III. Irreducible tensors

Subtle moment:

1) wave function $\Psi_{JM}(\Omega) = <\Omega\,|\,JM>$. Transformation after a rotation:

$$<\Omega'\,|\,JM> = \sum_{M'=-J}^{J} <\Omega\,|\,JM'><JM'\,|\exp(-i\,\omega\,\mathbf{n}\,\hat{\mathbf{J}})\,|\,JM> =$$

$$= \sum_{M'=-J}^{J} <\Omega\,|\,JM'>D^{J}_{M'M}(\alpha,\beta,\gamma)$$

No other function can stand to the right!

2) multiplication operator $\hat{O} = \Psi_{JM}(\Omega)$. Transformation:

$$\hat{O}' = \exp(-i\,\omega\,\mathbf{n}\,\hat{\mathbf{J}})\,\hat{O}\,\exp(i\,\omega\,\mathbf{n}\,\hat{\mathbf{J}}) = \sum_{M'=-J}^{J} \Psi_{JM'}(\Omega)\,D^{J}_{M'M}(\alpha,\beta,\gamma)$$

A (ket) function is to stand to the right!

$$d\hat{O}/d\omega = -i\,\mathbf{n}\,\{\hat{\mathbf{J}}\,\hat{O}\} =$$

The ang.momentum operator acts only on *O*, but not on a function standing to the right of *O*.

$$= -i\,\mathbf{n}\,\hat{\mathbf{J}}\,\hat{O} + i\,\mathbf{n}\,\hat{O}\,\hat{\mathbf{J}} = -i\,\mathbf{n}\,[\hat{\mathbf{J}},\hat{O}]$$

This term compensates the unwanted action of **J** on a function to the right.

The ang.momentum operator acts both on *O* and a function standing to the right of *O*.

If we consider a function $\Psi_{JM}(\Omega)$ not as a ket vector, but as a multiplication operator,

$$[\hat{\mathbf{J}},\ \Psi_{JM}(\Omega)] = \{\hat{\mathbf{J}}\,\Psi_{JM}(\Omega)\}$$

Ang.momentum acts only on Ψ_{JM}

In cyclic coordinates (covariant components):

$$\hat{J}_{\pm 1}|\Psi_{JM}\rangle = \mp\sqrt{\frac{J(J+1)-M(M\pm 1)}{2}}\,|\Psi_{JM\pm 1}\rangle, \quad \hat{J}_0|\Psi_{JM}\rangle = M|\Psi_{JM}\rangle$$

Wave function

$$[\hat{J}_{\pm 1}, \Psi_{JM}] = \mp\sqrt{\frac{J(J+1)-M(M\pm 1)}{2}}\,\Psi_{JM\pm 1}, \quad [\hat{J}_0, \Psi_{JM}] = M\,\Psi_{JM} \qquad \text{(III.*)}$$

Multiplication operator

Definition. An irreducible tensor of the rank J is an object $\mathfrak{M}_J$, whose $2J + 1$ components with $M = -J, -J+1, \ldots, J-1, J$ obey the commutation rules

$$[\hat{J}_{\pm 1}, \mathfrak{M}_{JM}] = \mp\frac{1}{\sqrt{2}}e^{\pm i\delta}\sqrt{J(J+1)-M(M\pm 1)}\,\mathfrak{M}_{JM\pm 1}, \qquad [\hat{J}_0, \mathfrak{M}_{JM}] = M\mathfrak{M}_{JM}$$

or in a compact form $\quad [\hat{J}_\mu, \mathfrak{M}_{JM}] = e^{iM\delta}\sqrt{J(J+1)}\,C_{JM1\mu}^{JM+\mu}\mathfrak{M}_{JM+\mu}$

Prove that $\quad [\hat{\mathbf{J}}^2, \mathfrak{M}_{JM}] = J(J+1)\,\mathfrak{M}_{JM}$

The phase δ can be chosen arbitrary; to obtain a full analogy with (III.*), we take $\delta \equiv 0$.

