Vector/Tensor operators

Review

$\hat{\vec{r}} = \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix}$ $\quad \hat{\vec{p}} = \begin{pmatrix} \hat{p}_x \\ \hat{p}_y \\ \hat{p}_z \end{pmatrix}$

$$\hat{D}(R) = e^{-i\theta \vec{u}\cdot\hat{\vec{J}}/\hbar}$$

Vector

Definition of a vector operator: an operator whose 3 components consist of operators $\hat{V}_j, j=1,2,3$ that transform as

"Rotation group"

$SO(3) \sim SU(2)$

Lie algebra

$[\hat{J}_j, \hat{J}_k] = i\hbar\epsilon_{jkl}\hat{J}_l$

$$\hat{D}^\dagger(R)\,\hat{V}_j\,\hat{D}(R) = \sum_{k=1}^{3} R_{jk}\hat{V}_k$$

Ordinary 3D rotation matrix

Definition in terms of infinitesimal rotations

$$\boxed{[\hat{J}_k, \hat{V}_j] = i\hbar\epsilon_{kjl}\hat{V}_l}$$

Cartesian version of the transformation

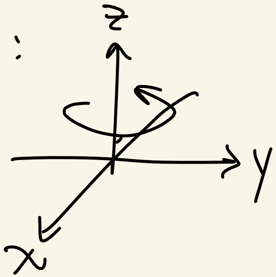
More generally, this can be generalized to tensor operators: an object that has as its components $\hat{T}_k^q$ where $\underbrace{-k \le q \le k}_{2k+1 \text{ components}}$

$$D^\dagger T_k^q D = \sum_{q'} T_{\underset{\text{"}j\text{"}}{\underset{\shortparallel}{k}}}^{q'} D^{(k)}_{qq'}(R)$$

Spherical vectors/tensors

$|j,m\rangle$ $\{\hat{J}^2, \hat{J}_z\}$

Analogous to vectors in spin-j subspace, it is convenient to use as a basis the eigenstates of $\hat{J}_z$:



Eigenvectors of rotations about the z axis:

$$\hat{z}, \quad \hat{x} \pm i\hat{y}$$

$j=1$ "vector"

$$\hat{V}_0^{(1)} = \hat{V}_z$$

$m=0$

$$\hat{V}_{\pm 1}^{(1)} = \mp\left(\frac{\hat{V}_x + i\hat{V}_y}{\sqrt{2}}\right)$$

Spherical vector operator

$$[\hat{J}_z, \hat{V}_m^{(1)}] = m\hat{V}_m^{(1)}$$

$$[\hat{J}_\pm, \hat{V}_m^{(1)}] = \sqrt{2 - m(m\pm 1)}\;\hat{V}_{m\pm 1}^{(1)}$$

$$\sqrt{j(j+1) - m(m\pm 1)}$$

Spherical tensor operators T_k^q ← "m", ← "j" Y_ℓ^m

"Things" that transform as spin-k representation / subspace

Definition:

$$\boxed{\begin{aligned} [\hat{J}_z, \hat{T}_k^q] &= q\,\hat{T}_k^q \\ [\hat{J}_\pm, \hat{T}_k^q] &= \sqrt{k(k+1)-q(q\pm 1)}\;\hat{T}_k^{q\pm 1} \end{aligned}}$$

Higher rank tensors also appear classically

Classical

Dyad/dyadic $\overleftrightarrow{T} = \vec{U}\vec{V}$ outer product

$$3\left\{\begin{pmatrix} U \end{pmatrix}\overbrace{\begin{pmatrix} V \end{pmatrix}}^{3} = \begin{pmatrix} \quad \end{pmatrix}\right.$$

9 components

Vectors are denoted by uppercase letters $\vec{A}, \vec{B}, \vec{U}, \vec{V}$

$$T_{jk} = U_j V_k$$

$$\overleftrightarrow{T} = \underset{\text{scalar}}{T_0} + \underset{\text{vector}}{T_1} + T_2$$

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$$T_{jk} = (T_0)_{jk} + (T_1)_{jk} + (T_2)_{jk}$$

$$\begin{pmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{pmatrix}$$

Symmetric & Antisymmetric

3 vector components T_1

5 tensor components

-1 from trace

(General T_{jk} may not be a dyad $U_j V_k$)

