Chapter 4
General Propertis of Irreducible Vectors & Operators

The states of a system are classified according to the IRs of the symmetry group of the system.

Eg., $Y_{l\,m}$ ~ spherical symmetry;
Bloch functions ~ translational symmetry.

Physical observables are also classified according to IRs of the underlying symmetry groups.

Eg., x, p transform as vectors under rotations;
$T_{\mu\,\nu}$, $F_{\mu\,\nu}$ transform as second rank tensors under Lorentz transformations.

A systematic study of the consequences of the above- described properties of state vectors and physical observables allows the full structure due to symmetry to be exposed and utilized.

In this chapter, we
- define irreducible sets of state vectors and operators,
- find procedure to decompose arbitrary vectors and operators into their irreducible components,
- and study the full range of implications on physically measurable quantities due to a symmetry group.

This general formalism will then be applied to specific groups to be discussed in the remainder the book.

Reminder:
Repeated indices imply summation only when they're staggered & un-barred:

$$a^\mu b_\mu \equiv \sum_\mu a^\mu b_\mu$$

but no summation for

$$a_\mu b_\mu \quad \text{or} \quad a^{\bar{\mu}} b_\mu = a^\mu b_{\bar{\mu}}$$

4.1 Irreducible Basis (IB) Vectors

- Definition 4.1:

Let $U(G)$ be a unitary rep of G on an inner product space V.
Let $\left\{ \hat{e}_i{}^\mu ;\ i = 1, \ldots, n_\mu \right\}$ be an orthonormal basis that spans an invariant subspace V^μ of V.
Let $D^\mu(g)$ be an (matrix) IR of G.

If

(4.1-1) $$U(g) \,|\, e_i{}^\mu \rangle = \left| \, e_j{}^\mu \right\rangle D^\mu(g)^j{}_i \qquad g \in G$$

$\left\{ \hat{e}_i{}^\mu ;\ i = 1, \ldots, n_\mu \right\}$ is said to be an irreducible set transforming according to the μ-rep,
ie., it is an irreducible basis (IB) of V^μ.
$\hat{e}_i{}^\mu$ is said to belong to, or transform according to, the ith row of the μ-rep.

- Theorem 4.1:

If the IRs D^μ & D^ν are not equivalent, then $V^\mu \perp V^\nu$.

- Proof:

Since we assume that the bases are orthonormal and that the representations are unitary, we have, $\forall\ i = 1, \ldots, n_\mu$, $j = 1, \ldots, n_\nu$:

$$\langle e^j{}_\nu \,|\, e^\mu{}_i \rangle = \langle e^j{}_\nu \,|\, U^\dagger(g)\, U(g) \,|\, e^\mu{}_i \rangle \qquad [\ U^\dagger U = E\ ]$$

$$= D_\nu{}^\dagger(g)^j{}_k \langle e^k{}_\nu \,|\, e^\mu{}_l \rangle\, D^\mu(g)^l{}_i \qquad [\text{ from 4.1-1 }]$$

$$= \frac{1}{n_G} \sum_g D_\nu{}^\dagger(g)^j{}_k\, D^\mu(g)^l{}_i \langle e^k{}_\nu \,|\, e^\mu{}_l \rangle$$

$$= \frac{1}{n_{\bar{\mu}}} \delta^\mu{}_\nu\, \delta^j{}_i\, \delta^l{}_k \langle e^k{}_\nu \,|\, e^\mu{}_l \rangle \qquad [\text{ Orthogonality of IRs }]$$

$$= \frac{1}{n_{\bar{\mu}}} \delta^\mu{}_\nu\, \delta^j{}_i \langle e^l{}_{\bar{\mu}} \,|\, e^\mu{}_l \rangle$$

$$= \delta^\mu{}_\nu\, \delta^j{}_i \qquad [\text{ Orthonormality of } \{e^\mu{}_l\}\ ]$$

Note: the ranges of the repeated- indices- summations are

$l = 1, \ldots, n_\mu$ and $k = 1, \ldots, n_\nu$

Thus, for $\mu \neq \nu$

$$\langle e^j{}_\nu \,|\, e^\mu{}_i \rangle = 0\ \forall\ i, j$$

ie., $V^\mu \perp V^\nu$.

Hermitian operators

Let H be a hermitian operator, ie., $H^\dagger = H$.
Let $|e_i\rangle$ be an eigenstate of H with eigenvalue λ_i, ie.,

$$H\,|e_i\rangle = \lambda_i\,|e_i\rangle$$

$$= H^\dagger|e_i\rangle \qquad [\ H^\dagger = H\ ]$$

Taking the adjoint,

$$\langle e^i \,|\, H^\dagger = \langle e^i \,|\, \lambda_{\bar{i}}^*$$

$$= \langle e^i \,|\, H$$

Hence

$$\langle e^j \,|\, H \,|\, e_i \rangle = \lambda_i \langle e^j \,|\, e_i \rangle \qquad [\ H\,|e_i\rangle = \lambda_i\,|e_i\rangle\ ]$$

$$= \lambda_{\bar{j}}^* \langle e^j \,|\, e_i \rangle \qquad [\ \langle e^j \,|\, H = \langle e^j \,|\, \lambda_{\bar{j}}^*\ ]$$

which means

$$(\lambda_i - \lambda_j{}^*) \langle e^j \,|\, e_i \rangle = 0$$

For $j = i$, we have

$$\lambda_i = \lambda_i{}^*$$

since $\langle e^j \,|\, e_i \rangle \neq 0$.

Thus, all eigenvalues of a hermitian operator are real.

For $i \neq j$, if

$$\lambda_i \neq \lambda_j$$

we have

$$\langle e^j \,|\, e_i \rangle = 0$$

so that all eigenvectors corresponding to different eigenvalues are orthogonal.

In case of an n-fold degeneracy, ie., there are n independent eigenvectors with the same eigenvalue λ_i, we can re-label them as

$$| e_{i\alpha} \rangle \qquad \alpha = 1, 2, \ldots, n$$

These vectors span an n-Dim subspace from which n orthonormal basis vectors can always be found. Thus we can always choose $| e_{i\alpha} \rangle$ as such an orthonormal set.

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Theorem 4.1 can be regarded as a generalization of the orthogonality of eigenvectors of a hermitian operator (see last section).

For $\mu = \nu$ (i.e. the two representations are equivalent). There are two possibilities:

(i) $V^\mu \cap V^\nu = \emptyset$, then $\langle e^j{}_\nu | e^\mu{}_i \rangle = 0$.
(typically, the two spaces are distinguished by the eigenvalues of some other operator outside the group under consideration);

(ii) $V^\mu \cap V^\nu \neq \emptyset$, then $V^\mu = V^\nu$.
and $| e^\mu{}_i \rangle = | e^\nu{}_j \rangle S^j{}_i$,
where S is a unitary matrix (indeed, $\langle e^j{}_\nu | e^\mu{}_i \rangle = S^j{}_i$).

- Examples:

Consider the Hilbert space of electron wave functions in a hydrogen atom.
$G = R_3$ − the group of rotations. Then [Messiah, Schiff]
1. States corresponding to different angular momenta (i.e. different IRs of R_3) are necessarily orthogonal to each other, irrespective of the "radial quantum number".
2. States corresponding to the same angular momenta are also mutually orthogonal if they correspond to different radial quantum numbers.
3. Nonvanishing scalar products are obtained only if both the angular momenta and the radial quantum numbers are the same.

