrt{(l-(-l+1))(l+(-l+1)+1)}Y_l^{-l+2}(\theta,\varphi)$$

$\boxed{2l-1}$ $\boxed{2}$

⋮ ⋮

$$L_+ Y_l^{m-1}(\theta,\varphi) = \hbar\sqrt{(l-(m-1))(l+(m-1)+1)}\ \boxed{Y_l^m(\theta,\varphi)}$$

$\boxed{l-m+1}$ $\boxed{l+m}$

↓ ↓

$$\boxed{\frac{(2l)!}{(l-m)!}} \qquad \boxed{(l+m)!}$$

2°: Obtendo $Y_l^m(\theta,\varphi)$ a partir de $Y_l^l(\theta,\varphi)$

$$Y_l^m(\theta,\varphi) = \sqrt{\frac{(l-m)!}{(2l)!\,(l+m)!}}\left(\frac{L_+}{\hbar}\right)^{l+m} Y_l^{-l}(\theta,\varphi)$$

- Usando:
  - $Y_l^{-l}(\theta,\varphi) = \frac{1}{2^l\, l!}\sqrt{\frac{(2l+1)!}{4\pi}}(\operatorname{sen}\theta)^l e^{-il\varphi}$
  - $(L_\pm)^p\left[e^{in\varphi}F(\theta)\right] = (\mp\hbar)^p e^{i(n\pm p)\varphi}(\operatorname{sen}\theta)^{p\pm n}\frac{d^p}{d(\cos\theta)^p}\left[(\operatorname{sen}\theta)^{\mp n}F(\theta)\right]$

Com $\begin{cases} n = -l \\ p = l+m \end{cases}$

- Encontramos:

$$Y_l^m(\theta,\varphi) = \frac{(-1)^{l+m}}{2^l\, l!}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\, e^{im\varphi}(\operatorname{sen}\theta)^m \frac{d^{l+m}}{d(\cos\theta)^{l+m}}(\operatorname{sen}\theta)^{2l}$$

Comparação

- Comparando as duas equações:

$$Y_l^m(\theta,\varphi) = \frac{(-1)^l}{2^l\, l!}\sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}}\, e^{im\varphi}(\operatorname{sen}\theta)^{-m}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\operatorname{sen}\theta)^{2l}$$

$$Y_l^m(\theta,\varphi) = \frac{(-1)^{l+m}}{2^l\, l!}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\, e^{im\varphi}(\operatorname{sen}\theta)^{m}\frac{d^{l+m}}{d(\cos\theta)^{l+m}}(\operatorname{sen}\theta)^{2l}$$

Comparação

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$$Y_l^m(\theta,\varphi) = \frac{(-1)^l}{2^l\, l!}\sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}}\, e^{im\varphi}(\text{sen}\,\theta)^{-m}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\text{sen}\,\theta)^{2l}$$

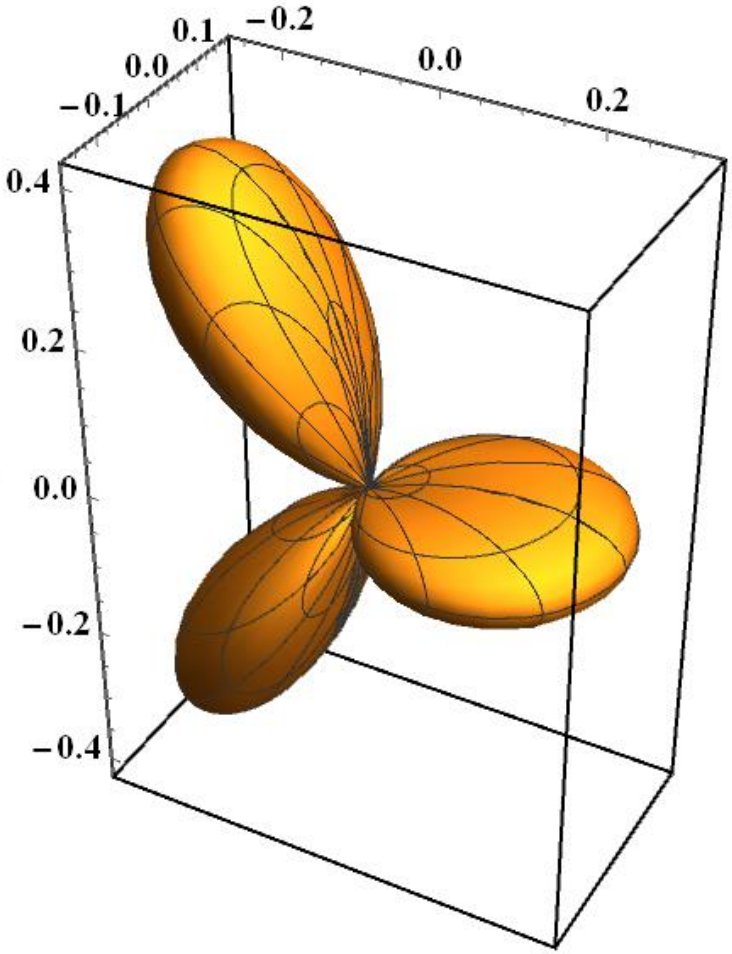
$$Y_l^m(\theta,\varphi) = \frac{(-1)^{l+m}}{2^l\, l!}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\, e^{im\varphi}(\text{sen}\,\theta)^{m}\frac{d^{l+m}}{d(\cos\theta)^{l+m}}(\text{sen}\,\theta)^{2l}$$

