Advanced Quantum Mechanics

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Lecture #6

Symmetries and Quantum Mechanics

Recap of Last Class

•Irreps of Rotation Group: constraints on quantum numbers

• Matrix element of operators within the irrep.

Orbital Angular Momentum and Spin

Irreps of Lie Groups and Orthogonality

Finite groups —-> orthogonality relations between irrep matrices and characters —-> reduction of a representation into its irreducible parts.

$$\sum_{a=1}^{g} T_{ip}^{(\alpha)}(G_a) T_{jq}^{(\beta)}(G_a)^* = \delta_{\alpha\beta} \delta_{ij} \delta_{pq} \frac{g}{s_{\alpha}} \qquad \sum_{p=1}^{n} c_p \chi_p^{(\alpha)} \chi_p^{(\beta)*} = g \delta_{\alpha\beta}$$

$$\sum_{p=1}^{n} c_p \chi_p^{(\alpha)} \chi_p^{(\beta)*} = g \delta_{\alpha\beta}$$

Involves sum over group elements

For continuous compact groups

$$\int d\vec{a}\rho(\vec{a})T_{ip}^{(\alpha)}[G(\vec{a})]T_{jq}^{(\beta)}[G(\vec{a})]^* = \delta_{\alpha\beta}\delta_{ij}\delta_{pq}\int d\vec{a}\rho(\vec{a})/s_{\alpha}$$

Integral Haar Measure

$$\int d\vec{a} \rho(\vec{a}) \chi^{(\alpha)}(\vec{a}) \chi^{(\beta)}(\vec{a})^* = \delta_{\alpha\beta} \int d\vec{a} \rho(\vec{a}) \qquad \qquad \text{Group Volume plays the role of young group g}$$

$$G_{a}G_{b} = G_{c} \to G(\vec{a})G(\vec{b}) = G(\vec{c})$$

$$\rho(\vec{a}) = \left[Det\left[\frac{\partial F_{i}[\vec{a}, \vec{b}]}{\partial b_{j}}|_{b=0}\right]\right]^{-1}$$

$$c^{(i)} = F_{i}[\vec{a}, \vec{b}]$$

The measure depends on parametrization. e.g.: different for axis-angle vs Euler angle parametrization of rotation

Irreps of Lie Groups and Orthogonality

With this caveat of the measure, orthogonality reduction of a representation into irreps can now be studied

$$T = \bigoplus_{\alpha} m^{(\alpha)} T^{(\alpha)}$$

$$\frac{1}{V} \int d\vec{a} \rho(\vec{a}) \chi^{(\beta)*}(\vec{a}) \chi(\vec{a}) = m^{(\beta)}$$

Direct Product Representations

$$\chi^{(\alpha \times \beta)}(\vec{a}) = \chi^{(\alpha)}(\vec{a})\chi^{(\beta)}(\vec{a})$$

$$T^{(\alpha \times \beta)} = \bigoplus_{\gamma} m^{(\gamma)} T^{(\gamma)} \qquad m^{(\gamma)} = \frac{1}{V} \int d\vec{a} \rho(\vec{a}) \chi^{(\gamma)*}(\vec{a}) \chi^{(\alpha)}(\vec{a}) \chi^{(\beta)}(\vec{a})$$

R₂: Irreps

Generator:
$$L_z = -i \frac{\partial}{\partial \theta}$$

Group Combination Rule:
$$\theta_c = \theta_a + \theta_b$$
 $\rho(\theta) = 1$

$$\theta_c = \theta_a + \theta_b$$

$$\rho(\theta) = 1$$

$$V = \int_0^{2\pi} d\theta = 2\pi$$

$$T(a+2\pi) = T(a) \Rightarrow T'(0) = im$$
 $m = 0, \pm 1, \pm 2...$ $T(\theta) = e^{im\theta}$

