

Operadores vectoriales

Las tres magnitudes $\{v_x, v_y, v_z\}$ son las componentes de un vector \vec{v} si ante una rotación R_{ij} se transforman como $v'_i = R_{ij} v_j$.

$\vec{v} = \{v_x, v_y, v_z\}$ es un vector si ante una rotación R se transforma como $v'_i = R_{ij} v_j$.

Un ket $|\alpha\rangle \in \mathcal{H}$ ante una rotación se transforma en el ket $|\alpha'\rangle = U(R) |\alpha\rangle$.

Decimos que $\vec{V} = \{V_x, V_y, V_z\}$ es un operador vectorial si $\langle V_i \rangle' = R_{ij} \langle V_j \rangle$.

$$\langle V_i \rangle' = \langle \alpha' | V_i | \alpha' \rangle = R_{ij} \langle \alpha | V_j | \alpha \rangle$$

$$\langle \alpha | U^\dagger(R) V_i U(R) | \alpha \rangle = R_{ij} \langle \alpha | V_j | \alpha \rangle$$

$$U^\dagger(R) V_i U(R) = R_{ij} V_j$$

Operadores vectoriales: transformado de un operador

Sea $|\alpha'\rangle = U(R)|\alpha\rangle$. Se define V'_i , el operador transformado de V_i , como :

$$\langle\alpha'|V'_i|\alpha'\rangle = \langle\alpha|V_i|\alpha\rangle$$

$$\langle\alpha|U^\dagger(R) V'_i U(R)|\alpha\rangle = \langle\alpha|V_i|\alpha\rangle$$

$$U^\dagger(R) V'_i U(R) = V_i$$

$$V'_i = U(R) V_i U^\dagger(R)$$

Definición de operador vectorial en términos de operadores transformados:

$$U^\dagger(R) V_i U(R) = R_{ij} V_j$$

$$U^\dagger(R^{-1}) V_i U(R^{-1}) = (R^{-1})_{ij} V_j$$

$$U(R) V_i U^\dagger(R) = R_{ji} V_j$$

$$V'_i = U(R) V_i U^\dagger(R) = V_j R_{ji}$$

Operadores tensoriales

Generalizamos la definición de operador vectorial $U(\mathbf{R}) V_i U^\dagger(\mathbf{R}) = V_j R_{ji}$ a operadores tensoriales de rango arbitrario k .

Los $2k+1$ operadores T_q^k ($q = -k, k$) son las componentes de un operador tensorial si ante rotaciones se transforman según la representación irreducible de dimensión $2k+1$ del grupo de las rotaciones:

$$U(\mathbf{R}) T_q^k U^\dagger(\mathbf{R}) = \sum_{q'} T_{q'}^k D_{q'q}^k(\mathbf{R})$$

Esta definición es equivalente a:

$$\left\{ \begin{array}{l} [J_z, T_q^k] = \hbar q T_q^k \\ [J_+, T_q^k] = \hbar \sqrt{k(k+1)-q(q+1)} T_{q+1}^k \\ [J_-, T_q^k] = \hbar \sqrt{k(k+1)-q(q-1)} T_{q-1}^k \end{array} \right.$$

Operadores tensoriales: rotación infinitesimal, $D_{q'q}^k(\boldsymbol{\varepsilon}) = \langle kq' | U(\boldsymbol{\varepsilon}) | kq \rangle$

$$U(\boldsymbol{\varepsilon}) T_q^k U^\dagger(\boldsymbol{\varepsilon}) = \sum_{q'} T_{q'}^k D_{q'q}^k(\boldsymbol{\varepsilon})$$

$$(1 - \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot \mathbf{J}) T_q^k (1 + \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot \mathbf{J}) = \sum_{q'} T_{q'}^k \langle kq' | (1 - \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot \mathbf{J}) | kq \rangle$$

$$T_q^k - \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot \mathbf{J} T_q^k + \frac{i}{\hbar} T_q^k \boldsymbol{\varepsilon} \cdot \mathbf{J} = \sum_{q'} T_{q'}^k \delta_{qq'} - \frac{i}{\hbar} T_{q'}^k \langle kq' | \boldsymbol{\varepsilon} \cdot \mathbf{J} | kq \rangle$$

$$-\frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{J}, T_q^k] = -\frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot \sum_{q'} T_{q'}^k \langle kq' | \mathbf{J} | kq \rangle$$

$$[\mathbf{J}, T_q^k] = \sum_{q'} T_{q'}^k \langle kq' | \mathbf{J} | kq \rangle$$