- A mudança $m \to -m$ é suficiente exceto por um fator $(-1)^{\mathrm{m}}$ e o sinal da parte imaginária:

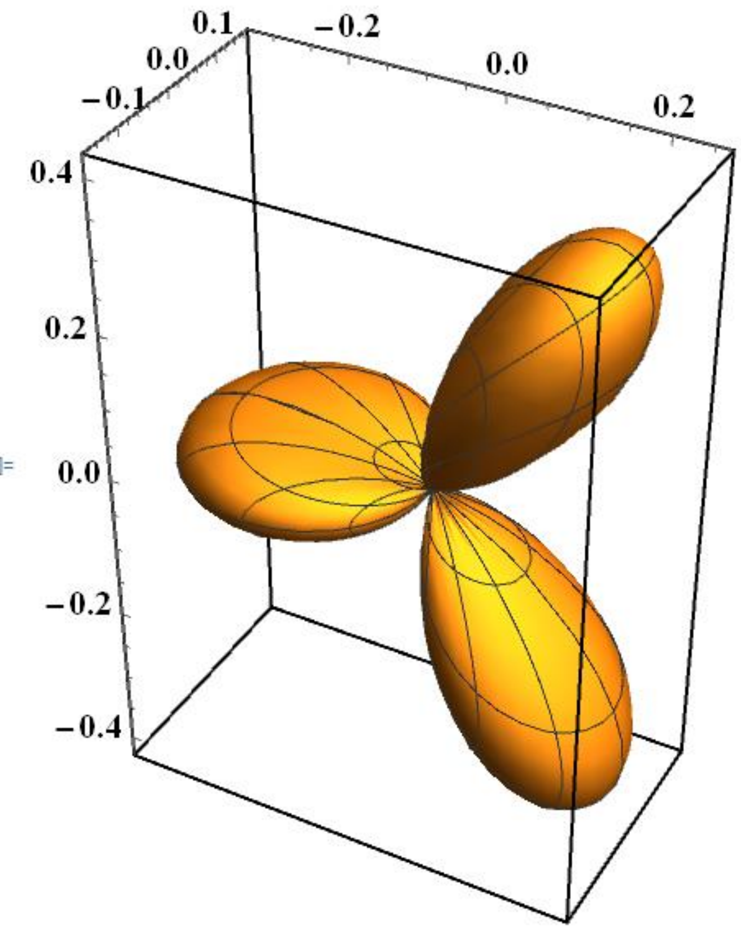
$$Y_l^{-m}(\theta,\varphi) = (-1)^m\left(Y_l^m(\theta,\varphi)\right)^*$$