$$m = 0, \pm 1, \pm 2...$$

$$T(\theta) = e^{im\theta}$$

The Fourier Expansion
$$\ \psi(r,\theta) = \sum \psi_m(r) e^{im\theta}$$

is reduction of a function into irreducible components

Direct Product Representation:

$$T^{(m\times n)}(\theta) = T^{(m)}(\theta)T^{(n)}(\theta) = T^{(m+n)}(\theta)$$

R₃: Characters, Orthogonality, Reduction

Characters corresponding to the different irreps of R_{3:}

Rotations by the same angle about any axis are in the same conjugacy class and hence have the same character. So the character can only depend on the angle of rotation and not on the axis of rotation. Use this flexibility to choose rotations about z axis to calculate the character

We have seen before that (2j+1) dim irreps of R_3 are labelled by j=0,1/2,1,... and the (2j+1) irreps of R_2 (m=-j to m=+j) form a basis set in this invariant subspace. So

$$D^{(j)}(\theta)=\oplus_{m=-j}^{m=j}T^{(m)}(\theta)$$
 Reduction on restriction to subgroup Irrep of R₃ Irreps of R₂

$$D^{(j)}(\theta)_{mm'} = T^{(m)}(\theta)\delta_{mm'}$$

$$\chi^{(j)}(\theta) = \sum_{m=-j}^{j} e^{im\theta} = e^{-ij\theta} (1 + e^{i\theta} + e^{2i\theta} + \dots e^{i2j\theta})$$
$$= e^{-ij\theta} \frac{e^{i(2j+1)\theta} - 1}{e^{i\theta} - 1} = \frac{\sin[(j+1/2)\theta]}{\sin[\theta/2]}$$

Check this from explicit form of rotation matrices

R₃: Characters, Orthogonality, Reduction

$$\chi^{(j_1)}(\theta)\chi^{(j_2)}(\theta) = \frac{\sin[(j_1+1/2)\theta]\sin[(j_2+1/2)\theta]}{\sin^2[\theta/2]}$$

$$= \frac{\cos[(j_1-j_2)\theta] - \cos[(j_1+j_2+1)\theta]}{2\sin^2[\theta/2]}$$

$$= \frac{\cos[(j_1-j_2)\theta] - \cos[(j_1+j_2)\theta] + 2\sin[(j_1+j_2+1/2)\theta]\sin[\theta/2]}{2\sin^2[\theta/2]}$$

$$= \frac{2\sin[j_1\theta]\sin[j_2\theta] + 2\sin[(j_1+j_2+1/2)\theta]\sin[\theta/2]}{2\sin^2[\theta/2]}$$

$$= \chi^{(j_1+j_2)}(\theta) + \chi^{(j_1-1/2)}(\theta)\chi^{(j_2-1/2)}(\theta)$$

$$= \chi^{(j_1+j_2)}(\theta) + \chi^{(j_1+j_2-1)}(\theta) + \dots + \chi^{(j_1-j_2)}(\theta) \quad \text{Assume j}_1 >= j_2$$

$$D^{(j_1 \times j_2)} = \bigoplus_{i=0}^{2j_2} D^{(j_1 - j_2 + i)}$$

Addition of Angular momenta

Example: Spin-Orbit Coupling in electrons

Need Relativistic QM to treat this properly!!

Semi Classical Picture:

Electrons move in the Electric field due to the nucleus

$$\vec{E} = -\nabla V_c(r)$$

Moving charge in E field ---> Magnetic Field

$$\vec{B} = -\frac{\vec{v}}{c} \times \vec{E}$$

Electrons have spin (magnetic dipole moment)

$$\vec{\mu}_B = -\frac{e}{mc}\vec{S}$$

$$H = -\vec{\mu}_B \cdot \vec{B} = -\frac{e\vec{S}}{mc} \cdot \left[\frac{\vec{p}}{mc} \times \frac{\vec{r}}{r} \frac{dV_c}{dr} \right] = \frac{1}{m^2 c^2 r} \frac{dV_c}{dr} \vec{L} \cdot \vec{S}$$

Overestimates co-eff by 2.