Operadores tensoriales: rotación infinitesimal, $D_{q'q}^k(\epsilon) = \langle kq' | U(\epsilon) | kq \rangle$

$$U(\epsilon) T_q^k U^\dagger(\epsilon) = \sum_{q'} T_{q'}^k D_{q'q}^k(\epsilon)$$

$$\left(1 - \frac{i}{\hbar} \epsilon \cdot \mathbf{J}\right) T_q^k \left(1 + \frac{i}{\hbar} \epsilon \cdot \mathbf{J}\right) = \sum_{q'} T_{q'}^k \langle kq' | \left(1 - \frac{i}{\hbar} \epsilon \cdot \mathbf{J}\right) | kq \rangle$$

$$T_q^k - \frac{i}{\hbar} \epsilon \cdot \mathbf{J} T_q^k + \frac{i}{\hbar} T_q^k \epsilon \cdot \mathbf{J} = \sum_{q'} T_{q'}^k \delta_{qq'} - \frac{i}{\hbar} T_{q'}^k \langle kq' | \epsilon \cdot \mathbf{J} | kq \rangle$$

$$-\frac{i}{\hbar} \epsilon \cdot [\mathbf{J}, T_q^k] = -\frac{i}{\hbar} \epsilon \cdot \sum_{q'} T_{q'}^k \langle kq' | \mathbf{J} | kq \rangle$$

$$[\mathbf{J}, T_q^k] = \sum_{q'} T_{q'}^k \langle kq' | \mathbf{J} | kq \rangle$$

$$\left\{ \begin{array}{l} [J_z, T_q^k] = \sum_{q'} T_{q'}^k \hbar q \langle kq' | kq \rangle = \hbar q T_q^k \\ [J_+, T_q^k] = \sum_{q'} T_{q'}^k \hbar \sqrt{k(k+1)-q(q+1)} \langle kq' | kq+1 \rangle = \hbar \sqrt{k(k+1)-q(q+1)} T_{q+1}^k \\ [J_-, T_q^k] = \sum_{q'} T_{q'}^k \hbar \sqrt{k(k+1)-q(q-1)} \langle kq' | kq-1 \rangle = \hbar \sqrt{k(k+1)-q(q-1)} T_{q-1}^k \end{array} \right.$$

Teorema de Wigner-Eckart

$$\langle \alpha j m | T_{m_1}^{j_1} | \alpha' j' m' \rangle = \langle j m | j_1 j' m_1 m' \rangle \langle \alpha j || T^{j_1} || \alpha' j' \rangle$$

$$\frac{1}{\hbar} \langle \alpha j m | [J_-, T_{m_1}^{j_1}] | \alpha' j' m' \rangle = \frac{1}{\hbar} \langle \alpha j m | J_- T_{m_1}^{j_1} | \alpha' j' m' \rangle - \frac{1}{\hbar} \langle \alpha j m | T_{m_1}^{j_1} J_- | \alpha' j' m' \rangle$$

$$\sqrt{j_1(j_1+1)-m_1(m_1-1)} \langle j m | T_{m_1-1}^{j_1} | j' m' \rangle =$$

$$\sqrt{j(j+1)-m(m+1)} \langle j m+1 | T_{m_1}^{j_1} | j' m' \rangle - \sqrt{j'(j'+1)-m'(m'-1)} \langle j m | T_{m_1}^{j_1} | j' m'-1 \rangle$$

Teorema de Wigner-Eckart

$$\langle \alpha j m | T_{m_1}^{j_1} | \alpha' j' m' \rangle = \langle j m | j_1 j' m_1 m' \rangle \langle \alpha j || T^{j_1} || \alpha' j' \rangle$$