4.2 Projection Operators

- Theorem 4.2:

Let $U(G)$ be a rep of G on V, and $D^\mu(G)$ be a matrix IR of G.
Define operators

(4.2-1) $$P^j{}_{\mu\, i} = \frac{n_\mu}{n_G} \sum_g D^{-1}{}_\mu(g)^j{}_i \, U(g)$$

Then $\forall \; | x \rangle \in V$, $\{ P^j{}_{\mu\, i} | x \rangle, \; i = 1, \ldots, n_\mu \}$ is an IB for V^μ.
We also say that $P^j{}_{\mu\, i} | x \rangle$ transform according to the ith row of the μ-rep.

For unitary reps,

$$P^j{}_{\mu\, i} = \frac{n_\mu}{n_G} \sum_g D^\dagger{}_\mu(g)^j{}_i \, U(g)$$

$$= \frac{n_{\bar{\mu}}}{n_G} \sum_g \left[D^\mu(g)^i{}_j \right]^* U(g)$$

- Proof:

$$U(g)\, P^{j}{}_{\mu\, i} \,|\, x \,\rangle = \frac{n_\mu}{n_G} \sum_{g'} U(g)\, U(g')\,|\, x\,\rangle\, D^{-1}{}_{\mu}(g')^{j}{}_{i}$$

$$= \frac{n_\mu}{n_G} \sum_{g'} U(g\, g')\,|\, x\,\rangle\, D^{-1}{}_{\mu}(g')^{j}{}_{i}$$

$$= \frac{n_\mu}{n_G} \sum_{g''} U(g'')\,|\, x\,\rangle\, D^{-1}{}_{\mu}\big(g^{-1}\, g''\big)^{j}{}_{i} \qquad [\, g'' = g\, g' \,]$$

$$= \frac{n_\mu}{n_G} \sum_{g''} U(g'')\,|\, x\,\rangle\, D^{-1}{}_{\mu}(g'')^{j}{}_{k}\; D^{-1}{}_{\mu}\big(g^{-1}\big)^{k}{}_{i} \qquad [\text{ see note below }]$$

$$= \mathrm{P}^{j}{}_{\mu\, k} \,\big|\, x\, \big\rangle\, D^{-1}{}_{\mu}\big(g^{-1}\big)^{k}{}_{i}$$

$$= \mathrm{P}^{j}{}_{\mu\, k} \,\big|\, x\, \big\rangle\, D_{\mu}(g)^{k}{}_{i}$$

Note:
If

$$D(a\, b) = D(a)\, D(b)$$

we must have

$$D^{-1}(a\, b) = D^{-1}(b)\, D^{-1}(a)$$

so that

$$D(a\, b)\, D^{-1}(a\, b) = D(a)\, D(b)\, D^{-1}(b)\, D^{-1}(a) = I$$

$$D^{-1}(a\, b)\, D(a\, b) = D^{-1}(b)\, D^{-1}(a)\, D(a)\, D(b) = I$$

- Theorem 4.3:

Let $\left\{ \hat{e}^{\nu}{}_{k},\;\; k = 1, \ldots, n \right\}$ be an IB, then

(4.2-2) $\qquad P^{j}{}_{\mu\, i} \,\big|\, e^{\nu}{}_{k} \,\big\rangle = \big|\, e^{\bar{\mu}}{}_{i} \,\big\rangle\, \delta^{\nu}{}_{\mu}\, \delta^{j}{}_{k}$

Thus,

if $\qquad \mu \neq \nu, \qquad P^{j}{}_{\mu\, i} \,\big|\, e^{\nu}{}_{k} \,\big\rangle = 0$;

and if $\qquad \mu = \nu, \qquad P^{j}{}_{\mu\, i} \,\big|\, e^{\bar{\mu}}{}_{k} \,\big\rangle = \big|\, e^{\mu}{}_{i} \,\big\rangle\;\; \delta^{j}{}_{k}$.

Let

$$|\, x\,\rangle = |\, e^{\mu}{}_{i}\,\rangle\, x^{i}$$

then

$$P^{j}{}_{\mu\, i}\,|\, x\,\rangle = P^{j}{}_{\mu\, i} \,\big|\, e^{\bar{\mu}}{}_{k} \,\big\rangle\, x^{k}$$

$$= |\, e^{\mu}{}_{i}\,\rangle\;\; \delta^{j}{}_{k}\, x^{k}$$

$$= |\, e^{\mu}{}_{i}\,\rangle\;\, x^{j}$$

ie, $P^{j}{}_{\mu\, i}$ kicks $|\, x\,\rangle$ into the direction $|\, e^{\mu}{}_{i}\,\rangle$ with magnitude x^{j}.

Obviously, $P^{\bar{i}}{}_{\mu\, i}$ is the projector onto $|\, e^{\mu}{}_{i}\,\rangle$.

- Proof:

$$P^{j}{}_{\mu i}\,|\,e^{\nu}{}_{k}\,\rangle = \frac{n_\mu}{n_G}\sum_g U(g)\,|\,e^{\nu}{}_{k}\,\rangle\, D^{\dagger}{}_{\mu}(g)^{j}{}_{i} \qquad \text{[unitary IR]}$$

$$= \;|\,e^{\nu}{}_{l}\,\rangle\,\frac{n_\mu}{n_G}\sum_g D^{\nu}(g)^{l}{}_{k}\; D^{\dagger}{}_{\mu}(g)^{j}{}_{i}$$

$$= \;|\,e^{\nu}{}_{l}\,\rangle\;\delta^{\nu}{}_{\mu}\,\delta^{l}{}_{i}\;\delta^{j}{}_{k} \qquad \text{[Great Orthogonality Theorem]}$$

$$= \;|\,e^{\nu}{}_{i}\,\rangle\;\delta^{\nu}{}_{\mu}\,\delta^{j}{}_{k}$$

$$= \;\left|\,e^{\overline{\mu}}{}_{i}\,\right\rangle\delta^{\nu}{}_{\mu}\,\delta^{j}{}_{k}$$

- **Matrix Form of $P^{j}{}_{\mu i}$**

By the definition

$$P^{j}{}_{\mu i} = \frac{n_\mu}{n_G}\sum_g D^{-1}{}_{\mu}(g)^{j}{}_{i}\,U(g)$$

the matrix elements of $P^{j}{}_{\mu i}$ in the IB $\{\,\hat{e}^{\nu}{}_{i}\,\}$ are

$$\left[P^{j}{}_{\mu i}\right]^{k}{}_{l} = \frac{n_\mu}{n_G}\sum_g D^{-1}{}_{\mu}(g)^{j}{}_{i}\,D^{\nu}(g)^{k}{}_{l}$$

$$= \;\delta^{\nu}{}_{\mu}\,\delta^{k}{}_{i}\;\delta^{j}{}_{l}$$

In other words, $P^{j}{}_{\mu i}$ in the IB $\{\,\hat{e}^{\mu}{}_{i}\,\}$ is matrix with only one nonzero element

$$\left[P^{j}{}_{\mu i}\right]^{\bar{i}}{}_{\bar{j}} = 1$$

Note that this is true even if the basis is not orthogonal.

- **Non-orthogonal basis**

Consider a non-orthogonal basis $\{\,\hat{e}_i\,\}$.