Another arbitrary phase: the common phase of all the components $\mathfrak{M}_{JM}$.
We can choose it, such that (like the phase of spherical functions for $J = L =$ integer)

$$(\mathfrak{M}_{JM})^* = (-1)^{-M}\,\mathfrak{M}_{J-M}$$

For quantum-mechanical applications another choice of the common phase is convenient:

$$\tilde{\mathfrak{M}}_J = i^J \mathfrak{M}_J \quad \Rightarrow \quad (\tilde{\mathfrak{M}}_{JM})^* = (-1)^{J-M}\,\tilde{\mathfrak{M}}_{J-M}$$

The tilded operator is Hermitian

$$\tilde{\mathfrak{M}}_J^{\dagger} = \tilde{\mathfrak{M}}_J \qquad \langle b \,|\, \tilde{\mathfrak{M}}_{JM} \,|\, a\rangle = (\langle a \,|\, (\tilde{\mathfrak{M}}_{JM})^* \,|\, b\rangle)^*$$

Covariant and contravariant components:

$$\mathfrak{M}_J = \sum_M \mathbf{e}_J^M \cdot \mathfrak{M}_{JM} = \sum_M \mathbf{e}_{JM} \cdot \mathfrak{M}_J^M$$

Covariant ($\mathfrak{M}_{JM}$) Contravariant ($\mathfrak{M}_J^M$)

Basis of unit IR tensors of the rank J: $\mathbf{e}_J^M \cdot \mathbf{e}_{J'M'} = \delta_{JJ'}\delta_{MM'}$

Contravariant

$$\mathfrak{M}_J^M = (\mathfrak{M}_{JM})^* = (-1)^{-M}\,\mathfrak{M}_{J-M},$$

$$\tilde{\mathfrak{M}}_J^M = (\tilde{\mathfrak{M}}_{JM})^* = (-1)^{J-M}\,\tilde{\mathfrak{M}}_{J-M}$$

Covariant

Transformation of IR tensors under rotation

It follows from the commutation rules defining an IR tensor that

$$\mathfrak{M}_{JM'}(X') = \hat{D}(\alpha, \beta, \gamma)\, \mathfrak{M}_{JM'}(X)\, [\hat{D}(\alpha, \beta, \gamma)]^{-1} = \sum_{M} \mathfrak{M}_{JM}(X)\, D^{J}_{MM'}(\alpha, \beta, \gamma),$$

$$\tilde{\mathfrak{M}}_{JM'}(X') = \hat{D}(\alpha, \beta, \gamma)\, \tilde{\mathfrak{M}}_{JM'}(X)\, [\hat{D}(\alpha, \beta, \gamma)]^{-1} = \sum_{M} \tilde{\mathfrak{M}}_{JM}(X)\, D^{J}_{MM'}(\alpha, \beta, \gamma).$$

I.e., $\mathfrak{M}_{JM}(X)$ and $\tilde{\mathfrak{M}}_{JM}(X)$ transform exactly like a wave function $\Psi_{JM}(\Omega)$.

Transformation of IR tensors under inversion ($\mathbf{r} \to -\mathbf{r}$)

$$\mathfrak{M}_{J} = \mathfrak{M}_{J}^{(+1)} + \mathfrak{M}_{J}^{(-1)}$$

$$\hat{P}_{r} \mathfrak{M}_{J}^{(\pi_J)} \hat{P}_{r}^{-1} = \pi_J \mathfrak{M}_{J}^{(\pi_J)}, \quad (\pi_J = \pm 1)$$

$\mathfrak{M}_{J}^{(\pi_J)}$ or $\tilde{\mathfrak{M}}_{J}^{(\pi_J)}$ is (i) a true (polar) tensor, if the parity $\pi_J = (-1)^J$

(ii) a pseudotensor (an axial tensor), if $\pi_J = (-1)^{J+1}$

Prove that

(i) the radius-vector **r** is an IR polar tensor of the rank 1.

