Phys 521

Fall 2023

Wigner-Eckart

① Spherical Harmonics

Any spherically symmetric potential

$$V(\vec r) = V(|\vec r|)$$

will have wave functions

$$\psi_{n\ell m}(\vec r) = \langle \vec r | n \ell m \rangle = R_{n\ell}(r)\, Y_\ell^m(\theta, \phi)$$

n = energy quantum number

$Y_{\ell m}(\theta, \phi)$ spherical harmonics

Define states $|\ell, m\rangle$ and direction eigenkets $|\hat n\rangle$ such that

$$\langle \hat n | \ell, m \rangle = Y_\ell^m(\theta, \phi)$$

Orbital angular momentum operator

$$\vec L = \vec r \times \vec p = \varepsilon_{ijk}\, x_j\, p_k$$

Generators of rotations on space of functions

$$[L_i, L_j] = i\hbar\, \varepsilon_{ijk} L_k$$

simplest is $\hat L_z \doteq \frac{\hbar}{i}\frac{\partial}{\partial \phi}$

and

$$\hat L^2 \doteq -\hbar^2 \left[\frac{1}{s^2}\frac{\partial^2}{\partial \phi^2} + \frac{1}{s}\frac{\partial}{\partial \theta}\left(s \frac{\partial}{\partial \theta} \right) \right]$$

with $s \equiv \sin\theta$

and ladder operators:

$$L_\pm \doteq \frac{\hbar}{i} e^{\pm i\phi}\left(\pm i\frac{\partial}{\partial\theta} + \cot\theta\frac{\partial}{\partial\phi}\right)$$

then $L_z Y_\ell^m = m\hbar Y_\ell^m$

$$L^2 Y_\ell^m = \hbar^2 \ell(\ell+1) Y_\ell^m$$

from $\frac{\hbar}{i}\frac{\partial}{\partial\phi} Y_\ell^m = m\hbar Y_\ell^m$

we see $Y_\ell^m \propto e^{im\phi}$

We can get Y_ℓ^m themselves from

$$L_+ Y_{\ell\ell} = 0$$

$$\frac{\hbar}{i} e^{i\phi}\left[i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right] Y_{\ell\ell} = 0$$

gives $Y_\ell^\ell = C_\ell e^{i\ell\phi} \sin^\ell\theta$

generate all Y_ℓ^m from <u>lowering operator</u>

C_ℓ defined by

$$\langle \ell' m' | \ell m\rangle = \int_{4\pi} d\Omega \left(Y_{\ell'}^{m'}\right)^* Y_\ell^m = \delta_{mm'}\delta_{\ell\ell'}$$

Also convenient to define

$$Y_\ell^{-m} \equiv (-1)^m \left(Y_\ell^m\right)^*$$

Explicitly for $\ell = 1$:

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}} \sin\theta\, e^{i\phi} = -\sqrt{\frac{3}{8\pi}} \left(\frac{x+iy}{r}\right)$$

$$Y_1^{-1} = \sqrt{\frac{3}{8\pi}} \sin\theta\, e^{-i\phi} = \sqrt{\frac{3}{8\pi}} \left(\frac{x-iy}{r}\right)$$

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

② Spherical Basis

On HW # 3 we found transformation from cartesian rotation generators, to basis where $J_z = \mathrm{diag}(1, 0, -1)$

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 0 & 1 \\ -i & 0 & -i \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$ (see next page)

position vector $\vec{r}$,

$$\vec{r} = (\hat{x}, \hat{y}, \hat{z}) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = (\hat{x}\ \hat{y}\ \hat{z})\, S S^\dagger \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$(\hat{x}, \hat{y}, \hat{z})\, S \equiv \left(\hat{e}^{+1}, \hat{e}^{0}, \hat{e}^{-1}\right)$$

spherical basis

We found HW # 3:

$$R^c(\phi\hat{z}) = \begin{pmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

generator $$\frac{J_z^c}{\hbar} = i\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

diagonalize to get

$$\frac{J_z}{\hbar} = \mathrm{diag}(1\ 0\ -1) = S\,\frac{J_z^c}{\hbar}$$

$$S_{iq} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 & 0 & 1 \\ -i & 0 & -i \\ 0 & \sqrt{2} & 0 \end{pmatrix} ; \quad S^{\dagger}_{qi} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 & i & 0 \\ 0 & \sqrt{2} & 0 \\ 1 & i & 0 \end{pmatrix}$$