Uma Intuição: m ímpar → inversão da parte real

$\mathbf{Re}\left[Y_3^1(\theta,\varphi)\right]$

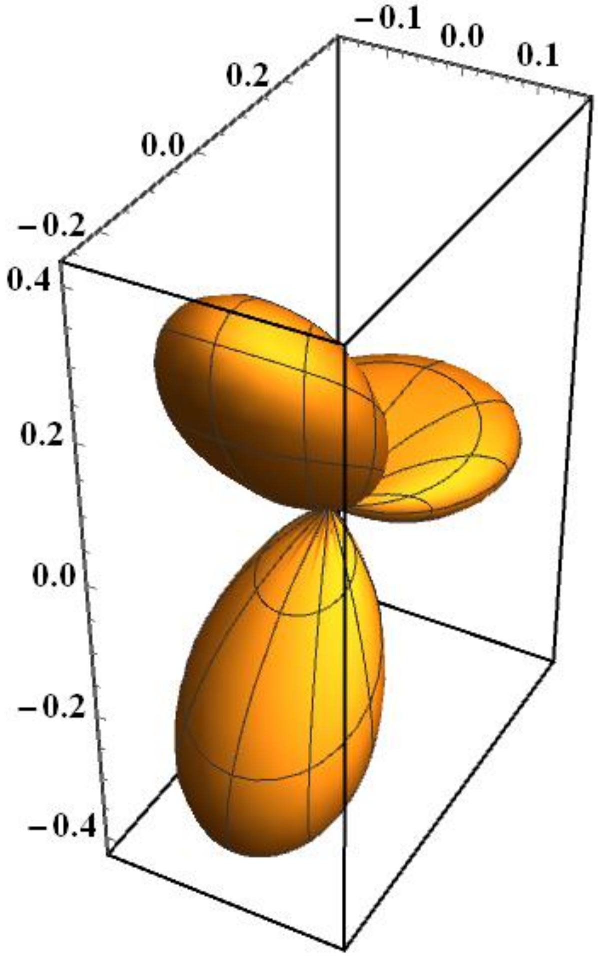


$\mathbf{Re}\left[Y_3^{-1}(\theta,\varphi)\right]$

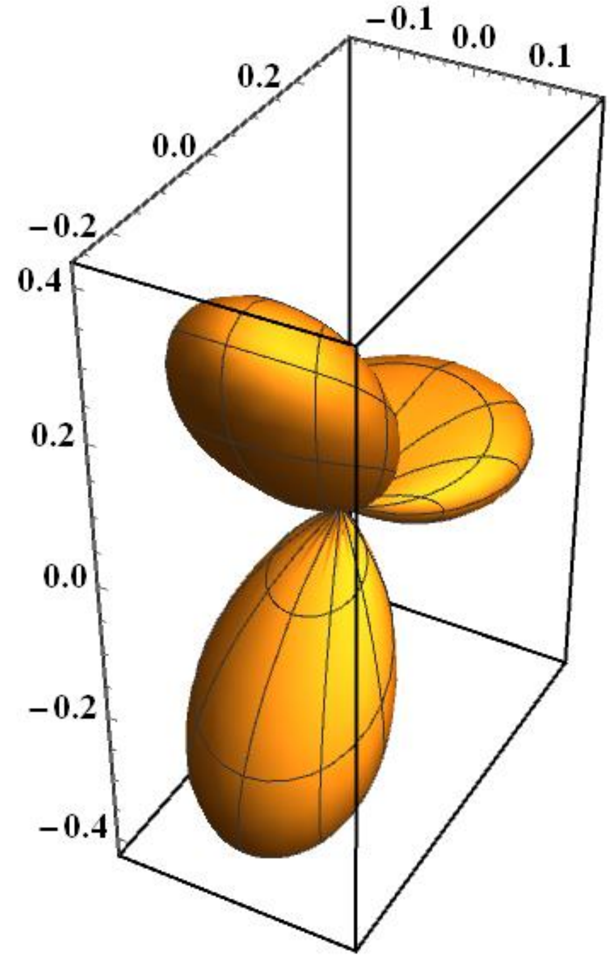


Uma Intuição: m ímpar → preservação da parte imaginária

$$\mathrm{Im}\left[Y_3^1(\theta,\varphi)\right]$$

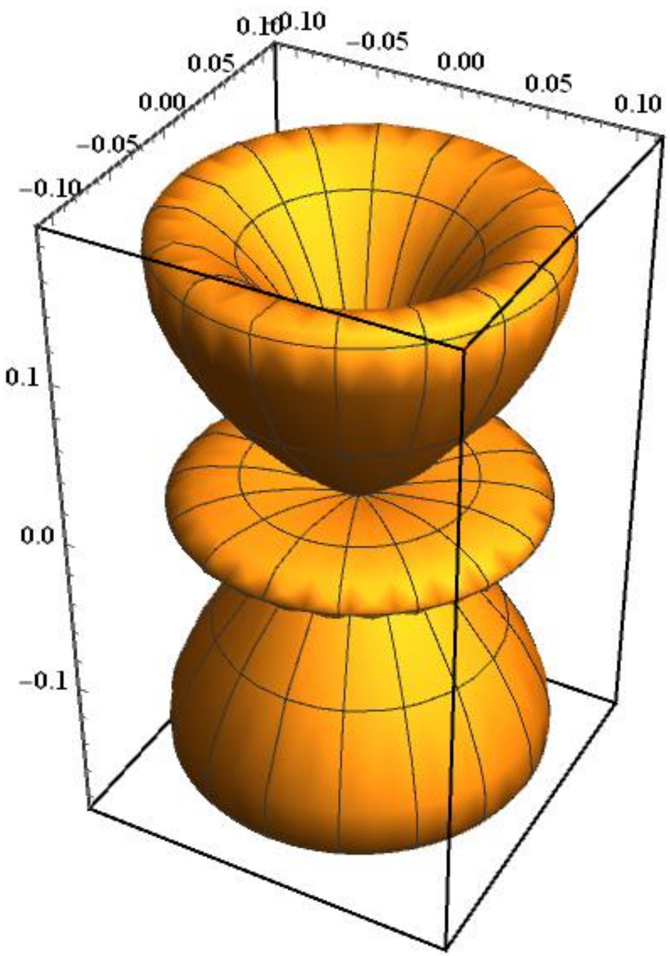