(ii) the angular momentum operator is an IR axial tensor of the rank 1.

Note, that the rank of the angular momentum operator is always 1, regardless of the quantum number J characterizing a particular system!

The angular momentum operator has only three cyclic components with

$$M = -1,\ 0,\ +1,$$

and so does the radius-vector.

How does the ang.momentum operator transform under inversion?

Direct product of two IR tensors of the ranks J_1 and J_2:

$(2J_1 + 1)(2J_2 + 1)$ components $\mathfrak{M}_{J_1M_1}\mathfrak{N}_{J_2M_2}$

The direct product can be reduced, i.e., represented as a linear combinations of terms, each of them transforming under rotations independently of the others:

$$\mathfrak{M}_{J_1M_1}\mathfrak{N}_{J_2M_2} = \sum_{J=|J_1-J_2|}^{J_1+J_2} C^{JM}_{J_1M_1J_2M_2}\mathfrak{L}_{JM}$$

Irreducible tensor product is an IR tensor defined as

$$\mathfrak{L}_{JM} = \sum_{M_1M_2} C^{JM}_{J_1M_1J_2M_2}\mathfrak{M}_{J_1M_1}\mathfrak{N}_{J_2M_2}$$

Prove that this object transform under rotations indeed as an IR tensor of the rank J.

Notation: $\mathfrak{L}_J \equiv \{\mathfrak{M}_{J_1} \otimes \mathfrak{N}_{J_2}\}_J$

For the IR tensor product of tilded IR tensors a standard relation holds

$$(\tilde{\mathfrak{L}}_{JM})^* = (-1)^{J-M}\tilde{\mathfrak{L}}_{J-M} \quad (\tilde{\mathfrak{L}}_{JM} = \{\tilde{\mathfrak{M}}_{J_1} \otimes \tilde{\mathfrak{N}}_{J_2}\}_{JM})$$

But an IR tensor product of non-tilded tensors under complex conjugation does not change in a way similar to its „factors“, i.e.

$$(\mathfrak{M}_{JM})^* = (-1)^{-M}\,\overline{\mathfrak{M}}_{J-M}, \quad \text{but} \quad (\mathfrak{L}_{JM})^* \neq (-1)^{-M}\,\mathfrak{L}_{J-M}$$

Commutator of the components of two IR tensors

$$\mathfrak{K}_{J_1M_1J_2M_2} \equiv [\mathfrak{M}_{J_1M_1}, \mathfrak{N}_{J_2M_2}] \equiv \mathfrak{M}_{J_1M_1}\mathfrak{N}_{J_2M_2} - \mathfrak{N}_{J_2M_2}\mathfrak{M}_{J_1M_1}$$

Commutator of an IR tensor product

$$\mathfrak{K}^{J_1J_2}_{JM} \equiv \{\mathfrak{M}_{J_1} \otimes \mathfrak{N}_{J_2}\}_{JM} - (-1)^{J_1+J_2-J}\{\mathfrak{N}_{J_2} \otimes \mathfrak{M}_{J_1}\}_{JM}$$

The factor $(-1)^{J_1+J_2-J}$ in front of the second term stems from

$$C^{c\gamma}_{a\alpha\, b\beta} = (-1)^{a+b-c}\, C^{c\gamma}_{b\beta\, a\alpha}$$

The commutator of an IR tensor product is also an IR tensor and can be expressed through the commutator of the components as

$$\mathfrak{K}^{J_1J_2}_{JM} = \sum_{M_1M_2} C^{JM}_{J_1M_1J_2M_2}\mathfrak{K}_{J_1M_1J_2M_2}$$

In a general case

$$\{\mathfrak{M}_{J_1} \otimes \mathfrak{N}_{J_2}\}_{JM} = (-1)^{J_1+J_2-J}\{\mathfrak{N}_{J_2} \otimes \mathfrak{M}_{J_1}\}_{JM} + \mathfrak{K}^{J_1J_2}_{JM}$$