i = cartesian x, y, z index

q = spherical $+1\ 0\ -1$ index

$S^{\dagger}S = I$ unitary transformation

$$S^{\dagger}_{qi}\begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}_i = V_q = \begin{cases} -\frac{1}{\sqrt{2}}(V_x - iV_y) & +1 \\ V_z & 0 \\ \frac{1}{\sqrt{2}}(V_x + iV_y) & -1 \end{cases} \qquad \underline{\underline{q=}}$$

with $\quad \hat{\varepsilon}^{\pm} = \mp(\hat{x} \pm i\hat{y})$

$$\varepsilon^0 = \hat{z}$$

and components

$$S^+ \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}}(x - iy) \\ z \\ \frac{1}{\sqrt{2}}(x+iy) \end{pmatrix} \equiv \begin{pmatrix} -r^{-1} \\ r^0 \\ -r^{+1} \end{pmatrix} = r\sqrt{\frac{4\pi}{3}} \begin{pmatrix} -Y_1^{-1} \\ Y_1^0 \\ -Y_1^1 \end{pmatrix}$$

then

$$\vec{F} = -r^{-1}\hat{\varepsilon}^{+1} - r^{+1}\hat{\varepsilon}^{-1} + r^0\hat{\varepsilon}^0$$

$$= \sum_{m=-1}^{+1} (-1)^m r^{-m} \hat{\varepsilon}^m$$

③ Tensor Operators

Under rotations, ordinary Cartesian vector transforms as

$$V_i' = R^c_{ij} V_j$$

$[R^c]$ is ordinary 3x3 rotation matrix in cartesian coordinates.

Recall expectation value of spin-½ operator.

$$|\psi_R\rangle = R^s_z|\psi\rangle \qquad \text{rotation of state about } \hat{z}$$

consider $\langle\psi|\hat{S}_x|\psi\rangle \to \langle\psi_R|\hat{S}_x|\psi_R\rangle$

$$= \langle\psi|R_z^{s^{-1}} S_x R^s_z|\psi\rangle$$

where $R_z^s = R^s(\phi\hat{z}) = e^{-i\phi\hat{S}_z/\hbar}$

then infinitessimally, $e^{-i\varepsilon\hat{S}_z/\hbar} = (1 - i\varepsilon\frac{\sigma_z}{2})$

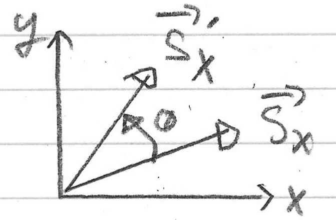
$$R_z^{s+}\hat{S}_x R_z^s = (1+i\varepsilon\tfrac{\sigma_z}{2})(\hbar\tfrac{\sigma_x}{2})(1-i\varepsilon\tfrac{\sigma_z}{2})$$

$$= \hbar\Big(\tfrac{\sigma_x}{2} + i\varepsilon\underbrace{\big[\tfrac{\sigma_z}{2},\tfrac{\sigma_x}{2}\big]}_{i\sigma_y/2}\Big) = \tfrac{\hbar}{2}(\sigma_x - \varepsilon\sigma_y) = \hat{S}_x - \varepsilon\hat{S}_y$$

For finite rotation,

$$R_z^{s+}\hat{S}_x R_z^s = \cos\phi\,\hat{S}_x - \sin\phi\,\hat{S}_y$$

Just like cartesian rotation of vector:



rotation $+\phi$ about $\hat{z}$

Cartesian tensors are generalizations of vectors. For example

$$T'_{ij} = \sum_{k,l} R^c_{ik} R^c_{jl} T_{kl}$$ rank 2 cartesian tensor

Such tensors are in general reducible under rotations.