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$$\sqrt{j_1(j_1+1)-m_1(m_1-1)} \langle j m | T_{m_1-1}^{j_1} | j' m' \rangle =$$

$$\sqrt{j(j+1)-m(m+1)} \langle j m+1 | T_{m_1}^{j_1} | j' m' \rangle - \sqrt{j'(j'+1)-m'(m'-1)} \langle j m | T_{m_1}^{j_1} | j' m'-1 \rangle$$

Idéntico a la relación de recurrencia de los coeficientes de CG con $j_2 m_2 \rightarrow j' m'$:

$$\sqrt{j_1(j_1+1)-m_1(m_1-1)} \langle j m | j_1 j_2, m_1-1 m_2 \rangle =$$

$$\sqrt{j(j+1)-m(m+1)} \langle j m+1 | j_1 j_2, m_1 m_2 \rangle - \sqrt{j_2(j_2+1)-m_2(m_2-1)} \langle j m | j_1 j_2, m_1 m_2-1 \rangle$$

Teorema de Wigner-Eckart

$$\langle \alpha j m | T_{m_1}^{j_1} | \alpha' j' m' \rangle = \langle j m | j_1 j' m_1 m' \rangle \langle \alpha j || T^{j_1} || \alpha' j' \rangle$$

$$\frac{1}{\hbar} \langle \alpha j m | [J_-, T_{m_1}^{j_1}] | \alpha' j' m' \rangle = \frac{1}{\hbar} \langle \alpha j m | J_- T_{m_1}^{j_1} | \alpha' j' m' \rangle - \frac{1}{\hbar} \langle \alpha j m | T_{m_1}^{j_1} J_- | \alpha' j' m' \rangle$$

$$\sqrt{j_1(j_1+1)-m_1(m_1-1)} \langle j m | T_{m_1-1}^{j_1} | j' m' \rangle =$$

$$\sqrt{j(j+1)-m(m+1)} \langle j m+1 | T_{m_1}^{j_1} | j' m' \rangle - \sqrt{j'(j'+1)-m'(m'-1)} \langle j m | T_{m_1}^{j_1} | j' m'-1 \rangle$$

Idéntico a la relación de recurrencia de los coeficientes de CG con $j_2 m_2 \rightarrow j' m'$:

$$\sqrt{j_1(j_1+1)-m_1(m_1-1)} \langle j m | j_1 j_2, m_1-1 m_2 \rangle =$$

$$\sqrt{j(j+1)-m(m+1)} \langle j m+1 | j_1 j_2, m_1 m_2 \rangle - \sqrt{j_2(j_2+1)-m_2(m_2-1)} \langle j m | j_1 j_2, m_1 m_2-1 \rangle$$

$$\sqrt{j_1(j_1+1)-m_1(m_1-1)} \langle j m | j_1 j_2, m_1-1 m_2 \rangle =$$

$$\sqrt{j(j+1)-m(m+1)} \langle j m+1 | j_1 j_2, m_1 m_2 \rangle - \sqrt{j'(j'+1)-m'(m'-1)} \langle j m | j_1 j', m_1 m'-1 \rangle$$

Descomposición en tensores irreducibles

$$T_q^k = \sum_{q_1 q_2} X_{q_1}^{k_1} Y_{q_2}^{k_2} \langle k_1 k_2, q_1 q_2 | kq \rangle$$

$$\hbar^{-1} [J_+, T_q^k] = \sum_{q_1 q_2} \hbar^{-1} \left\{ [J_+, X_{q_1}^{k_1}] Y_{q_2}^{k_2} + X_{q_1}^{k_1} [J_+, Y_{q_2}^{k_2}] \right\} \langle k_1 k_2, q_1 q_2 | kq \rangle =$$

$$= \sum_{q_1 q_2} X_{q_1+1}^{k_1} Y_{q_2}^{k_2} \sqrt{k_1(k_1+1)-q_1(q_1+1)} \langle k_1 k_2, q_1 q_2 | kq \rangle +$$