Define the overlap matrix $\mathbb{S}$ by

$$\left\langle e^{i}\,\middle|\,e_{j}\right\rangle = \mathbb{S}^{i}{}_{j}$$

with

$$\mathbb{S}^{i}{}_{j} = \delta^{i}{}_{j} \qquad \text{or} \qquad \mathbb{S} = I$$

for an orthonormal basis.

In matrix form, we set

$$| e_i \rangle \quad \Longrightarrow \quad \boldsymbol{e}_i = \begin{pmatrix} 0 \\ \vdots \\ x^i = 1 \\ \vdots \\ 0 \end{pmatrix}$$

$$\left\langle e^i \right| \quad \Longrightarrow \quad \boldsymbol{e}_i{}^T \, \mathbb{S} = \left(0 \;\; \cdots \;\; x_i = 1 \;\; \cdots \;\; 0 \right) \begin{pmatrix} \mathbb{S}^1{}_1 & \cdots & \mathbb{S}^1{}_n \\ \vdots & \mathbb{S}^i{}_j & \vdots \\ \mathbb{S}^n{}_1 & \cdots & \mathbb{S}^n{}_n \end{pmatrix}$$

$$= \left(\mathbb{S}^i{}_1, \, \ldots, \, \mathbb{S}^i{}_j, \, \ldots, \, \mathbb{S}^i{}_n \right)$$

so that

$$\left\langle e^i \,|\, e_j \right\rangle = \left(\mathbb{S}^i{}_1, \, \ldots, \, \mathbb{S}^i{}_k, \, \ldots, \, \mathbb{S}^i{}_n \right) \begin{pmatrix} 0 \\ \vdots \\ x^j = 1 \\ \vdots \\ 0 \end{pmatrix}$$

$$= \; \mathbb{S}^i{}_j$$

as required.

Next we set

$$| \, x \rangle = | \, e_i \rangle \, x^i \quad \Longrightarrow \quad \mathrm{x} = \begin{pmatrix} \mathrm{x}^1 \\ \vdots \\ \mathrm{x}^\mathrm{i} \\ \vdots \\ \mathrm{x}^\mathrm{n} \end{pmatrix}$$

$$\left\langle x \right| = \left\langle e^i \right| x_i \quad \Longrightarrow \quad \left(\mathrm{x}_1 \;\; \cdots \;\; \mathrm{x}_\mathrm{i} \;\; \cdots \;\; \mathrm{x}_\mathrm{n} \right) \begin{pmatrix} \mathbb{S}^1{}_1 & \cdots & \mathbb{S}^1{}_\mathrm{n} \\ \vdots & \mathbb{S}^\mathrm{i}{}_\mathrm{j} & \vdots \\ \mathbb{S}^\mathrm{n}{}_1 & \cdots & \mathbb{S}^\mathrm{n}{}_\mathrm{n} \end{pmatrix}$$

$$= \; \boldsymbol{x}^T \, \mathbb{S}$$

Hence

$$\langle x \,|\, y \rangle = \left\langle e^i \,|\, e_j \right\rangle x_i \, y^j = \; x_i \, \mathbb{S}^i{}_j \, y^j$$

becomes in matrix form

$$\boldsymbol{x}^T \, \mathbb{S} \, \boldsymbol{y} = \left(x_1 \;\; \cdots \;\; x_i \;\; \cdots \;\; x_n \right) \begin{pmatrix} \mathbb{S}^1{}_1 & \cdots & \mathbb{S}^1{}_n \\ \vdots & \mathbb{S}^i{}_j & \vdots \\ \mathbb{S}^n{}_1 & \cdots & \mathbb{S}^n{}_n \end{pmatrix} \begin{pmatrix} y^1 \\ \vdots \\ y^i \\ \vdots \\ y^n \end{pmatrix}$$

$$= \; x_i \, \mathbb{S}^i{}_j \, y^j$$

Let an operator U be defined as

$$U \; | \; e_i \rangle = \left| \; e_j \right\rangle D^j{}_i$$

so that

$$U \,|\, x \rangle = U \,|\, e_i \rangle \, x^i = \left| \; e_j \right\rangle D^j{}_i \, x^i$$

In matrix form, we have

$$U \quad \Longrightarrow \quad D = \begin{pmatrix} D^1{}_1 & \cdots & D^1{}_n \\ \vdots & D^i{}_j & \vdots \\ D^n{}_1 & \cdots & D^n{}_n \end{pmatrix}$$

$$U\,|\,x\,\rangle \quad \Longrightarrow \quad D\,\boldsymbol{x} = \begin{pmatrix} D^1{}_1 & \cdots & D^1{}_n \\ \vdots & D^i{}_j & \vdots \\ D^n{}_1 & \cdots & D^n{}_n \end{pmatrix} \begin{pmatrix} x^1 \\ \vdots \\ x^i \\ \vdots \\ x^n \end{pmatrix}$$

Thus

$$D^i{}_j = (\,0 \;\; \cdots \;\; x_i = 1 \;\; \cdots \;\; 0\,) \begin{pmatrix} D^1{}_1 & \cdots & D^1{}_n \\ \vdots & D^l{}_m & \vdots \\ D^n{}_1 & \cdots & D^n{}_n \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ x^j = 1 \\ \vdots \\ 0 \end{pmatrix}$$

$$= \boldsymbol{e}_i{}^T\, D\, \boldsymbol{e}_j$$

On the other hand, from

$$U\,|\,e_i\,\rangle = \big|\,e_j\,\big\rangle\, D^j{}_i$$

we have

$$\big\langle\, e^i \,\big|\, U \;\big|\; e_j \,\big\rangle = \big\langle\, e^i \,\big|\; e_k \,\big\rangle\, D^k{}_j$$

$$= \; \mathbb{S}^i{}_k\, D^k{}_j$$

or

$$D^i{}_j = \left(\mathbb{S}^{-1}\right)^i{}_k \,\big\langle\, e^k \,\big|\, U \;\big|\; e_j \,\big\rangle$$

which reduces to the more familiar form

$$D^i{}_j = \big\langle\, e^i \,\big|\, U \;\big|\; e_j \,\big\rangle$$

for orthonormal basis ($\mathbb{S} = I$).

■ Corollary 1:

(4.2-3) $$P^j{}_{\mu\, i}\, P^l{}_{\nu\, k} = P^l{}_{\nu\, i}\;\delta^{\bar{\nu}}{}_{\mu}\,\delta^j{}_k$$

$$= \; P^l{}_{\mu\, i}\,\delta^{\bar{\mu}}{}_{\nu}\,\delta^j{}_k$$

■ Proof:

From theorem 4.2, $\left\{\, P^l{}_{\nu\, k} |\, x\,\rangle \,,\;\; k = 1, \;\ldots\,,\, n \,\right\}$ is an IB for V^μ.