Example: Hyperfine Coupling between nuclei and electrons

Nuclei have spin : so nuclear spins can couple to the electronic orbital angular momentum

the magnetic dipole moment of electrons create a magnetic field at the nuclear core, which couples to the nuclear spin

$$H \sim \lambda_{hf} \vec{I} \cdot (\vec{L} + \vec{S}) = \lambda_{hf} \vec{I} \cdot \vec{J}$$

Generically, particles with spin can have spin-spin interactions of the above form

Addition of Angular momenta

$$[L_i, L_j] = i\epsilon_{ijk}L_k \qquad [S_i, S_j] = i\varepsilon_{ijk}S_k \qquad [L_i, S_j] = 0$$

Infinitesimal rotation affecting both subspaces:

$$(1 - i\vec{L} \cdot \hat{n}\delta\theta) \otimes (1 - i\vec{S} \cdot \hat{n}\delta\theta) \sim [1 - i(\vec{L} \otimes 1 + 1 \otimes \vec{S}) \cdot \hat{n}\delta\theta] = [1 - i\vec{J} \cdot \hat{n}\delta\theta]$$

$$ec{J}=ec{L}+ec{S}=ec{L}\otimes 1+1\otimes ec{S}$$
 $[J_i,J_j]=i\epsilon_{ijk}J_k$ J denotes total angular momentum.

Consider a Hamiltonian which is rotationally invariant in L and S subspaces individually.

 L^2 , S^2 , L_z , S_z provide good quantum numbers for the system.

Simultaneous eigenstates of L², S², Lz, Sz $|j_1,m_1;j_2,m_2\rangle=|j_1,j_2;m_1,m_2\rangle$

$$L^{2}|j_{1},j_{2};m_{1},m_{2}\rangle = j_{1}(j_{1}+1)|j_{1},j_{2};m_{1},m_{2}\rangle \qquad S^{2}|j_{1},j_{2};m_{1},m_{2}\rangle = j_{2}(j_{2}+1)|j_{1},j_{2};m_{1},m_{2}\rangle$$

$$L_z|j_1,j_2;m_1,m_2\rangle = m_1|j_1,j_2;m_1,m_2\rangle$$
 $S_z|j_1,j_2;m_1,m_2\rangle = m_2|j_1,j_2;m_1,m_2\rangle$

Addition of Angular momenta

Now add a L.S term to this Hamiltonian

$$[L^2,\vec{L}\cdot\vec{S}]=[L^2,L_i]S_i=0 \qquad \qquad \text{Similarly} \quad [S^2,\vec{L}\cdot\vec{S}]=0$$

So L² and S² are conserved quantities and provide good quantum numbers

It is obvious that L_z and S_z are no longer conserved.

$$[L_z, \vec{L} \cdot \vec{S}] = i[L_y S_x - L_x S_y] = -i[\vec{L} \times \vec{S}]_z \qquad [S_z, \vec{L} \cdot \vec{S}] = -i[L_y S_x - L_x S_y] = i[\vec{L} \times \vec{S}]_z$$

but $J_z=L_z+S_z$ is conserved.

Define $J_x=L_x+S_x$ and $J_y=L_y+S_y$, Then define $J^2=JiJi$

Finally
$$\vec{L}\cdot\vec{S}=\frac{1}{2}[J^2-L^2-S^2] \qquad \qquad [J^2,L^2]=0 \qquad \qquad [J^2,S^2]=0 \qquad \qquad \text{So \mathbb{J}^2 is conserved.}$$

We should work with simultaneous eigenstates of L2, S2, Jz, J2 $|j_1,j_2;j,m
angle$

However, we may be interested in expectations/ matrix elements of only the orbital or only the spin degrees of freedom. These are easy to evaluate in $|j_1,j_2;m_1,m_2\rangle$ basis

