Tensors and Tensor Operators.

Scalars - invariant under rotations.

Vectors - transform according to

$$x_i' = \sum_j a_{ij} x_j$$

a_{ij} - rotation matrix
x_i - vector component. (cartesian)

Tensors.
- Consider $T_{ij} = x_i(1)\, x_j(2)$

A general non-symmetric tensor of rank 2 has 9 independent components which transform according to a reducible 9×9 representation of rotation group.

$$T_{ij}' = \sum_{kl} a_{ik} a_{jl} T_{kl}$$

We can form a scalar $T_0 = \sum_k T_{kk}$, 1 component

an antisymmetric tensor $\hat{T}_{ij} = \frac{1}{2}(T_{ij} - T_{ji})$ 3 "

a symmetric tensor of 0 trace $\bar{T}_{ij} = \frac{1}{2}(T_{ij} + T_{ji}) - \frac{1}{3}\delta_{ij} T_0$

5 component

Since ~~transfor~~ rotations preserve trace and symmetry, each set of components transform among themselves forming 1, 3 and 5-D invariant subspaces.

- In each subspace of dimension $(2k+1)$, form linear combinations of the T_{ij}'s labelled by T_{kq}, $q = -k, \dots, k$ such that under rotations

$$T_{kq}' = \sum_p T_{kp} \mathcal{D}^k_{pq}(\alpha, \beta, \gamma)$$

Definition of an irreducible spherical tensor.

a vector "$\underset{\sim}{a}$" in terms of irreducible tensor components is

$$a_{\pm 1} = \mp \frac{1}{\sqrt{2}} (a_x \mp i a_y) \qquad a_0 = a_z$$

$$a_q' = \sum_p a_p \mathcal{D}^1_{pq}(\alpha, \beta, \gamma)$$

The direct product $a_{q_1} b_{q_2}$ transforms according to

$$(a_{q_1} b_{q_2})' = \sum_{p_1 p_2} a_{p_1} b_{p_2} \mathcal{D}^1_{p_1 q_1} \mathcal{D}^1_{p_2 q_2}$$

just as for angular momentum eigenfunctions - i.e. according to the reducible representation

$$\mathcal{D}^1 \times \mathcal{D}^1 = \mathcal{D}^2 + \mathcal{D}^1 + \mathcal{D}^0 .$$

construct irreducible representations as before by vector coupling

$$T_{KQ}(ab) = \sum_{q_1 q_2} a_{q_1} b_{q_2} \langle 1 1 q_1 q_2 | K Q \rangle$$

$K = 2, 1, 0.$

$\therefore$ Angular momentum eigenfunctions are just a special case of irreducible spherical tensor operators.

The condition $T_{kq}' = \sum_p T_{kp} \mathcal{D}^k_{pq}(\alpha,\beta,\gamma)$ can be expressed more conveniently in terms of commutation relations as follows

<u>Commutation Relations for T_{kq}.</u>

$$T_{kq}' = D\, T_{kq}\, D^\dagger = \sum_p T_{kp} \mathcal{D}^k_{pq}(\alpha,\beta,\gamma)$$

- Let D be the infinitesimal rotation $(1 - i\alpha J_\lambda)$, $\lambda = \pm 1, 0$.

Then $\mathcal{D}^k_{pq} = \langle kp | 1 - i\alpha J_\lambda | kq \rangle$

$$= \delta_{pq} - i\alpha \langle kp | J_\lambda | kq \rangle$$

$\therefore (1 - i\alpha J_\lambda)\, T_{kq}\, (1 + i\alpha J_\lambda)$ (since ~~$J_\lambda^\dagger = J_\lambda$~~ $DD^\dagger = 1$)

$$= T_{kq} - i\alpha \sum_p T_{kp} \langle kp | J_\lambda | kq \rangle$$

Equating coefficients of $i\alpha$ yields

$$[J_\lambda, T_{kq}] = \sum_p T_{kp} \langle kp | J_\lambda | kq \rangle$$

But $\langle jm | J_z | jm \rangle = m$

$$\langle j\, m\pm1 | J_\pm | jm \rangle = \{(j \pm m + 1)(j \mp m)\}^{1/2}$$

$$\therefore [J_z, T_{kq}] = q\, T_{kq}$$

$$[J_\pm, T_{kq}] = \{(k \pm q + 1)(k \mp q)\}^{1/2}\, T_{k\,q\pm1}$$

ie. J_z and $J_\pm$ have the same effect on the T_{kq}'s as they have on the angular momentum eigenvectors $|jm\rangle$. The result appears as a commutator only because the quantities are operators.

ie $(J_z T_{kq} - T_{kq} J_z)\,\Psi = (J_z T_{kq})\,\Psi$

General Tensor Product.

- Suppose irr. tensor operators R_k, $S_{k'}$.