For commuting tensors

$$\{\mathfrak{M}_{J_1} \otimes \mathfrak{N}_{J_2}\}_{JM} = (-1)^{J_1+J_2-J}\{\mathfrak{N}_{J_2} \otimes \mathfrak{M}_{J_1}\}_{JM}$$

It is easy to show (prove it!) that if all components of an IR tensor mutually commute, its IR tensor product to itself is zero if the product rank $I = 2(J - n) - 1$, where $n = 0, 1, 2, 3...$, i.e., that

$$\{\mathfrak{M}_J \otimes \mathfrak{M}_J\}_I = 0,$$

for $I = 2J - 1,\ 2J - 3, \ldots$ and $\mathfrak{K}^{JJ}_{IM} = 0$

Scalar product is defined for two IR tensors of the <u>same</u> rank

$$(\mathfrak{M}_J \cdot \mathfrak{N}_J) = \sum_M (-1)^{-M} \mathfrak{M}_{JM} \mathfrak{N}_{J-M} = \sum_M \mathfrak{M}_{JM} \mathfrak{N}^*_{JM} = \sum_M \mathfrak{M}_{JM} \mathfrak{N}_J^M$$

$$(\tilde{\mathfrak{M}}_J \cdot \tilde{\mathfrak{N}}_J) = \sum_M (-1)^{J-M} \tilde{\mathfrak{M}}_{JM} \tilde{\mathfrak{N}}_{J-M} = \sum_M \tilde{\mathfrak{M}}_{JM} \tilde{\mathfrak{N}}^*_{JM} = \sum_M \tilde{\mathfrak{M}}_{JM} \tilde{\mathfrak{N}}_J^M$$

$$(\mathfrak{M}_J \cdot \mathfrak{N}_J) = (-1)^{-J} (\tilde{\mathfrak{M}}_J \cdot \tilde{\mathfrak{N}}_J)$$ ⟵ Why?

A scalar product differs only by a numerical factor from an IR tensor product of the rank 0:

$$\{\mathfrak{M}_J \otimes \mathfrak{N}_J\}_{00} = \sum_{M_1 M_2} C^{00}_{JM_1 JM_2} \mathfrak{M}_{JM_1} \mathfrak{N}_{JM_2} = \frac{1}{\sqrt{2J+1}} \sum_M (-1)^{J-M} \mathfrak{M}_{JM} \mathfrak{N}_{J-M}$$

$$\{\tilde{\mathfrak{M}}_J \otimes \tilde{\mathfrak{N}}_J\}_{00} = \sum_{M_1 M_2} C^{00}_{JM_1 JM_2} \tilde{\mathfrak{M}}_{JM_1} \tilde{\mathfrak{N}}_{JM_2} = \frac{1}{\sqrt{2J+1}} \sum_M (-1)^{J-M} \tilde{\mathfrak{M}}_{JM} \tilde{\mathfrak{N}}_{J-M}$$

$$(\mathfrak{M}_J \cdot \mathfrak{N}_J) = (-1)^{-J} \sqrt{2J+1} \{\mathfrak{M}_J \otimes \mathfrak{N}_J\}_{00}$$

$$(\tilde{\mathfrak{M}}_J \cdot \tilde{\mathfrak{N}}_J) = \sqrt{2J+1} \{\tilde{\mathfrak{M}}_J \otimes \tilde{\mathfrak{N}}_J\}_{00}.$$

An arbitrary vector **A** can be considered as an IR tensor $\mathbf{A}_1$ of the rank 1.