Need to find the transformation between the bases

Basis Transformation

The reduction of $\mathcal{D}^{(j_1 imes j_2)}$ into irreps of rotation group (j,m basis) gives us required transformation

$$D^{(j_1 \times j_2)} = \oplus_{i=0}^{2j_2} D^{(j_1-j_2+i)} \qquad \text{Irreps j}_1 + \mathbf{j}_2, \ \mathbf{j}_1 + \mathbf{j}_2 - \mathbf{1}, \ \mathbf{j}_1 + \mathbf{j}_2 - \mathbf{2}, \ \dots \ | \ \mathbf{j}_1 - \mathbf{j}_2 \ |, \ \text{each occur once}$$
 in the reduction

$$|j_1, j_2; j, m\rangle = \sum_{m_1 m_2} C(j_1, j_2, j; m_1, m_2, m) |j_1, j_2; m_1, m_2\rangle$$

Clebsch Gordan Coefficients

Properties of a group

In general
$$\Psi_k^{(\gamma)t} = \sum_{ij} C(\alpha\beta\gamma t; ijk) \phi_i^{(\alpha)} \phi_j^{(\beta)}$$

From reduction of the direct product representation

$$\left(C(j_1,j_2,j;m_1,m_2,m)=0
ight)$$
 unless $|\mathbf{j_1-j_2}|$ < \mathbf{j} < $\mathbf{j_1+j_2}$

Clebsch Gordan Co-efficients

$$|j_1, j_2; j, m\rangle = \sum_{m_1 m_2} C(j_1, j_2, j; m_1, m_2, m) |j_1, j_2; m_1, m_2\rangle$$

$$C(j_1, j_2, j; m_1, m_2, m) = \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle$$

Now,

$$J_z - L_z - S_z |j_1, j_2; j, m\rangle = 0 \implies C(j_1, j_2, j; m_1, m_2, m)(m - m_1 - m_2) = 0$$

$$C(j_1,j_2,j;m_1,m_2,m)=0$$
 unless m=m₁+m₂ and $|j_1-j_2| < j < |j_1+j_2|$

$$J^{\pm}|j_1,j_2;j,m\rangle = \sum_{m_1m_2} C(j_1,j_2,j;m_1,m_2,m)|(L^{\pm}+S^{\pm})|j_1,j_2;m_1,m_2\rangle$$

$$c_{jm}^{\pm}|j_{1},j_{2};j,m\pm1\rangle = \sum_{m_{1}m_{2}}C(j_{1},j_{2},j;m_{1},m_{2},m)\left[c_{j_{1}m_{1}}^{\pm}|j_{1},j_{2};m_{1}\pm1,m_{2}\rangle + c_{j_{2}m_{2}}^{\pm}|j_{1},j_{2};m_{1},m_{2}\pm1\rangle\right]$$

$$c_{jm}^{\pm} = \sqrt{j(j+1) - m(m \pm 1)}$$

Clebsch Gordan Co-efficients

$$c_{jm}^{\pm}|j_{1},j_{2};j,m\pm 1\rangle = \sum_{m_{1}m_{2}}C(j_{1},j_{2},j;m_{1},m_{2},m)\left[c_{j_{1}m_{1}}^{\pm}|j_{1},j_{2};m_{1}\pm 1,m_{2}\rangle + c_{j_{2}m_{2}}^{\pm}|j_{1},j_{2};m_{1},m_{2}\pm 1\rangle\right]$$

$$c_{jm}^{\pm} = \sqrt{j(j+1) - m(m\pm 1)}$$

Take inner prod. with $\langle j_1, j_2; l_1, l_2|$ and remember the defn. of CG co-eff.

$$c_{jm}^{\pm}C(j_1,j_2,j;l_1,l_2,m\pm 1) = c_{j_1,l_1\mp 1}^{\pm}C(j_1,j_2,j;l_1\mp 1,l_2,m) + c_{j_2,l_2\mp 1}^{\pm}C(j_1,j_2,j;l_1,l_2\mp 1,m)$$