$$+ \sum_{q_1 q_2} X_{q_1}^{k_1} Y_{q_2+1}^{k_2} \sqrt{k_2(k_2+1)-q_2(q_2+1)} \langle k_1 k_2, q_1 q_2 | kq \rangle =$$

$$= \sum_{q_1 q_2} X_{q_1}^{k_1} Y_{q_2}^{k_2} \left\{ \underbrace{\sqrt{k_1(k_1+1)-q_1(q_1-1)} \langle k_1 k_2, q_1-1 q_2 | kq \rangle + \sqrt{k_2(k_2+1)-q_2(q_2-1)} \langle k_1 k_2, q_1 q_2-1 | kq \rangle}_{\sqrt{k(k+1)-q(q+1)} \langle k_1 k_2, q_1 q_2 | kq+1 \rangle} \right\}$$

$$= \sqrt{k(k+1)-q(q+1)} \sum_{q_1 q_2} X_{q_1}^{k_1} Y_{q_2}^{k_2} \langle k_1 k_2, q_1 q_2 | kq+1 \rangle$$

$$= \sqrt{k(k+1)-q(q+1)} T_{q+1}^k$$

La base cartesiana

- Para $j = 1$ tenemos la base $\{|1, 1\rangle, |1, 0\rangle, |1, -1\rangle\}$.
- Otra posibilidad es la base cartesiana $\{|x\rangle, |y\rangle, |z\rangle\}$, compuesta por kets invariantes ante rotaciones en $\hat{x}, \hat{y}, \hat{z}$, es decir los autoestados de J_x, J_y, J_z con autovalor 0.
- Claramente es $|z\rangle = |1, 0\rangle$ pues $U(\hat{z}, \phi) |1, 0\rangle = |1, 0\rangle$.
- Para obtener $|x\rangle, |y\rangle$ aplicamos rotaciones: $|x\rangle = U(\hat{y}, \frac{\pi}{2}) |z\rangle$ y $|y\rangle = U(\hat{z}, \frac{\pi}{2}) |x\rangle$.

$$\text{Usando: } d^1(\beta) = \frac{1}{2} \begin{pmatrix} 1 + \cos \beta & -\sqrt{2} \sin \beta & 1 - \cos \beta \\ \sqrt{2} \sin \beta & 2 \cos \beta & -\sqrt{2} \sin \beta \\ 1 - \cos \beta & \sqrt{2} \sin \beta & 1 + \cos \beta \end{pmatrix} \longrightarrow d^1\left(\frac{\pi}{2}\right) = \frac{1}{2} \begin{pmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}$$

$$|x\rangle = U(\hat{y}, \frac{\pi}{2}) |1, 0\rangle = \sum_m |1, m\rangle \langle 1, m | U(\hat{y}, \frac{\pi}{2}) |1, 0\rangle = \sum_m |1, m\rangle d_{m,0}^1\left(\frac{\pi}{2}\right) = \frac{-1}{\sqrt{2}} (|1, 1\rangle - |1, -1\rangle)$$

$$|y\rangle = U(\hat{z}, \frac{\pi}{2}) |x\rangle = e^{-i\frac{\pi}{2} J_z} \frac{-1}{\sqrt{2}} (|1, 1\rangle - |1, -1\rangle) = \frac{-1}{\sqrt{2}} (e^{-i\frac{\pi}{2}} |1, 1\rangle - e^{i\frac{\pi}{2}} |1, -1\rangle) = \frac{i}{\sqrt{2}} (|1, 1\rangle + |1, -1\rangle)$$

$$|z\rangle = |1, 0\rangle$$

Singlete y triplete de $\mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{3} \oplus \mathbf{5}$ en la base cartesiana

Sea S un tensor de rango cero. Sean T, V, W operadores vectoriales (tensores rango 1)

Los denotamos tanto por sus componentes esféricas como cartesianas.