For its cyclic components we have $A_1^{\mu} = (-1)^{\mu} A_{1-\mu}$ (non-tilded IR tensor).

$$A_{1\mu} \equiv A_{\mu}, \quad A^{1\mu} \equiv A^{\mu}$$

From two vectors we can construct IR tensor products of ranks 0, 1, and 2.

$$\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{00}, \quad \{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{1\mu}, \quad \{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{2\mu}$$

Rank 0

$$(\mathbf{A}_1 \cdot \mathbf{B}_1) = (\mathbf{A} \cdot \mathbf{B}) \qquad \{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{00} = -\frac{1}{\sqrt{3}}(\mathbf{A} \cdot \mathbf{B})$$

Scalar product of two IR tensors of the rank 1

Scalar product of two verctors (standartly defined)

Rank 1

$$\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_1 = \frac{i}{\sqrt{2}}[\mathbf{A} \times \mathbf{B}]$$

$$\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{1M} = \frac{i}{\sqrt{2}}[\mathbf{A} \times \mathbf{B}]_M = \sum_{M\nu} C_{1\mu 1\nu}^{1M} A_{\mu} B_{\nu}$$

Rank 2

$$\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{2M} = \sum_{\mu,\nu} C^{2M}_{1\mu 1\nu} A_\mu B_\nu = \sqrt{\frac{3|M|-2}{14|M|-12}} \sum_{\substack{\mu+\nu=M \\ \mu \geq \nu}} (A_\mu B_\nu + A_\nu B_\mu)$$

$$\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{2+2} = A_{+1} B_{+1},$$

$$\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{2+1} = \frac{1}{\sqrt{2}} (A_{+1} B_0 + A_0 B_{+1}),$$

$$\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{20} = \frac{1}{\sqrt{6}} (A_{+1} B_{-1} + 2 A_0 B_0 + A_{-1} B_{+1}),$$

$$\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{2-1} = \frac{1}{\sqrt{2}} (A_{-1} B_0 + A_0 B_{-1}),$$

$$\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_{2-2} = A_{-1} B_{-1}.$$

If **A** is a polar vector and **B** is an axial vector, how do their IR tensor products of ranks 0, 1, and 2 change under the inversion operator?

From three <u>commuting</u> vectors we can construct

$$\{\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_0 \otimes \mathbf{C}_1\}_1 = -\frac{1}{\sqrt{3}} (\mathbf{A} \cdot \mathbf{B}) \cdot \mathbf{C},$$

Rank 0 →

$$\{\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_1 \otimes \mathbf{C}_1\}_0 = -\frac{i}{\sqrt{6}} [\mathbf{A} \times \mathbf{B}] \cdot \mathbf{C},$$

$$\{\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_1 \otimes \mathbf{C}_1\}_1 = -\frac{1}{2} [[\mathbf{A} \times \mathbf{B}] \times \mathbf{C}] = \frac{1}{2} \mathbf{A} (\mathbf{B} \cdot \mathbf{C}) - \frac{1}{2} \mathbf{B} (\mathbf{A} \cdot \mathbf{C}),$$

← Rank 1

$$\{\{\mathbf{A}_1 \otimes \mathbf{B}_1\}_2 \otimes \mathbf{C}_1\}_1 = \sqrt{\frac{3}{5}} \left\{ \frac{1}{3} \mathbf{C} (\mathbf{A} \cdot \mathbf{B}) - \frac{1}{2} \mathbf{B} (\mathbf{A} \cdot \mathbf{C}) - \frac{1}{2} \mathbf{A} (\mathbf{B} \cdot \mathbf{C}) \right\}.$$

Expressions for tensor products of higher ranks (2 and 3) are cumbersome.

Cartesian tensors

An arbitrary Cartesian tensor $T_{ik}, \ (i, k = x, y, z)$ can be expressed as

$$T_{ik} = E\delta_{ik} + A_{ik} + S_{ik}$$

Term proportional to the unity tesor

Antisymmetric tensor

Symmetric tensor with a zero trace

$$E = \frac{1}{3}\,\mathrm{Sp}\,(T_{ik}) = \frac{1}{3}\sum_i T_{ii},$$

$$A_{ik} = \frac{1}{2}(T_{ik} - T_{ki}),$$

$$A_{ik} = -A_{ki}$$

$$S_{ik} = \frac{1}{2}\left(T_{ik} + T_{ki} - \frac{2}{3}\delta_{ik}\sum_l T_{ll}\right)$$