Recursion Relations for Clebsch Gordan co-eff.

$$D^{(1)\times(1/2)} = D^{(3/2)} + D^{(1/2)}$$

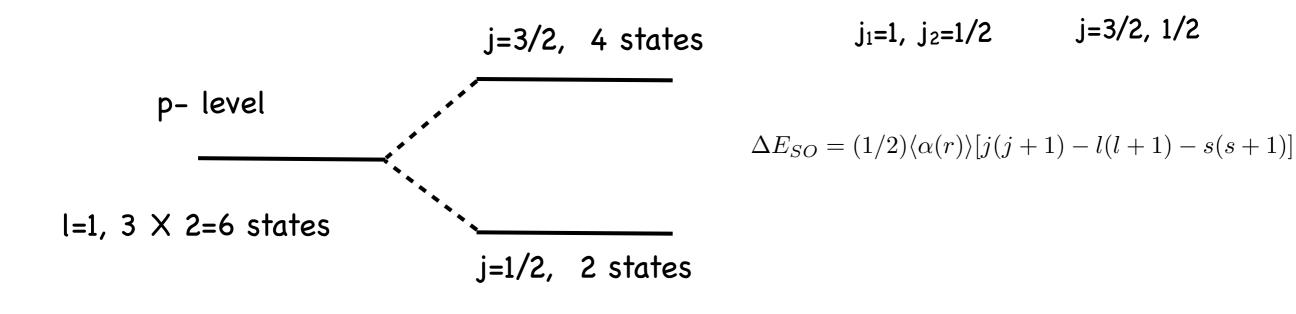
Clebsch Gordan Co-efficients

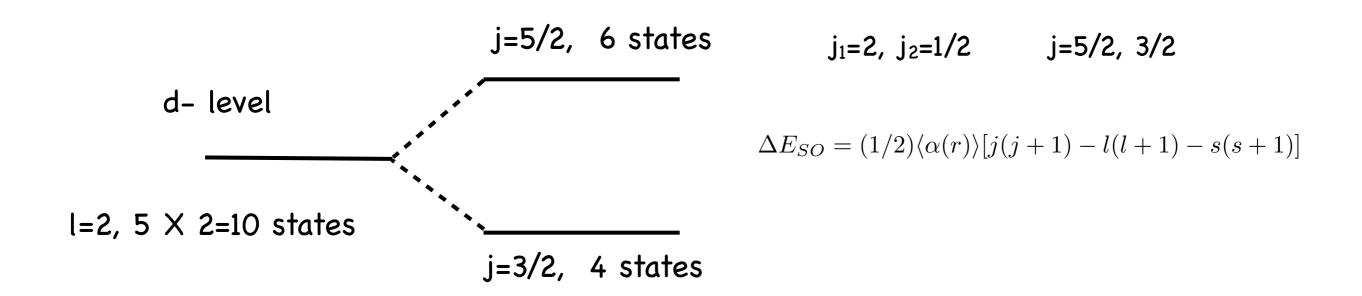
$$| 3/2, 1/2 \rangle = C(1,1/2,3/2; 1,-1/2,1/2) | 1, -1/2 \rangle + C(1,1/2,3/2; 0,1/2,1/2) | 0, 1/2 \rangle$$
 $| 3/2, -1/2 \rangle = C(1,1/2,3/2; -1,1/2,-1/2) | -1, 1/2 \rangle + C(1,1/2,3/2; 0,-1/2,-1/2) | 0, -1/2 \rangle$

$$| 1/2, 1/2 \rangle = C(1,1/2,1/2; 1,-1/2,1/2) | 1, -1/2 \rangle + C(1,1/2,1/2; 0,1/2,1/2) | 0, 1/2 \rangle$$

$$| 1/2, -1/2 \rangle = C(1,1/2,1/2; -1,1/2,-1/2) | -1, 1/2 \rangle + C(1,1/2,1/2; 0,-1/2,-1/2) | 0, -1/2 \rangle$$