For example dyadic of two vectors $\vec{A}, \vec{B}$

$$A_i B_j = \frac{\vec{A}\cdot\vec{B}}{3}\delta_{ij} + \frac{1}{2}\left(A_i B_j - A_j B_i\right)$$

$$+ \left[\frac{A_i B_j + B_j \cdot A_i}{2} - \frac{\vec{A}\cdot\vec{B}}{3}\delta_{ij}\right]$$

SU(2) decomposition into <u>spherical tensors</u>

$$\underset{\sim}{3} \times \underset{\sim}{3} = \underset{\sim}{1} + \underset{\sim}{3} + \underset{\sim}{5}$$

where $\underset{\sim}{5}$ is traceless (unlike moment of inertia tensor)

Wigner-Eckart theorm concerns states $\propto Y_{\ell m}$, $|\alpha, \ell m\rangle$

where α are any other quantum number, for example $|n \ell m\rangle$ of hydrogen.

We want to rotate tensor like basis $|\ell, m\rangle$:

$|\hat{n}'\rangle = R|\hat{n}\rangle$ direction eigenket rotates

$$\langle n'|\ell m\rangle = \langle n|\left(R^{\dagger}|\ell m\rangle\right)$$

$$R^{\dagger}|\ell, m\rangle = \sum_{m'} |\ell m'\rangle \underbrace{\langle \ell m'|R^{\dagger}|\ell m\rangle}_{\mathcal{D}^{(\ell)}_{m'm}(R^{\dagger})}$$

rotation of basis $|\ell, m\rangle$

so

$$\langle \hat{n}' | \ell m \rangle = \sum_{m'} \langle \hat{n} | \ell m' \rangle \mathcal{D}^{(\ell)}_{m'm}(R^\dagger)$$

or

$$Y_\ell^m(\hat{n}') = \sum_{m'} Y_\ell^{m'} \underbrace{\mathcal{D}^{(\ell)}_{m'm}(R^\dagger)}_{\left(\mathcal{D}^{(\ell)}_{m'm}\right)^\dagger = \mathcal{D}^{(\ell)*}_{\underset{\checkmark}{mm'}}(R)}$$

note order

Under change of basis, spherical tensor of rank k, dim 2k+1   -k ≤ m ≤ k

$$R^\dagger T_k^m R = \sum_{m'} T_k^{m'} \mathcal{D}^{k*}_{mm'}(R)$$

or taking hermitian conjugate (hermitian operator)

$$\boxed{R\, T_k^m R^\dagger = \sum_{m'} T_k^{m'} \mathcal{D}^{k}_{m'm}(R)}$$

Note in notation of Cummins, Shankar rank index lower case like Y_ℓ^m. Opposite of Sakurai!

Or equivalently,

$$[J_\pm, T_k^m] = \pm\hbar\left[k(k+1) \mp (m \pm 1))\right]^{1/2} T_k^{m\pm1}$$

$$[J_z, T_k^m] = \hbar m\, T_k^m$$

WE #8

we have selection rule (m-rule)

$\langle \alpha' j' m' | T_k^q | \alpha j m \rangle = 0$ unless $m' = q + m$

<u>Example</u> spherical position operator r_1^q (rank 1, vector)

$$\left.\begin{aligned} r_1^{\pm} &= r\sqrt{\frac{8\pi}{3}}\, Y_1^{\pm 1} \\ r_1^{0} &= r\sqrt{\frac{4\pi}{3}}\, Y_1^{0} \end{aligned}\right\} \equiv C_m r Y_\ell^q$$

$$\langle n'\ell' n' | r_1^q | n\ell m \rangle = \int d^3r\, R_{n'\ell'} Y_{\ell'}^{m'} C_m r Y_\ell^q R_{n\ell} Y_\ell^m$$

$$= C_m \underbrace{\int_0^\infty r^3 dr\, R_{n'\ell'} R_{n\ell}}_{\equiv \text{ reduced matrix element}} \underbrace{\int d\Omega\, Y_{\ell'}^{m'} Y_\ell^q Y_\ell^m}_{\text{Clebsch Gordon}}$$

$$= \langle n'\ell' \| r_1 \| n\ell \rangle \langle \ell m; 1 q | \ell' m' \rangle$$

this is example of Wigner-Eckart theorem.

recall C.G. coefficients (as written by Commins, Wikipedia, similar to particle data group)

$$|JM\rangle = \sum_{m_1, m_2} |j_1 m_1\rangle |j_2 m_2\rangle \underbrace{\langle j_1 m_1; j_2 m_2 | JM \rangle}_{C.G.}$$