$$S_{ik} = S_{ki}, \quad \sum_i S_{ii} = 0$$

Reducing a Cartesian tensor to IR tensors

Rank 0

$$\mathcal{T}_{00} = E$$

Rank 1 An antisymmetric Cartesian (true) tensor can be expressed through an (axial) vector

$$A_{ik} = \varepsilon_{ikl}\mathcal{A}_l, \quad \mathcal{A}_i = \frac{1}{2}\sum_{kl}\varepsilon_{ikl}A_{kl}$$

and, hence, through an IR (pseudo)tensor of the rank 1:

$$\mathcal{T}_{10} = \mathcal{A}_z = A_{xy}, \qquad \mathcal{T}_{1\pm1} = \mp\frac{1}{\sqrt{2}}(\mathcal{A}_x \pm i\mathcal{A}_y) = \mp\frac{1}{\sqrt{2}}(A_{yz} \pm iA_{zx})$$

Rank 2 A symmetric Cartesian tensor with zero trace yields an IR tensor of the rank 2:

$$\mathcal{T}_{20} = S_{zz},$$

$$\mathcal{T}_{2\pm1} = \mp\sqrt{\frac{2}{3}}(S_{zx} \pm iS_{zy}),$$

$$\mathcal{T}_{2\pm2} = \sqrt{\frac{1}{6}}(S_{xx} - S_{yy} \pm 2iS_{xy}).$$

Differential operations as IR tensors

$$\operatorname{grad}\Phi = \{\nabla_1 \otimes \Phi\}_1,$$
$$\operatorname{div}\mathbf{A} = -\sqrt{3}\,\{\nabla_1 \otimes \mathbf{A}_1\}_0,$$
$$\operatorname{rot}\mathbf{A} = -i\sqrt{2}\,\{\nabla_1 \otimes \mathbf{A}_1\}_1,$$
$$\Delta = \nabla^2 = -\sqrt{3}\,\{\nabla_1 \otimes \nabla_1\}_0,$$
$$\operatorname{grad}\operatorname{div}\mathbf{A} = -\sqrt{3}\,\{\nabla_1 \otimes \{\nabla_1 \otimes \mathbf{A}_1\}_0\}_1,$$
$$\operatorname{rot}\operatorname{rot}\mathbf{A} = -2\,\{\nabla_1 \otimes \{\nabla_1 \otimes \mathbf{A}_1\}_1\}_1,$$
$$\operatorname{div}\operatorname{grad}\Phi = -\sqrt{3}\,\{\nabla_1 \otimes \{\nabla_1 \otimes \Phi\}_1\}_0 = -\sqrt{3}\,\{\nabla_1 \otimes \nabla_1\}_0\,\Phi,$$
$$\operatorname{rot}\operatorname{grad}\Phi = -i\sqrt{2}\,\{\nabla_1 \otimes \{\nabla_1 \otimes \Phi\}_1\}_1 = 0,$$
$$\operatorname{div}\operatorname{rot}\mathbf{A} = i\sqrt{6}\,\{\nabla_1 \otimes \{\nabla_1 \otimes \mathbf{A}_1\}_1\}_0 = 0.$$

$$\nabla = \mathbf{n}\frac{\partial}{\partial r} - \frac{i}{r}\,[\mathbf{n} \times \hat{\mathbf{L}}]$$
$$\nabla_\mu = \sqrt{\frac{4\pi}{3}}\left(Y_{1\mu}\frac{\partial}{\partial r} - \frac{\sqrt{2}}{r}\,\{\mathbf{Y}_1 \otimes \hat{\mathbf{L}}_1\}_{1\mu}\right)$$

$\hat{\mathbf{L}}_1 \equiv \hat{\mathbf{L}}$ is the orbital momentum operator,

$\mathbf{Y}_1$ is the IR tensor of the rank 1, whose cyclic components are ther sperical functions $Y_{1\mu}(\mathbf{n})$ [to be defined later], and $\mathbf{n} = \mathbf{r} / r$.