In fact,

$$P^l{}_{\nu\, k} |\, x\,\rangle = P^l{}_{\nu\, k} |\, e^\mu{}_i\,\rangle\, x^i{}_\mu \qquad\qquad |\; x\;\rangle \in V$$

$$= \;|\; e^\mu{}_k\;\rangle\;\delta^\mu{}_\nu\,\delta^l{}_i\,x^i{}_\mu$$

$$= \;|\; e^\mu{}_k\;\rangle\;\delta^\mu{}_\nu\;\, x^l{}_\mu$$

$$= \;|\,e^\nu{}_k\;\rangle\;\; x^l{}_{\bar{\nu}}$$

Thus

$$P^j{}_{\mu\, i}\, P^l{}_{\nu\, k}\,|\,x\;\rangle = P^j{}_{\mu\, i}|\; e^\nu{}_k\;\rangle\;\; x^l{}_{\bar{\nu}}$$

$$= \;|\,e^\nu{}_i\;\rangle\;\delta^\nu{}_\mu\;\;\delta^j{}_k\,x^l{}_{\bar{\nu}}$$

$$= \;\mathrm{P}^l{}_{\nu\, i}|\,x\;\rangle\,\delta^{\bar{\nu}}{}_\mu\,\delta^j{}_k$$

Since the relation is valid $\forall\, | x \rangle \in V$, we have

$$P^{j}{}_{\mu i}\, P^{l}{}_{\nu k} = P^{l}{}_{\nu i}\, \delta^{\bar{\nu}}{}_{\mu}\, \delta^{j}{}_{k}$$
$$= \; P^{l}{}_{\mu i}\, \delta^{\bar{\mu}}{}_{\nu}\, \delta^{j}{}_{k}$$

- Corollary 2:

The n_G operators $U(g)$, $g \in G$, can be written as linear combinations of $P^{j}{}_{\mu i}$ $\left(\mu = 1, \ldots, n_c ;\; i,\; j = 1, \ldots, n_\mu \right)$:

(4.2-4) $$U(g) = P^{j}{}_{\mu i}\, D^{\mu}(g)^{i}{}_{j}$$

- **Proof:**

By definition

$$P^{j}{}_{\mu i} = \frac{n_\mu}{n_G} \sum_g D^{-1}{}_{\mu}(g)^{j}{}_{i}\, U(g)$$

Hence

$$D^{\mu}(g')^{i}{}_{j}\, P^{j}{}_{\mu i} = \frac{n_\mu}{n_G} \sum_g D^{\mu}(g')^{i}{}_{j}\, D^{-1}{}_{\mu}(g)^{j}{}_{i}\, U(g)$$
$$= \sum_g \delta_{g g'}\, U(g) \qquad \text{[Completeness Theorem]}$$
$$= \; U(g)$$

- Corollary 3:

(4.2-5) $$U(g)\, P^{l}{}_{\nu k} = \; P^{l}{}_{\bar{\nu} i}\; D^{\bar{\nu}}(g)^{i}{}_{k}$$

- **Proof:**

Combining

$$P^{j}{}_{\mu i}\, P^{l}{}_{\nu k} = \delta^{\nu}{}_{\bar{\mu}}\, \delta^{j}{}_{k}\, P^{l}{}_{\bar{\mu} i}$$

and

$$U(g) = P^{j}{}_{\mu i}\, D^{\mu}(g)^{i}{}_{j}$$

we have

$$U(g)\, P^{l}{}_{\nu k} = P^{j}{}_{\mu i}\, P^{l}{}_{\nu k}\, D^{\mu}(g)^{i}{}_{j}$$
$$= \; \delta^{\nu}{}_{\mu}\, \delta^{j}{}_{k}\, P^{l}{}_{\mu i}\, D^{\mu}(g)^{i}{}_{j}$$

This relation follows directly from Equations (4.2-3) and (4.2-4). It is, of course, merely a restatement of Theorem 4.2 in pure operator form.

- Definition 4.2:

$$P_{\mu i} \equiv P^{\bar{i}}{}_{\mu i}$$

are the projection operators onto the basis vector $\hat{e}^{\mu}{}_{i}$ and

$$P \equiv \sum_i P_{\mu i} = \mathrm{P}^{i}{}_{\mu i}$$

are the projection operators onto the irreducible invariant space V_μ (spanned by $\left\{ \hat{e}^{\mu}{}_{i},\; i = 1, \ldots, n_\mu \right\}$).

✸

We must establish that $P_{\mu i}$ are indeed projection operators. This can be shown as follows:

$$P_{\mu i} P_{\nu k} = P^{\bar{i}}{}_{\mu i} P^{\bar{k}}{}_{\nu k}$$
$$= P^{\bar{k}}{}_{\mu i} \delta^{\bar{\mu}}{}_{\nu} \delta^{\bar{i}}{}_{k} \qquad [\, P^{j}{}_{\mu i} P^{l}{}_{\nu k} = P^{l}{}_{\mu i} \delta^{\bar{\mu}}{}_{\nu} \delta^{j}{}_{k} \,]$$
$$= P^{\bar{i}}{}_{\mu i} \delta^{\bar{\mu}}{}_{\nu} \delta^{\bar{i}}{}_{k}$$
$$= P_{\mu i} \delta^{\bar{\mu}}{}_{\nu} \delta^{\bar{i}}{}_{k}$$

Similarly,

$$P_{\mu} P_{\nu} = P^{i}{}_{\mu i} P^{j}{}_{\nu j}$$
$$= P^{j}{}_{\mu i} \delta^{\bar{\mu}}{}_{\nu} \delta^{i}{}_{j} \qquad [\, P^{j}{}_{\mu i} P^{l}{}_{\nu k} = P^{l}{}_{\mu i} \delta^{\bar{\mu}}{}_{\nu} \delta^{j}{}_{k} \,]$$
$$= P^{i}{}_{\mu i} \delta^{\bar{\mu}}{}_{\nu}$$
$$= P_{\mu} \delta^{\bar{\mu}}{}_{\nu}$$

- Theorem 4.4:

The projection operators P_{μ} and $P_{\mu i}$ are complete in the sense that $\sum_{\mu} P_{\mu} = E$.

- Proof:

Let $\{ \hat{e}^{\nu}{}_{k} \}$ be an IB for invariant subspace V^{ν}.
According to Theorem 4.3:

$$P_{\mu i} \,|\, e^{\nu}{}_{k} \rangle = P^{\bar{i}}{}_{\mu i} \,|\, e^{\nu}{}_{k} \rangle = \left| e^{\bar{\mu}}{}_{i} \right\rangle \delta^{\nu}{}_{\mu} \delta^{\bar{i}}{}_{k}$$

and $$P_{\mu} \,|\, e^{\nu}{}_{k} \rangle = P^{i}{}_{\mu i} \,|\, e^{\nu}{}_{k} \rangle = \left| e^{\bar{\mu}}{}_{i} \right\rangle \delta^{\nu}{}_{\mu} \delta^{i}{}_{k} = \left| e^{\bar{\mu}}{}_{k} \right\rangle \delta^{\nu}{}_{\mu}$$

hence $$\sum_{\mu} P_{\mu} \,|\, e^{\nu}{}_{k} \rangle = \,|\, e^{\mu}{}_{k} \rangle \delta^{\nu}{}_{\mu} = |\, e^{\nu}{}_{k} \rangle$$

Since this holds for all $|\, e^{\nu}{}_{k} \rangle$, we have

$$\sum_{\mu} P_{\mu} = \mathrm{E}$$

provided the space V is fully reducible (as we always assume it is). QED

■ Summary

If $U(G)$ is a rep of G on V, then

$$V = \sum_{\mu \alpha \oplus} V_{\mu}{}^{\alpha}$$

where μ is the IR label
($\mu = 1, \ldots, n_c$; $n_c =$ number of distinct classes),
and $\alpha = 1, \ldots, a_{\mu}$
(a_{μ} = number of occurrences of the μ-rep in the reduction of $U(G)$).