- ▶ componentes esféricas $\{T_{+1}, T_0, T_{-1}\}$, que se transforman según $D_{mm'}^1(\alpha, \beta, \gamma)$
- ▶ componentes cartesianas, $\{T_x, T_y, T_z\}$, que se transforman según $R_{ij}(\alpha, \beta, \gamma)$

$$\begin{cases} T_{+1} = \frac{1}{\sqrt{2}} (T_x + iT_y) \\ T_{-1} = \frac{-1}{\sqrt{2}} (T_x - iT_y) \\ T_0 = T_z \end{cases} \quad \begin{cases} T_x = \frac{-1}{\sqrt{2}} (T_{+1} - T_{-1}) \\ T_y = \frac{i}{\sqrt{2}} (T_{+1} + T_{-1}) \\ T_z = T_0 \end{cases}$$

Sea $V^1 \otimes W^1$. Usando CG escribimos el $\mathbf{1}$ y $\mathbf{3}$ (T^0 y T^1) de $\mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{3} \oplus \mathbf{5}$:

$$\begin{cases} T_{+1}^1 = \frac{1}{\sqrt{2}} (V_1 W_0 - V_0 W_1) \\ T_{-1}^1 = \frac{1}{\sqrt{2}} (V_0 W_{-1} - V_{-1} W_0) \\ T_0^1 = \frac{1}{\sqrt{2}} (V_1 W_{-1} - V_{-1} W_1) \\ T_0^0 = \frac{1}{\sqrt{3}} (V_1 W_{-1} - V_0 W_0 + V_{-1} W_1) \end{cases} \quad \Rightarrow \quad \begin{cases} T_x = V_y W_z - V_z W_y \\ T_y = V_z W_x - V_x W_z \\ T_z = V_x W_y - V_y W_x \\ T_0^0 = V_x W_x + V_y W_y + V_z W_z \end{cases}$$

Ejemplo de operadores tensoriales: momentos multipolares

Campo electromagnético de una distribución de carga $\rho(\mathbf{r})$ y corriente $\mathbf{J}(\mathbf{r})$:

$$\mathbf{E}(\mathbf{r}) = -\nabla\Phi(\mathbf{r}) \quad \mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$$

donde el potencial eléctrico y magnético, dado $\rho(\mathbf{r})$ y $\mathbf{J}(\mathbf{r})$, son :

$$\Phi(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \quad \mathbf{A}(\mathbf{r}) = \frac{1}{c} \int \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$$

Desarrollo en armónicos esféricos de $|\mathbf{r} - \mathbf{r}'|^{-1}$:

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell+1} \frac{r'^{\ell}}{r^{\ell+1}} Y_{\ell m}^*(\theta', \phi') Y_{\ell m}(\theta, \phi) \quad (\text{con } r' < r)$$

$$\Phi(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' = \sum_{\ell, m} \frac{4\pi}{2\ell+1} \underbrace{\int \rho(\mathbf{r}') r'^{\ell} Y_{\ell m}^*(\theta', \phi') d\mathbf{r}'}_{q_{\ell m}} \frac{1}{r^{\ell+1}} Y_{\ell m}(\theta, \phi)$$

$$\Phi(\mathbf{r}) = 4\pi \sum_{\ell, m} \frac{4\pi}{2\ell+1} q_{\ell m} \frac{1}{r^{\ell+1}} Y_{\ell m}(\theta, \phi)$$

Ejemplo de operadores tensoriales: momentos multipolares

Los momentos eléctricos multipolares son :

$$q_{\ell m} = \int \rho(\mathbf{r}) r^\ell Y_{\ell m}^*(\theta, \phi) d\mathbf{r}$$

y los operadores correspondientes :

$$Q_{\ell m} = \int q r^\ell Y_{\ell m}^*(\theta, \phi) |\mathbf{r}\rangle \langle \mathbf{r}| d\mathbf{r}$$

Verificar que $Q_{\ell m}$ es un operador esférico irreducible de rango ℓ :

$$[L_+, Q_{\ell m}] = \hbar \sqrt{\ell(\ell+1) - m(m+1)} Q_{\ell, m+1}$$

$$[L_-, Q_{\ell m}] = \hbar \sqrt{\ell(\ell+1) - m(m-1)} Q_{\ell, m-1}$$

$$[L_z, Q_{\ell m}] = \hbar m Q_{\ell m}$$