	Trace	Antisymmetric	Traceless symmetric
	$\dfrac{\mathrm{Tr}(T)}{3}\delta_{jk}$	$\dfrac{T_{jk} - T_{kj}}{2}$	$\dfrac{T_{jk} + T_{kj}}{2} - \dfrac{\mathrm{Tr}(T)}{3}\delta_{jk}$
Special case $\overleftrightarrow{T} = \vec{U}\vec{V}$	$\dfrac{\vec{U}\cdot\vec{V}}{3}\delta_{jk}$	$\dfrac{1}{2}\epsilon_{jkl}(\vec{U}\times\vec{V})_l$	$\dfrac{U_j V_k + U_k V_j}{2} - \dfrac{\vec{U}\cdot\vec{V}}{3}\delta_{jk}$
# components	1	3	5
	$j=0$	$j=1$	$j=2$

Why do we get $j = 0, 1, 2$

Clebsch-Gordan series

$$\overleftrightarrow{T} = \vec{U}\,\vec{V} = \vec{U} \otimes \vec{V} = \bigoplus_{J=|j_1-j_2|}^{j_1+j_2=2} \mathcal{H}_J = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2$$

$$\vec{U}\uparrow 1 \qquad \vec{V}\uparrow 1$$

$$|j_1 - j_2| = 1 - 1 = 0$$

Another example

Two-level systems

$$|\hat{n}\rangle\langle\hat{n}| = \frac{\hat{\mathbb{1}} + \hat{n}\cdot\vec{\sigma}}{2}$$

Trace 1

Transforms like a vector

$$\begin{pmatrix} \hat{\sigma}_x \\ \hat{\sigma}_y \\ \hat{\sigma}_z \end{pmatrix} \text{ is a vector operator}$$

$$|\hat{n}\rangle \otimes \langle\hat{n}|$$

$$\tfrac{1}{2} \qquad \tfrac{1}{2}$$

$$\mathcal{H}_{1/2} \otimes \mathcal{H}_{1/2} = \bigoplus_{J=0}^{1} \mathcal{H}_J = \mathcal{H}_0 + \mathcal{H}_1$$

Application to determine whether a matrix element $\langle \psi_f | \hat{V} | \psi_i \rangle$ vanishes or not based solely on rotational symmetry (SSR)

$\langle \alpha' j' m' |$ $\quad$ $| \alpha j m \rangle$

Label for other d.o.f.

Wigner-Eckart theorem

Proportional const.

"Reduced matrix element" ← Sakurai

$\mathcal{H}_{j'} \leftarrow \mathcal{H}_k \otimes \mathcal{H}_j$

$$\langle \alpha' j' m' | \hat{T}_k^q | \alpha j m \rangle = \underbrace{\langle j', m' | j, m, k, q \rangle}_{\text{C-G coefficients}} \overbrace{\langle \alpha, j' || T_k || \alpha, j \rangle}$$

"Double bar notation"

Important

Doesn't depend on m, m', q "directional quantity"

C-G coefficients

(Conventionally defined to be real, so we can also write it as $\langle j, m, k, q | j', m' \rangle$

Does not depend on the "direction"

$$\cancel{\langle \alpha' j' || T_k || \alpha j \rangle^*} = \cancel{\langle \alpha j || T_k^\dagger || \alpha' j' \rangle}$$

Sketch of the proof idea of WE thm

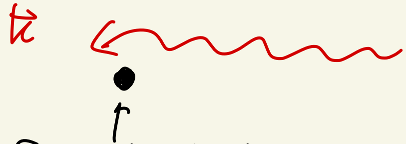
<u>Claim</u> $\hat{T}^q_k|jm\rangle$ transforms like elements in $\mathcal{H}_k \otimes \mathcal{H}_j$

- $\hat{R}\left(\hat{T}^q_k|jm\rangle\right) = \hat{R}\hat{T}^q_k\hat{R}^\dagger \hat{R}|jm\rangle$

$$= \sum_{q'm'} \underbrace{D^{(k)}_{q'q}(R)\, D^{(j)}_{m'm}(R)}\; T^{q'}_k |jm'\rangle$$