A complete set of basis vectors corresponding to this reduction can be labelled as $|\,\alpha, \mu, i\,\rangle$ where $i = 1, \ldots, n_\mu$ (n_μ = dim of the μ-rep). The effects of the above- defined operators on these vectors are:

(4.2-6) $$P_\mu \,|\, \alpha, \nu, k \,\rangle = |\, \alpha, \mu, k \,\rangle\, \delta^{\bar{\mu}}{}_\nu$$

(4.2-7) $$P_{\mu i} \,|\, \alpha, \nu, k \,\rangle = |\, \alpha, \mu, i \,\rangle\, \delta^{\bar{\mu}}{}_\nu\, \delta^{\bar{i}}{}_k$$

(4.2-8) $$P^j{}_{\mu i} \,|\, \alpha, \nu, k \,\rangle = |\, \alpha, \mu, i \,\rangle\, \delta^{\bar{\mu}}{}_\nu\, \delta^j{}_k$$

Although $P^j{}_{\mu i}$ are not projection operators in the strict sense, they are the most useful among the three because they can be used to construct irreducible basis vectors from arbitrary vectors according to Theorem 4.2. (N.B. The projection operators $P_{\mu i}$ do not have this property.)

- Example 1:

Let V be the space of square integrable functions $f(x)$ of the variable x.
G be the group (e, I_s) where I_s, the space inversion operation, changes x to $-x$.
Since $G \simeq C_2$, it has two 1-D IRs (given by Table 3.1).

The two projection operators are:

$P_1 = E + U(I_s)$ and $P_2 = E - U(I_s)$

where we have used $U(e) = E$.
(For 1-D reps, the i, j indices on $P^j{}_{\mu i}$ are, of course, unnecessary.)

Given any function $f(x)$, the "parity" operator $U(I_s)$ transforms it into $f(-x)$. Hence

$P_1\, f(x) = f(x) + f(-x) \equiv f_+(x)$ even under parity

and $P_2\, f(x) = f(x) - f(-x) \equiv f_-(x)$ odd under parity

- Example 2:

Let V be the space of state- vectors for a particle on a 1-D lattice.
G be the symmetry group of discrete translations T_d, as discussed in Chap. 1.
We have learned that

the IRs are labelled by k ($-\pi/b \le k \le \pi/b$), and
the rep functions are $\{e^{-i k n b}\}$.

Starting with a localized state $|\, y \,\rangle$ where $-b/2 \le y \le b/2$, we can project out its irreducible components

(4.2-9) $$\begin{aligned} |\, k, y \,\rangle = P_k \,|\, y \,\rangle &= \sum_n T(n)\,|\, y \,\rangle\, e^{i k n b} \\ &= \sum_n |\, n b + y \,\rangle\, e^{i k n b} \end{aligned}$$

These states are eigenstates of translations with eigenvalue, $e^{-i k m b}$:

$$\begin{aligned} T(m)\,|\, k, y \,\rangle &= \sum_n T(m+n)\,|\, y \,\rangle\, e^{i k n b} \\ &= \sum_{n'} T(n')\,|\, y \,\rangle\, e^{i k (n' - m) b} \\ &= |\, k, y \,\rangle\, e^{-i k m b} \\ &= |\, k, y + m b \,\rangle \end{aligned}$$

confirming Eq. (1.3-3).

Hence

$$|\langle k,\ y+m\,b\ |k,\ y+m\,b\rangle|^2 = |\langle k,\ y\ |k,\ y\rangle|^2\left|e^{-i\,k\,m\,b}\right|^2$$
$$= \ |\langle k,\ y\ |k,\ y\rangle|^2$$

ie., the probabilities for finding the electron in any of the "cells" on the lattice are equal to each other. These states are normal mode states analogous to plane wave states in continuum quantum mechanics.

Note that if

$|\ x\rangle = |\ l\,b + y\rangle$ for any integer l,

then

$$\begin{aligned} P_k\,|x\rangle &= P_k\,|\,l\,b+y\,\rangle \\ &= \sum_n T(n)\,|\,l\,b+y\ \rangle\,e^{i\,k\,n\,b} \\ &= \sum_n |\,(\,l+n)\,b+y\ \rangle\,e^{i\,k\,n\,b} \\ &= e^{-i\,k\,l\,b}\sum_m |\,m\,b+y\ \rangle\,e^{i\,k\,m\,b} \qquad [\ m=l+n\ ] \\ &= e^{-i\,k\,l\,b}\,P_k\left|\,y\right\rangle \\ &= |\ k,\ y\,\rangle\,e^{-i\,k\,l\,b} \end{aligned}$$

Hence, to obtain all distinct irreducible states, it suffices to start with localized states within just one unit cell and apply the projection operators.

■ ✱

The last example illustrates how the projection operators can be used to transform from a given basis

$|\ x\rangle = |\ n\,b+y\,\rangle \equiv |\,n,\ y\,\rangle$, representing localized states,

to an IB

$|\ k,\ y\,\rangle = P_k\,|\,0,\ y\,\rangle$, representing normal modes.

The localized states may represent the physical system at some initial (or intermediate) time. In order to predict the time development of these states, it is necessary to express them in terms of the normal mode vectors, because only the latter have simple time evolution behavior – as a consequence of the commutativity of the Hamiltonian with symmetry transformations.

This fact underlines the importance of the systematic utilization of IB for all applicable symmetries of a given physical system. We shall use this type of transformation of bases extensively in later chapters when we study the IRs of many symmetry groups.

A second type of application concerns the reduction of direct product reps to their irreducible components, and the evaluation of C-GCs.

Let $D^{\mu}(G)$ ($\mu = 1,\ 2,\ \ldots,\ n_c$) be an IR of G realized on V_μ with basis $\left\{\hat{e}^{\mu}{}_{i}\,,\ i=1,\ \ldots,\ n_\mu\right\}$.

Consider the direct product rep $D^{\mu\times\nu}$ realized on $V_\mu \times V_\nu$.

How do we find the irreducible invariant subspaces of $V_\mu \times V_\nu$ described in Sec. 3.8?

One systematic method is to use the projection operators of this section.

Specifically, we can start with the original basis vectors $|\ k,\ l\ \rangle = \hat{e}^{\mu}{}_{k} \times \hat{e}^{\nu}{}_{l}$ operators: $P^{j}{}_{\lambda\,i}\left|\,k,\ l\ \right\rangle$.

For fixed ($\lambda,\ j,\ k,\ l$), the n_λ vectors ($i\ = 1,\ \ldots,\ n_\lambda$) span a irreducible invariant subspace (provided the projection does not yield null vectors). By selecting different sets of ($\lambda,\ j,\ k,\ l$) , one can generate all the irreducible invariant subspaces.

The transformation matrix between the original and the new basis gives the C-GCs. A concrete example of using this procedure to reduce $D^{3\times3}(S_3)$ is given as an exercise [cf. Problem 4.2].

4.3 Irreducible Operators (IOs) & the Wigner-Eckart Theorem

- Definition 4.3: (IOs)

A set of operators $\left\{ O^{\mu}{}_{i}\,,\ i = 1, \ldots, n_{\mu} \right\}$ on V transforming under G as:

(4.3-1) $$U(g)\, O^{\mu}{}_{i}\, U(g)^{-1} = O^{\mu}{}_{j}\, D^{\mu}(g)^{j}{}_{i}$$

where $g \in G$, and $D^{\mu}(G)$ is a matrix IR of G, is said to be a set of irreducible operators (IOs) corresponding to the μ-rep. They are sometimes also referred to as irreducible tensors.