$$\mathrm{Im}\left[Y_3^{-1}(\theta,\varphi)\right]$$

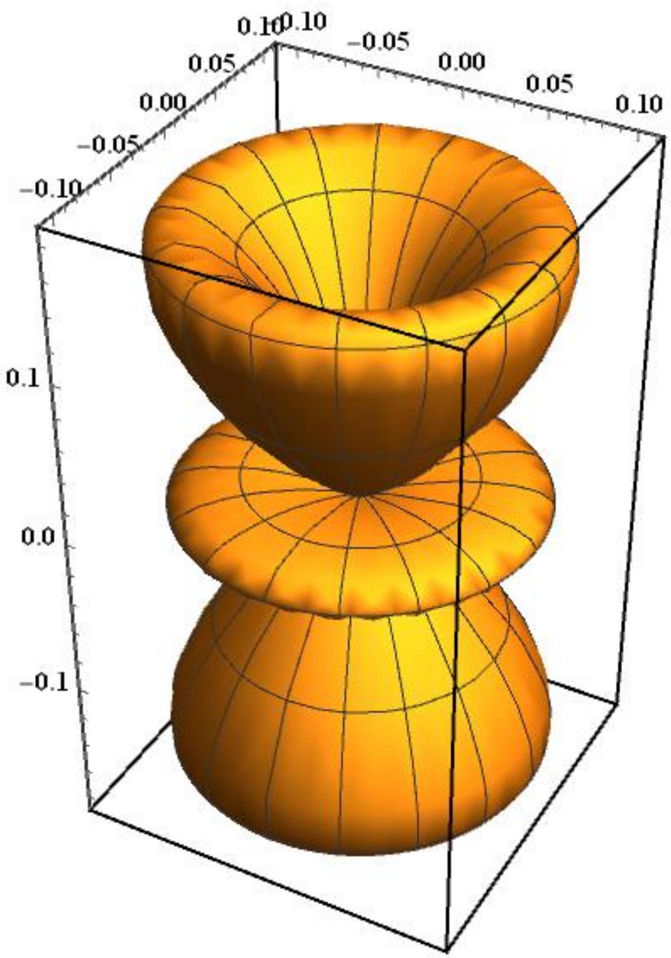


Uma Intuição: o módulo quadrado é sempre preservado!

$$\left|Y_3^1(\theta,\varphi)\right|^2$$



$$\left|Y_3^{-1}(\theta,\varphi)\right|^2$$



Obrigado!

Referência: Cohen-Tannoudji, C., Diu, B., & Lalöe F. (1977), Quantum Mechanics, Vol. 1. John Wiley.