The irr. tensor product of rank K is

$$T_{KQ}(R_k, S_{k'}) = \sum_{qq'} R_{kq} S_{k'q'} \langle k k' q q' | KQ \rangle$$

If R and S are operators, then
$T(R,S) \neq T(S,R)$.

The scalar product is

$$T_{00}(R_k, S_k) = \frac{(-1)^k}{\sqrt{2k+1}} \sum_q (-1)^q R_{kq} S_{k-q}$$

$$= \frac{(-1)^k}{\sqrt{2k+1}} \underset{\sim}{R}_k \cdot \underset{\sim}{S}_k \quad \text{for } k = 1.$$

If ~~k = k' and K = 1~~ $R = S$ then, from exchange symmetry, $T_{KQ}(R_k, R_k)$ vanishes unless K = even (integral k) or K = odd ($\frac{1}{2}$-integral k). $(-1)^{K-k-k'}$

- Generalization of $\underset{\sim}{r} \times \underset{\sim}{r} = 0$.

(Doesn't apply if R is an operator - e.g.
$\underset{\sim}{J} \times \underset{\sim}{J} = i \underset{\sim}{J}$ $\quad (J_x J_y - J_y J_x) = i J_z$)

~~Tensor Operators.~~

~~The general requirement~~
~~general rule for operators~~

$$\cancel{T_{kq}' = O T_{kq} O^{+} = \sum_p T_{kp} \mathcal{D}^k_{pq}(\alpha, \beta, \gamma)}$$

~~reduces to the commutation relations~~

$$\cancel{[J_z, T_{kq}] = q\, T_{kq}}$$

$$[J_\pm, T_{kq}] = [(k \pm q + 1)(k \mp q)]^{1/2}\, T_{kq\pm1}$$

~~for infinitesimal rotations. - Defines irr. tensor operators.~~

~~- The spherical harmonics obey the above commutation relations and so they form a particular example of spherical tensors.~~

Matrix Elements of Tensor Operators.

- Evaluate $\langle \alpha J M | T_{kq} | \alpha' J' M' \rangle$.

Regard T_{kq} as an angular momentum eigenfunction.

$T_{kq} | \alpha' J' M' \rangle$ is a simple product-type eigenfunction which transforms according to the reducible rep. $D_k \times D_{J'}$ of rotation group. The irreducible components are

$$| \beta K Q \rangle = \sum_{q M'} T_{kq} | \alpha' J' M' \rangle \langle K Q | J' k M' q \rangle$$

The inverse transform is

$$T_{kq} | \alpha' J' M' \rangle = \sum_{KQ} | \beta K Q \rangle \langle K Q | J' k M' q \rangle$$

$$\therefore \langle \alpha J M | T_{KQ} | \alpha' J' M' \rangle = \sum_{KQ} \langle \alpha J M | \beta K Q \rangle \langle K Q | J' k M' q \rangle$$

$$= \langle \alpha J M | \beta J M \rangle \langle J M | J' k M' q \rangle$$

$\langle \alpha J M | \beta J M \rangle$ is independent of M

Put $\langle \alpha J M | \beta J M \rangle = (-1)^{2k} \langle \alpha J \| T_k \| \alpha' J' \rangle$

$$\therefore \langle \alpha J M | T_{KQ} | \alpha' J' M' \rangle = (-1)^{k} \langle \alpha J \| T_k \| \alpha' J' \rangle \langle \cancel{KQ}^{JM} | J' k M' q \rangle$$

Examples of Tensor Products.

1. - The electric dipole transition operator is

$$\hat{e}\cdot\vec{r} = -e_1 r_{-1} - e_{-1} r_1 + e_0 r_0 = \sum_q (-1)^q e_q r_{-q}$$

where $e_{\pm 1} = \mp \frac{1}{\sqrt{2}}(e_x \pm i e_y)$

$$e_0 = e_z$$

2. The spin - orbit interaction is of the form

$$H_{SO} = \sum_i f(r_i)\, \vec{l}_i \cdot \vec{s}_i$$

$$= \sum_i f(r_i) \sum_q (-1)^q l_q\, s_{-q}$$

where l_q operates only on the orbital part and s_q only on the spin part of the wavefunction.