✸

Given IOs $\{ O^{\mu}{}_{i} \}$ and IB $\{ \hat{e}^{\nu}{}_{j} \}$, how does the set of vectors $O^{\mu}{}_{i} \left| e^{\nu}{}_{j} \right\rangle$ behave under group transformations? We have,

(4.3-2) $$\begin{aligned} U(g)\, O^{\mu}{}_{i} \left| e^{\nu}{}_{j} \right\rangle &= U(g)\, O^{\mu}{}_{i}\, U(g)^{-1}\, U(g) \left| e^{\nu}{}_{j} \right\rangle \\ &= O^{\mu}{}_{k}\, D^{\mu}(g)^{k}{}_{i}\, U(g) \left| e^{\nu}{}_{j} \right\rangle \\ &= O^{\mu}{}_{k} \left| e^{\nu}{}_{l} \right\rangle D^{\mu}(g)^{k}{}_{i}\, D^{\nu}(g)^{l}{}_{j} \end{aligned}$$

i.e. these states transform according to the direct product rep $D^{\mu\times\nu}$.

Thus $O^{\mu}{}_{i} \left| \begin{smallmatrix} \nu \\ j \end{smallmatrix} \right\rangle$ transforms like $\left| \begin{smallmatrix} \mu\,\nu \\ i\,j \end{smallmatrix} \right\rangle$.

However, for a given $i,\ j$, it should formally be a vector (not the direct product of 2 vectors). Hence, we write

(4.3-3) $$O^{\mu}{}_{i} \left| \begin{matrix} \nu \\ j \end{matrix} \right\rangle = c \left| \begin{matrix} \lambda \\ \alpha\, l \end{matrix} \right\rangle \left\langle \begin{matrix} \alpha\, l \\ \lambda \end{matrix} \,\middle|\, \begin{matrix} \mu\,\nu \\ i\,j \end{matrix} \right\rangle$$

where c is a constant that depends on O, μ, ν but not on $i,\ j$.

We can now evaluate the matrix element $\left\langle \begin{matrix} l \\ \lambda \end{matrix} \middle| O^{\mu}{}_{i} \middle| \begin{matrix} \nu \\ j \end{matrix} \right\rangle$ making use of Theorem 4.1 and arrive at the far-reaching result:

- Theorem 4.5 (Wigner-Eckart):

Let $\{ O^{\mu}{}_{i} \}$ be a set of IOs then

(4.3-4) $$\left\langle \begin{matrix} l \\ \lambda \end{matrix} \middle| O^{\mu}{}_{i} \middle| \begin{matrix} \nu \\ j \end{matrix} \right\rangle = \sum_{\alpha} \left\langle \begin{matrix} \alpha\, l \\ \bar{\lambda} \end{matrix} \,\middle|\, \begin{matrix} \mu\,\nu \\ i\,j \end{matrix} \right\rangle \langle\, \lambda \,|\, O^{\mu} \,|\, \nu \,\rangle_{\alpha}$$

where

$$\langle\, \lambda \,|\, O^{\mu} \,|\, \nu \,\rangle_{\alpha} \equiv \frac{1}{n_{\lambda}} \left\langle \begin{matrix} k \\ \bar{\lambda} \end{matrix} \,\middle|\, \begin{matrix} \lambda \\ \alpha\, k \end{matrix} \right\rangle$$

is called the reduced matrix element.

- **Proof:**

Assuming unitary reps,

$$\begin{aligned} \left\langle \begin{matrix} l \\ \lambda \end{matrix} \middle| O^{\mu}{}_{i} \middle| \begin{matrix} \nu \\ j \end{matrix} \right\rangle &= \left\langle \begin{matrix} l \\ \lambda \end{matrix} \middle| U^{-1}(g)\, U(g)\, O^{\mu}{}_{i}\, U^{-1}(g)\, U(g) \middle| \begin{matrix} \nu \\ j \end{matrix} \right\rangle \\ &= \left\langle \begin{matrix} l' \\ \lambda \end{matrix} \middle| O^{\mu}{}_{i'} \middle| \begin{matrix} \nu \\ j' \end{matrix} \right\rangle D_{\lambda}{}^{\dagger}(g)^{l}{}_{l'}\, D^{\mu}(g)^{i'}{}_{i}\, D^{\nu}(g)^{j'}{}_{j} \\ &= \left\langle \begin{matrix} l' \\ \lambda \end{matrix} \middle| O^{\mu}{}_{i'} \middle| \begin{matrix} \nu \\ j' \end{matrix} \right\rangle D_{\lambda}{}^{\dagger}(g)^{l}{}_{l'} \left\langle \begin{matrix} i'\, j' \\ \bar{\mu}\ \bar{\nu} \end{matrix} \,\middle|\, \begin{matrix} \sigma \\ \alpha\, k' \end{matrix} \right\rangle D^{\sigma}(g)^{k'}{}_{k} \left\langle \begin{matrix} \alpha\, k \\ \sigma \end{matrix} \,\middle|\, \begin{matrix} \mu\,\nu \\ i\,j \end{matrix} \right\rangle \qquad [3.8\text{-}9] \end{aligned}$$

Since this relation is independent of g, we have

$$\left\langle \begin{matrix} l \\ \lambda \end{matrix} \middle| O^\mu{}_i \middle| \begin{matrix} \nu \\ j \end{matrix} \right\rangle = \frac{1}{n_G} \sum_g \left\langle \begin{matrix} l' \\ \lambda \end{matrix} \middle| O^\mu{}_{i'} \middle| \begin{matrix} \nu \\ j' \end{matrix} \right\rangle D_\lambda{}^\dagger(g)^l{}_{l'} \left\langle \begin{matrix} i'\ j' \\ \bar{\mu}\ \bar{\nu} \end{matrix} \middle| \begin{matrix} \sigma \\ \alpha\, k' \end{matrix} \right\rangle D^\sigma(g)^{k'}{}_k \left\langle \begin{matrix} \alpha\, k \\ \sigma \end{matrix} \middle| \begin{matrix} \mu\, \nu \\ i\ j \end{matrix} \right\rangle$$

$$= \frac{1}{n_\sigma} \left\langle \begin{matrix} l' \\ \lambda \end{matrix} \middle| O^\mu{}_{i'} \middle| \begin{matrix} \nu \\ j' \end{matrix} \right\rangle \left\langle \begin{matrix} i'\ j' \\ \bar{\mu}\ \bar{\nu} \end{matrix} \middle| \begin{matrix} \sigma \\ \alpha\, k' \end{matrix} \right\rangle \left\langle \begin{matrix} \alpha\, k \\ \sigma \end{matrix} \middle| \begin{matrix} \mu\, \nu \\ i\ j \end{matrix} \right\rangle \delta^\sigma_\lambda\, \delta^l_k\, \delta^{l'}_{k'}$$

$$= \frac{1}{n_\lambda} \left\langle \begin{matrix} l' \\ \lambda \end{matrix} \middle| O^\mu{}_{i'} \middle| \begin{matrix} \nu \\ j' \end{matrix} \right\rangle \left\langle \begin{matrix} i'\ j' \\ \bar{\mu}\ \bar{\nu} \end{matrix} \middle| \begin{matrix} \bar{\lambda} \\ \alpha\, l' \end{matrix} \right\rangle \left\langle \begin{matrix} \alpha\, l \\ \lambda \end{matrix} \middle| \begin{matrix} \mu\, \nu \\ i\ j \end{matrix} \right\rangle$$