Physical application: Dipole selection rule

super



feels the local $\vec{E}$ field

Polarization

$$\vec{E}(\vec{r},t) = \mathrm{Re}\left[\hat{\epsilon}\, E(\vec{r})\, e^{-i\omega t}\right]$$

I've already combined the factor $e^{i\vec{k}\cdot\vec{r}}$

Interaction Hamiltonian

$q\vec{r}$ ← Vector operator

$$\hat{H}_{int} = -\hat{\vec{d}}\cdot\vec{E}(\vec{r},t)$$

$$= -\frac{1}{2}\left[\hat{\vec{d}}\cdot\vec{\epsilon}\, E(\vec{r})\, e^{-i\omega t} + \hat{\vec{d}}\cdot\vec{\epsilon}^{\,*} E^{*}(\vec{r})\, e^{i\omega t}\right]$$

From perturbation theory

absorption of photons

emission of photons

Focus on the absorption part $\hat{\vec{d}}\cdot\vec{\epsilon}$

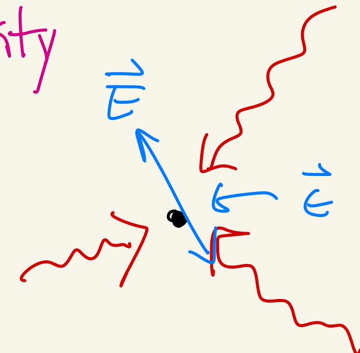
Not $\vec{\epsilon}^{\,*}$

Rate of transition $\propto \left|\langle \psi_f | \hat{d}\cdot\vec{\epsilon}_L E(\vec{r}) | \psi_i\rangle\right|^2$

$e^{i\vec{k}\cdot\vec{r}}$

$$= \underbrace{\left|\langle \psi_f | \hat{d}\cdot\vec{\epsilon}\, | \psi_i\rangle\right|^2}_{\text{We want to know}} \; \underbrace{\left|E(\vec{r})\right|^2}_{\text{Intensity}}$$

Atom can't "see"

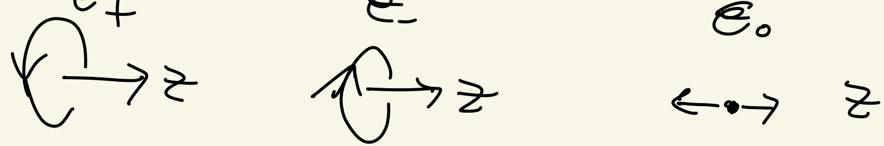


Independent of the direction of propagation $\vec{k}$

Only depends on $\vec{\epsilon}$

Expand $\vec{\epsilon}$ in the spherical basis

$\vec{e}_+$ $\quad$ $\vec{e}_-$ $\quad$ $\vec{e}_0$ $\quad$ $\vec{\epsilon}_0 = \epsilon_z$



$$\epsilon_{\pm} = \mp\frac{(\epsilon_x \pm i\epsilon_y)}{\sqrt{2}}$$

Jargon

"คำศัพท์เฉพาะทาง"

σ_+ light $\quad$ σ_- light $\quad$ π light

Dipole selection rule $\quad \vec{d}\cdot\vec{E}$

Direction $\quad$ doesn't depend on q

$$\langle \alpha', j', m' | \hat{d}^{\,q}_{k=1} | \alpha, j, m\rangle = \langle j' m' | 1\, q, j\, m\rangle \boxed{\langle \alpha' j' \| d_k \| \alpha\, j\rangle}$$

Directionless

For this ↑ to not vanish

$$m + \underset{0,\pm 1}{q} = m'$$

If the light propagates in the z direction, there will only be $\sigma_\pm$ components


$z \Rightarrow q = \pm 1 \Rightarrow \boxed{m' - m = \pm 1}$ SSR for m'

But if the light propagates in direction other than z $\quad m' - m = \begin{cases} \pm 1 \\ 0 \end{cases}$

$$\underbrace{|j-1| \leq j' \leq j+1}_{\Downarrow}$$

No $j = 0 \rightarrow j' = 0$ (forbidden transition)

Example of using rotational symmetry to derive SSR ?