3. The spin - spin interaction is of the form

$$H_{SS} = g(r_{12}) \left\{ \frac{(s_1\cdot r_{12})(s_2\cdot r_{12})}{r_{12}^{\;2}} - \frac{1}{3}(s_1\cdot s_2) \right\}$$

$$= \sum_{q=-2}^{2} (-1)^q L_{2,q}\, S_{2,-q}$$

$$L_{2,q} = \sqrt{\frac{8\pi}{15}}\; \frac{g(r_{12})}{r_{12}^{\;2}}\; \mathcal{Y}_2^{\,m}(\hat{r}_{12})$$

$$S_{2,q} = \sqrt{\frac{2\pi}{15}}\; (s_1\cdot\nabla_{\hat{r}})(s_2\cdot\nabla_{\hat{r}})\; \mathcal{Y}_2^{\,m}(\hat{r})$$

$\mathcal{Y}_l^{\,m}(\hat{r}) = r^l\, Y_l^{\,m}(\hat{r})$ is called a solid spherical harmonic.

e.g. $Y_2^0(\hat{r}) = \sqrt{\frac{5}{16\pi}}\,(2z^2 - x^2 - y^2)$

and $S_{2,0} = \frac{2}{\sqrt{24}}\left(2\sigma_{1z}\sigma_{2z} - \sigma_{1x}\sigma_{2x} - \sigma_{1y}\sigma_{2y}\right)$

The process of forming products of the type

$$(\vec{a}_1\cdot\nabla)(\vec{a}_2\cdot\nabla)\cdots(\vec{a}_\ell\cdot\nabla)\,Y_\ell^m(\hat{r})$$

is called polarization (Dirac). Since the dot products are all scalars, the complete expression has the same transformation properties as $Y_\ell^m(\hat{r})$. The same result could be obtained by repeated application of vector coupling.

Why does e_1 represent circular polarization?

$$e_1 = -\frac{1}{\sqrt{2}}(e_x + i e_y) \qquad e_x = -\frac{1}{\sqrt{2}}(e_1 - e_{-1})$$

$$e_{-1} = \frac{1}{\sqrt{2}}(e_x - i e_y) \qquad e_y = \frac{i}{\sqrt{2}}(e_1 + e_{-1})$$

If $e_1 = 1$, $e_{-1} = 0$, $e_0 = 0$, then

$$\hat{e} = \frac{1}{\sqrt{2}}(-\hat{i} + i\hat{j})$$

$$= \frac{1}{\sqrt{2}}\left(e^{i\pi}\,\hat{i} + e^{i\pi/2}\,\hat{j}\right)$$

$$\vec{A} = \hat{e}\,e^{i(k\cdot r - \omega t)}$$

$$= \frac{1}{\sqrt{2}}\left(e^{i(k\cdot r - \omega t + \pi)}\,\hat{i} + e^{i(k\cdot r - \omega t + \pi/2)}\,\hat{j}\right)$$

Due: Dec. 19, 1994

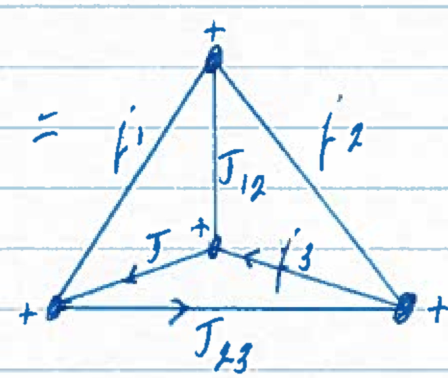
Physics 64-550 Final Problem Set.

1. Complete the proof of the rules for separating graphs across one, two and three lines, as outlined in the hand-out notes.

2. Prove graphically that the recoupling coefficient for three angular momenta is given by

$$\langle (j_1 j_2) J_{12}, j_3 ; J \mid j_1 (j_2 j_3) J_{23} ; J \rangle$$

$$= (-1)^{j_1 + j_2 + j_3 + J} \left[(2J_{12}+1)(2J_{23}+1) \right]^{1/2} \begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_3 & J & j_{23} \end{Bmatrix}$$

where $\begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_3 & J & j_{23} \end{Bmatrix} =$ 

3. Prove that the reduced matrix element of the angular momentum operator $\vec{L}$ is given by

$$\langle l \| \vec{L} \| l' \rangle = \hbar \, \delta_{l,l'} \left[l(l+1)(2l+1) \right]^{1/2}$$

4. The electric dipole oscillator strength for an atomic transition $\gamma LM \to \gamma' L' M'$ is defined by (in atomic units)

$$F(\gamma LM \to \gamma' L' M') = \frac{2}{3}(E'-E)\sum_{\hat{e}} \left| \langle \gamma' L' M' | \hat{e}\cdot\vec{r} | \gamma L M \rangle \right|^2$$

The averaged oscillator strength $\bar{F}$ is obtained by summing over M' and averaging over M; i.e.

$$\bar{F}(\gamma L \to \gamma' L') = \frac{1}{(2L+1)} \sum_{M,M'} F(\gamma LM \to \gamma' L' M')$$

Use the Wigner-Eckart Theorem to prove that

$$\bar{F}(\gamma L \to \gamma' L') = \frac{2}{3}\,\frac{(E'-E)}{2L+1} \left| \langle \gamma' L' \| \vec{r} \| \gamma L \rangle \right|^2$$