$$= \sum_\alpha \left\langle \begin{matrix} \alpha\, l \\ \lambda \end{matrix} \middle| \begin{matrix} \mu\, \nu \\ i\ j \end{matrix} \right\rangle \langle\, \lambda \,|\, O^\mu \,|\, \nu \,\rangle_\alpha$$

where

$$\langle\, \lambda \,|\, O^\mu \,|\, \nu \,\rangle_\alpha = \frac{1}{n_\lambda} \left\langle \begin{matrix} l' \\ \lambda \end{matrix} \middle| O^\mu{}_{i'} \middle| \begin{matrix} \nu \\ j' \end{matrix} \right\rangle \left\langle \begin{matrix} i'\ j' \\ \bar{\mu}\ \bar{\nu} \end{matrix} \middle| \begin{matrix} \bar{\lambda} \\ \alpha\, l' \end{matrix} \right\rangle$$

$$= c\, \frac{1}{n_\lambda} \left\langle \begin{matrix} l' \\ \lambda \end{matrix} \middle| \begin{matrix} \mu\, \nu \\ i'\ j' \end{matrix} \right\rangle \left\langle \begin{matrix} i'\ j' \\ \bar{\mu}\ \bar{\nu} \end{matrix} \middle| \begin{matrix} \bar{\lambda} \\ \alpha\, l' \end{matrix} \right\rangle$$

$$= c\, \frac{1}{n_\lambda} \left\langle \begin{matrix} l' \\ \lambda \end{matrix} \middle| \begin{matrix} \bar{\lambda} \\ \alpha\, l' \end{matrix} \right\rangle$$

Setting $c = 1$ completes the proof.

■ ✸

Thus the multitude of $\left\langle \begin{matrix} l \\ \lambda \end{matrix} \middle| O^\mu{}_i \middle| \begin{matrix} \nu \\ j \end{matrix} \right\rangle$ are all determined by a few $\langle\, \lambda \,|\, O^\mu \,|\, \nu \,\rangle_\alpha$.

All the i-, j-, and l- dependence are contained in the C-GCs $\left\langle \begin{matrix} \alpha\, l \\ \lambda \end{matrix} \middle| \begin{matrix} \mu\, \nu \\ i\ j \end{matrix} \right\rangle$, which are specified by group representation theory, hence can be looked up in published tables.
The specific properties of the states and the operator enter only thru $\langle\, \lambda \,|\, O^\mu \,|\, \nu \,\rangle_\alpha$.

In many important application such as 3-D rotational symmetry, each IR (λ) only occurs once in the reduction of the direct product ($\mu \times \nu$); then $\alpha = 1$ and there only one $\langle\, \lambda \,|\, O^\mu \,|\, \nu \,\rangle_\alpha$ for each (μ, ν, λ).
Under normal circumstances, the regularities exhibited by the Wigner- Eckart theorem exhaust all the structure of the relevant matrix elements required by invariance under the symmetry group.

To illustrate the usefulness of the Wigner- Eckart theorem, we sketch its application to electromagnetic transitions in atoms (visible light, x-ray) and nuclei (γ-ray). Since the electromagnetic interaction is invariant under 3-D rotation, the symmetry group is the rotation group R_3 [see Chapters 7 and 8 for details]. The electromagnetic transitions involve the emission of a "photon"(angular momentum (s, λ) while the atomic nuclear system jumps from an initial state of angular momentum $|\, j, m\, \rangle$ to a final state of angular momentum $|\, j', m' \rangle$. In each case, the first "quantum number" s (or j, or j') corresponds to the magnitude of angular momentum, the second λ (or m, or m') to its component along an arbitrary chosen "quantization axis", and λ takes on $2s + 1$ values: $-s, -s + 1, \ldots, s$ (similarly for m and m'). The energy levels for the initial and final states, and the a priori possible transitions are depicted in Fig. 4.1 for the case of $i = j' = 1$, and we shall assume $s = 1$ as well.

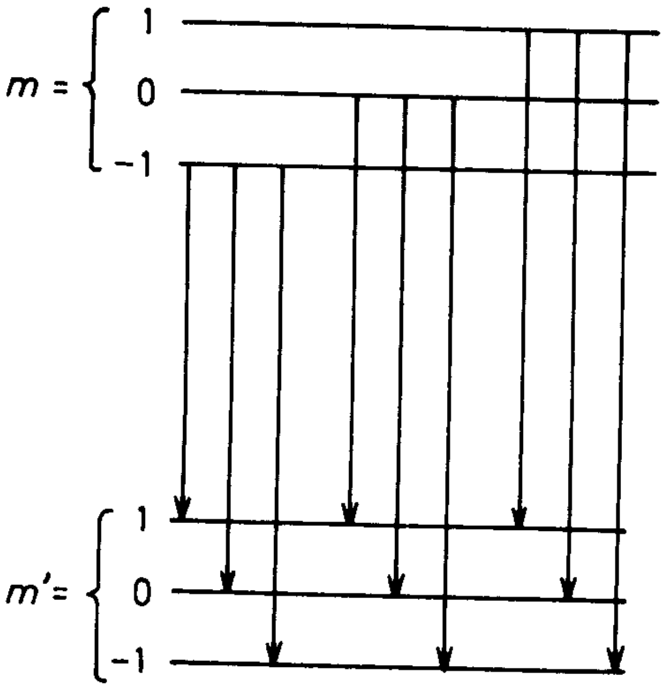

Fig. 4.1 Possible transitions without symmetry consideration.

The probability (intensity) for each transition is, according to quantum mechanics [Messiah, Schiff], proportional to $|\, f\, |^2$ where $f = \left\langle \begin{array}{c} j' \\ m' \end{array} \right| O^s{}_\lambda \left| \begin{array}{c} j \\ m \end{array} \right\rangle$ and $O^s{}_\lambda$, is the "multipole transition operator" [cf. Sec. 8.7] for the process. This permits the use of the Wigner- Eckart theorem which implies $f = f_0 \left\langle \begin{array}{c} m' \\ j' \end{array} \right| \left. \begin{array}{c} s\ j \\ \lambda\ m \end{array} \right\rangle$, where f_0 is the "reduced matrix element", and $\left\langle \begin{array}{c} m' \\ j' \end{array} \right| \left. \begin{array}{c} s\ j \\ \lambda\ m \end{array} \right\rangle$ is the relevant C-GC. [α in Theorem 4.5 is identical to 1 for the group R_3 .] As a consequence, all 9 potential transitions are determined by one constant f_0. The C-GCs $\left\langle \begin{array}{c} m' \\ 1 \end{array} \right| \left. \begin{array}{c} 1\ 1 \\ \lambda\ m \end{array} \right\rangle$ vanish unless $m' = \lambda + m$, and the non- zero elements are given in Table 4.1. From this information we can predict that, unless there are other reasons forbidding the transition, there should be 7 distinct transitions. These are depicted in Fig. 4.2 with their relative intensities (also called "branching ratios") labelling the lines. [In reality, there is also space inversion symmetry (parity conservation), which forbids about half of the transitions shown in Fig. 4.2. We shall reconsider this example in Chap. 11.]

