9-10. Summary of lectures on rotational symmetry

O(3) group: continuous rotations of a sphere

eigenstates of Ham. for motion in central potential form basis for representation of O(3)

ie $\psi_{orb}(x,y,z) \propto Y_\ell^m(\theta,\varphi)$ form $(2\ell+1)$ dimensional rep^{n} $D^{(\ell)}$

$$R_z(\alpha)\, Y_\ell^m = e^{-im\alpha}\, Y_\ell^m$$

(in natural basis)

multi-e $\quad R_z(\alpha)|L,m_L\rangle = e^{-im_L\alpha}\, \underbrace{|L,m_L\rangle}_{\text{form rep}^{n}\ D^{(L)}}$

Character $\quad \chi^{(L)}(\alpha) = \dfrac{\sin(L+\frac{1}{2})\alpha}{\sin\frac{\alpha}{2}}$ $\quad$ proper rot^{n}

$\chi^{(L)}(\bar{\alpha}) = \underbrace{(-1)^{\sum_i l_i}}_{\text{parity}}\ \chi(\alpha)$ $\quad$ improper rot^{n}

Spin wavefn^{s} can also form basis

$$R_z(\alpha)|S,m_s\rangle = e^{-im_s\alpha}\,|S,m_s\rangle$$

(in natural basis)

if $S=\frac{1}{2}$ $\quad R(2\pi)|\tfrac{1}{2},\tfrac{1}{2}\rangle = e^{-i\frac{1}{2}2\pi}\,|\tfrac{1}{2}\,\tfrac{1}{2}\rangle = (-1)\,|\tfrac{1}{2},\tfrac{1}{2}\rangle$

change sign upon rot^{n} by 2π

Conventional point groups do not capture full symmetry properties of half-integer spin wavef^{n}, extra element

$$\bar{E} = R(2\pi) \qquad \bar{E}\,\psi_{spin} = (-1)^{2S}\,\psi_{spin}$$

if Hamiltonian spherical $\longrightarrow$ lower symmetry p.g. G

decompose $D^{(S)}$ into irr.^{s} of double group

$$d\text{-}G = \{\underbrace{R}_{\text{operation of } G}, \bar{E}R\}$$

ingeneral

for given angular momentum $\vec{J}$

$|J, m_J\rangle$ form rep^{n} $D^{(J)}$

$2J+1$ $\longrightarrow$ Γ_i – irr^{s} of $D^{(J)}$ in point group of Hamiltonian

spherical

Ham of lower sym.

characters

$$\chi^{(J)}(\alpha) = \frac{\sin\left(J+\frac{1}{2}\right)\alpha}{\sin\frac{\alpha}{2}}$$

if environment centrosymmetric

$$\chi^{(J)}(\bar{\alpha}) = \underbrace{(-1)^{\sum l_i}}_{\text{parity}}\,\chi(\alpha)$$

if half-odd J, use double group $d\text{-}G$

$$\chi(\bar{E}\alpha) = (-1)^{2S}\,\chi(\alpha)$$

$$\chi(\bar{E}\bar{\alpha}) = (-1)^{2S}\,\chi(\bar{\alpha})$$

spin wavef^{n} invariant under spacial inversion by def^{n}

Double Groups

Example, d–432

	d–432		E	$\bar{E}$	3[8]	$\bar{E}3$ [8]	[6] same class 2_z[3] $\bar{E}2_z$[3]	[12] 2_d[6] $\bar{E}2_d$[6]	4_z[6]	$\bar{E}4_z$[6]
same as 432	Γ_1	A_1	1	1	1	1	1	1	1	1
	Γ_2	A_2	1	1	1	1	1	−1	−1	−1
	Γ_3	E	2	2	−1	−1	2	0	0	0
	Γ_4	T_1	3	3	0	0	−1	−1	1	1
	Γ_5	T_2	3	3	0	0	−1	1	−1	−1
new irr's	Γ_6		2	−2	1	−1	0	0	$\sqrt{2}$	$-\sqrt{2}$
	Γ_7		2	−2	1	−1	0	0	$-\sqrt{2}$	$\sqrt{2}$
	Γ_8		4	−4	−1	1	0	0	0	0

A complete listing of double groups may be found in G. F. Koster et al, Properties of the Thirty-Two Point Groups (MIT Press, Cambridge MA, 1963)