WE #9

Wigner-Eckart theorem:

$$\langle \alpha_2 j_2 m_2 | T_k^q | \alpha_1 j_1 m_1 \rangle = \langle \alpha_2 j_2 || T_k || \alpha_1 j_1 \rangle \langle j_1 m_1 ; k q | j_2 m_2 \rangle$$

Selection rules

$\langle \alpha_2 j_2 m_2 | T_k^q | \alpha_1 j_1 m_1 \rangle \neq 0$ only if

$$m_2 = m_1 + q$$

and triangle rul,

$$j_2 = j_1 + k, j_1 + k - 1, \ldots |j_1 - k|$$

For scalar (rank $k=0$) amplitude $\neq 0$ for $j_1 = j_2$

For vector (rank $k=1$) amplitude $\neq 0$ only for

$$j_2 = j_1 + 1, j_1, j_1 - 1$$

For vector, we have the projection theorem,

$$\langle \alpha j m' | A_1^q | \alpha j m \rangle =$$

$$\frac{\langle \alpha' j m | \vec{J} \cdot \vec{A} | \alpha j m \rangle}{\hbar^2 j(j+1)} \langle j m' | J^q | j m \rangle$$

WE #10

Application of projection theorem, Landé g-factor

For electron in hydrogen atom

$$\vec{\mu} = \vec{\mu}_s + \vec{\mu}_l = -\mu_B\left(2\vec{S}+\vec{L}\right) = -g_j\,\mu_B\,\vec{J}$$

$\vec{J} = \vec{L}+\vec{S}$ and g_j is Landé g-factor.

$$\mu_B = \frac{e\hbar}{2mc}$$

projection theorem for $q=0$, state $|n j m\rangle$

$$\langle jm|A_1^0|jm\rangle = \frac{m}{\hbar j(j+1)}\langle jm|\vec{J}\cdot\vec{A}|jm\rangle$$

for $\vec{A} = \vec{\mu} = -\mu_B\left(2\vec{S}+\vec{L}\right)$

$$\vec{J}\cdot\vec{A} = -\mu_B\left(\vec{S}+\vec{L}\right)\cdot\left(2\vec{S}+\vec{L}\right)$$

$$= -\mu_B\left(L^2+\vec{L}\cdot\vec{S}\right) - 2\mu_B\left(S^2+\vec{L}\cdot\vec{S}\right)$$

with $\langle jm|L^2|jm\rangle = \hbar^2 l(l+1)$

$$\langle jm|S^2|jm\rangle = \hbar^2 s(s+1)$$

$$\langle jm|\vec{L}\cdot\vec{S}|jm\rangle = \frac{1}{2}\langle jm|J^2-L^2-S^2|jm\rangle$$

$$= \frac{\hbar^2}{2}\left[j(j+1)-l(l+1)-s(s+1)\right]$$

We get

$$\langle\mu_z\rangle = \langle j\, m | \mu^0 | j\, m\rangle = \frac{-\mu_B m}{\hbar j(j+1)} \hbar^2 \left[\frac{1}{2}\left(j(j+1) - l(l+1) - s(s+1)\right) + l(l+1) + s(s+1)\right]$$

$$= \frac{-\mu_B m \hbar}{j(j+1)} \frac{1}{2}\left[j(j+1) + l(l+1) + s(s+1)\right]$$

and $\langle \mu_z \rangle = -g_j \mu_B \langle j m | J_z | j m\rangle = -g_j m \hbar \mu_B$

gives $g_j = \frac{1}{2j(j+1)}\left[j(j+1) + s(s+1) + l(l+1)\right]$

<u>note</u>: for $q \neq 0$

$$\langle \alpha j m | \vec{u} | \alpha j m\rangle = \frac{\langle \alpha j m | \vec{J}\cdot\vec{\mu} | \alpha j m\rangle}{\hbar^2 j(j+1)} \langle \alpha m | J_1^q | j m\rangle$$

$$\langle \alpha m \,|\, q \,|\, \alpha m\rangle = \delta_{m,m+q}$$

$= 0$ unless $q = 0$

So $\vec{\mu}_{\text{effective}} = -g_j \mu_B \vec{J}$