Spin-Orbit coupling and fine structure





Two spin 1/2: Singlet and Triplet states

Two spin 1/2 particles interacting with a spin-spin interaction

$$H = -J\vec{S}_1 \cdot \vec{S}_2$$

Ferromagnets are governed by such terms coming from Coulomb interaction

$$|j_1, j_2; m_1, m_2\rangle$$
 $|1/2, 1/2\rangle, |1/2, -1/2\rangle, |-1/2, 1/2\rangle, |-1/2, -1/2\rangle$

Eigenstates:
$$j=1(1/2+1/2)$$
 and

$$j=0 (1/2-1/2)$$

$$m=0$$

$$|1/2,1/2\rangle \quad \frac{1}{\sqrt{2}}(|1/2,-1/2\rangle + |-1/2,1/2\rangle) \ |-1/2,-1/2\rangle \qquad \qquad \frac{1}{\sqrt{2}}(|1/2,-1/2\rangle - |-1/2,1/2\rangle)$$

Triplet States

Singlet States

Use Clebsch Gordon to calculate this

Scalars, Vectors and Tensors

Notion of scalar, vector, tensor quantities based on their transformation under rotation:

Scalar is invariant under rotation R(x) = x

Example: distance between points

A Vector has same transformation properties as Cartesian co-ordinates

$$R(\vec{x}) = \hat{R}\vec{x} \Rightarrow R(x_i) = x_i' = R_{ij}x_j$$

Example: position, momentum, etc.

Cartesian Tensor of Rank n has same transformation properties as that of product of n co-ord.

$$R(x_{ijk...n}) = x'_{ijk...n} = R_{ii'}R_{jj'}R_{kk'}...R_{nn'}x_{i'j'k'...n'}$$

Example (Rank 2): stress, conductivity, quadrupole moment, moment of inertia etc. Any $T_{ij} = u_i \ v_j$, where u_i and v_j are components of vectors

Scalar, Vector and Tensor Operators

QM Equivalent of Rotation:
$$\hat{A} o \mathcal{D}^\dagger \hat{A} \mathcal{D}$$

$$\hat{A} \to \mathcal{D}^{\dagger} \hat{A} \mathcal{I}$$

$$\mathcal{D} = e^{-i\vec{L}.\hat{n}\theta}$$

$$\mathcal{D}^{\dagger}\hat{A}\mathcal{D} = \hat{A}$$

Invariant under rotation

Consider Infinitesimal rotation about j axis:
$$\mathcal{D}^\dagger \hat{A} \mathcal{D} = (1+iL_j\theta)\hat{A}(1-iL_j\theta) = \hat{A}+i\theta[L_j,\hat{A}]$$

For Scalar Operator
$$[L_j,\hat{A}]=0$$

So a scalar operator commutes with all the angular momentum operators

Vector Operator: A set D operators in D dim which transform according to $\mathcal{D}^\dagger \hat{A}_i \mathcal{D} = R_{ij} \hat{A}_j$

3 D: For infinitesimal rotation about j axis, $\vec{r'}=\vec{r}+\hat{j} imes \vec{r} heta \Rightarrow \hat{A}_i o \hat{A}_i+arepsilon_{ijk}\hat{A}_k heta$

But,
$$\mathcal{D}^{\dagger}\hat{A}_{i}\mathcal{D}=(1+iL_{j}\theta)\hat{A}_{i}(1-iL_{j}\theta)=\hat{A}_{i}-i\theta[\hat{A}_{i},L_{j}]$$

So, for vector Operators $[\hat{A}_i, L_i] = i \varepsilon_{ijk} \hat{A}_k$

Example: position, momentum, orbital ang. momentum, spin, dipole moment etc.

Irreducible Set of Operators

Irreducible Set of Operators:

A set of operators, which transform among themselves as

$$S_i^{(\alpha)'} \equiv T(G_a) S_i^{(\alpha)} T(G_a^{-1}) = \sum_j T_{ji}^{(\alpha)} (G_a) S_j^{(\alpha)} \qquad \text{are called irreducible operators} \\ \text{transforming according to} \quad T^{(\alpha)}$$

- Scalar operators transform according to the 1 dim. j=0 irrep of the rotation group
- Vector operators transform according to the 3 dim. j=1 irrep of the rotation group.
- Spinor operators transform according to the 2 dim. j=1/2 irrep of rotation group

What about Tensor Operators?

Reduction of Cartesian Tensors

Reducibility of Cartesian Tensors:

Consider the cartesian Tensor $T_{ij}=U_iV_j$ $ec{U}, \ ec{V}$ being vectors

Since U_i and V_j transform according to j=1 irrep

$$\mathcal{D}^{(1\times 1)} = \mathcal{D}^{(0)} \oplus \mathcal{D}^{(1)} \oplus \mathcal{D}^{(2)}$$

UiVj transform according to

So generic Cartesian tensors are reducible

Scalar (j=0) Vector (j=1) Traceless symmetric 1 dim 3 dim Tensor (j=2) 5 dim

Same criterion holds for QM operators

Reduction of
$$\mathsf{L_i}\mathsf{L_j}$$
: $L_iL_j = \frac{1}{3}L^2\delta_{ij} + \frac{1}{2}i\epsilon_{ijk}L_k + \left(\frac{\{L_i,L_j\}}{2} - \frac{L^2}{3}\right)$

Scalar (j=0) Vector (j=1) Traceless symmetric 1 dim 3 dim Tensor (j=2) 5 dim

Example : Quadrupole moment operator $Q_{ij}\sim r_ir_j-rac{r^2}{3}\delta_{ij}$ is irreducible set corr. to j=2

Irreducibile Rank k Tensor Operators: Spherical Tensors

A set of 2k+1 irreducible operators which transform according to k irrep of rotation group are called spherical tensors of rank k if

$$\mathcal{D}T_q^{(k)}\mathcal{D}^{\dagger} = \sum_{q'} \mathcal{D}_{q'q}^{(k)} T_{q'}^{(k)}$$

$$[L_z, T_q^{(k)}] = q T_q^{(k)}$$
 $[L^{\pm}, T_q^{(k)}] = \pm \sqrt{(k \mp q)(k \pm q + 1)} T_{q\pm 1}^{(k)}$

We are using irreps of rotation group and the |j,m> basis to define spherical tensors

Eigenfunctions corresponding to |j,m> basis are the Spherical Harmonics, so the idea is to take linear combinations of $x_ix_jx_l....$ corresponding to $Y^l_{m.}$

The same linear combinations of symmetrized $u_i v_j w_l \dots$ gives the spherical tensor operators.

Example with
$$p_i p_j$$
: $Y^2_0 = N(3 z^2/r^2 - 1) \rightarrow N(3 p_z^2 - p^2)$

$$Y^{2}_{-2} = N \sqrt{(3/2) (x-iy)^{2}/r^{2}} \rightarrow N \sqrt{(3/2) (p_{x}-ip_{y})^{2}}$$
 $Y^{2}_{2} = N \sqrt{(3/2) (x+iy)^{2}/r^{2}} \rightarrow N \sqrt{(3/2) (p_{x}+ip_{y})^{2}}$

$$Y^{2}_{-1} = N \sqrt{6} (x-iy)z/r^{2} \rightarrow N \sqrt{6} (p_{x}-ip_{y})p_{z}$$
 $Y^{2}_{1} = N \sqrt{6} (x+iy)z/r^{2} \rightarrow N \sqrt{6} (p_{x}+ip_{y})p_{z}$