$m'\backslash m$	-1	0	1
-1	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{3}}$	0
0	$-\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{3}}$	$\sqrt{\frac{1}{2}}$
1	0	$\sqrt{\frac{1}{3}}$	$-\sqrt{\frac{1}{2}}$

Table 4.1 C-GCs $\left\langle \begin{array}{c} m' \\ 1 \end{array} \right| \left. \begin{array}{cc} 1 & 1 \\ m' - m & m \end{array} \right\rangle$

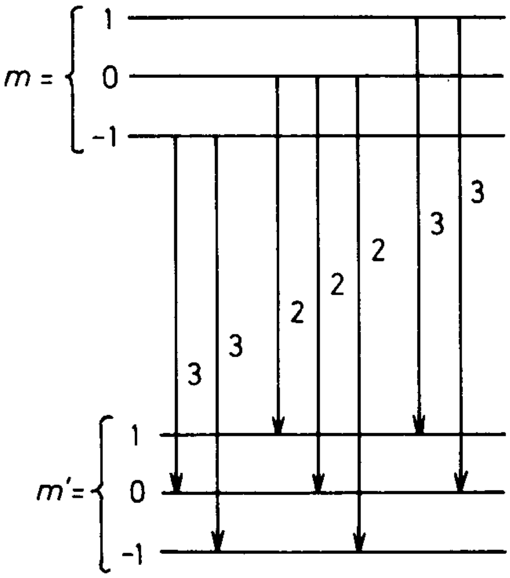

Fig. 4.2 Allowed transitions and branching ratios.

Supplementary

In non-relativistic quantum mechanics, every state of a system is assumed to be a vector $|\psi\rangle$ of a Hilbert space $\mathcal{H}$. Equivalently, we say that $\mathcal{H}$ is the solution space of the Schrodinger eq

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)|\psi\rangle = 0$$

where H is the hamiltonian of the system.

For a spinless particles, it is assumed that the eigenstates $\{|\boldsymbol{r}\rangle\}$ of the position operator **r** to be a basis of $\mathcal{H}$:

$$\boldsymbol{r}\,|\,\boldsymbol{r}\,\rangle = \boldsymbol{r}\,|\,\boldsymbol{r}\,\rangle \qquad (\text{ eigen-equation })$$

$$\langle\,\boldsymbol{r}\,|\,\boldsymbol{r}\,'\rangle = \delta(\boldsymbol{r} - \boldsymbol{r}\,') \qquad (\text{ orthonormality })$$

$$\int |\boldsymbol{r}\rangle\, d\boldsymbol{r}\,\langle\,\boldsymbol{r}| = 1 \qquad (\text{ completeness })$$

Note: the same symbol **r** is used to denote the position operator, its eigenvalue, and the label of its eigenstate.

Completeness of $\{|\,\mathbf{r}\,\rangle\}$ means

$$|\psi\rangle = \int |r\rangle\, d r\,\langle\, r|\,\psi\,\rangle$$

and

$$\langle\,\boldsymbol{r}|\left(i\hbar\frac{\partial}{\partial t} - H\right)|\psi\rangle = 0$$

$$= \; i\hbar\frac{\partial}{\partial t}\langle\,\boldsymbol{r}|\psi\,\rangle - \int\langle\boldsymbol{r}|\,H\,|\,\boldsymbol{r}\,'\rangle d\boldsymbol{r}\,'\langle\,\boldsymbol{r}\,'|\,\psi\,\rangle$$

Setting

$$\langle\boldsymbol{r}|\,H\,|\,\boldsymbol{r}\,'\rangle = \langle\boldsymbol{r}|\,H\,|\,\boldsymbol{r}\,\rangle\delta(\,\boldsymbol{r} - \boldsymbol{r}\,')$$

we have

$$\left\{i\hbar\frac{\partial}{\partial t} - \langle\,\boldsymbol{r}|\,H\,|\,\boldsymbol{r}\,\rangle\right\}\langle\,\boldsymbol{r}\,|\,\psi\,\rangle = \; 0$$

which is the usual wavefunction form of the Schrodinger equation if we set

$$\psi(\boldsymbol{r}, t) = \langle\,\boldsymbol{r}\,|\,\psi\,\rangle$$

In general, any set of eigenstates $\{ \mid a \rangle \}$ of an operator A can be used as a basis of $\mathcal{H}$. However, it may happen that in order to span $\mathcal{H}$, more than one vector with the same eigenvalue of A are required. A is then said to be degenerate with respect to $\mathcal{H}$.

The assumption of non-degeneracy of **r** seemed self-evident to the pioneer developers of the quantum theory but it broke down after spin was discovered.

■ CSCO

An alternative basis for $\mathcal{H}$ is the simultaneous eigenstates of a Complete Set of Commutating Operators (CSCO).

Note: These operators are assumed to be observables, ie, they are hermitian.

Note: Given a degenerate operator A , the corresponding CSCO contains all operators which commute with A as well as with each other.

The proof is as follows:

Consider a degenerate operator A & the set of its eigenstates $\{ \mid a_{i\alpha} \rangle \}$ that span $\mathcal{H}$. Thus

$$A \mid a_{i\alpha} \rangle = a_i \mid a_{i\alpha} \rangle \qquad (\alpha = 1 \ldots m_i \text{ labels the degeneracy })$$

With respect to this basis, A is diagonal:

$$A \begin{pmatrix} \vdots \\ |a_{i1}\rangle \\ \vdots \\ |a_{i m_i}\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} \ddots & & & 0 \\ & a_i & & \\ & & \ddots & \\ & & & a_i \\ 0 & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ |a_{i1}\rangle \\ \vdots \\ |a_{i m_i}\rangle \\ \vdots \end{pmatrix}$$

If B commutes with A, we have

$$A\,B\,|a_{i\alpha}\rangle = B\,A\,|a_{i\alpha}\rangle = a_i\,B\,|a_{i\alpha}\rangle$$

so that $B\,|a_{i\alpha}\rangle$ is also an eigenstate of A with the same eigenvalue, a_i, as $|a_{i\alpha}\rangle$. This means $B\,|a_{i\alpha}\rangle$ can only be a linear combination of $\{|a_{i\alpha}\rangle\}$ of fixed i. That is

$$B\,|a_{i\alpha}\rangle = \sum_\beta b_{i\beta} \left| a_{i\beta} \right\rangle$$

In other words, with respect to the basis $\{ \mid a_{i\alpha} \rangle \}$, B must be of the block diagonal form

$$B = \begin{pmatrix} \ddots & & 0 \\ & B_i & \\ 0 & & \ddots \end{pmatrix}$$

where B_i is a $m_i \times m_i$ matrix.

This means $\{ |a_{i\alpha}\rangle \}$ for a fixed i is an invariant subspace of B.

If every $|a_{i\alpha}\rangle$ for a fixed i is also an eigenvector of B, B_i will be diagonal. If not, B can be diagonalized by a similarity transformation $S\,B\,S^{-1}$. Furthermore, S can be of the same block diagonal structure as B since $\{ |a_{i\alpha}\rangle \}$ for a fixed i is an invariant subspace of B. Now, A is just the unit matrix multiplied by a_i in each of these subspaces, the similarity transformation thus leaves A unchanged. Hence, it is possible to find a set of basis such that both A & B are diagonal.

The same argument applies to all other operators in the CSCO, which means there exists a basis for which all these operators are diagoanl. Since the set also exhausts all such operators, every basis vector must have a distinct combination of eigenvalues of the members of the CSCO. Hence, the basis can be labelled uniquely in terms of the eigenvalues of the members of the CSCO.

In terms of group theory, the foregoing proof can be greatly simplified. It is easy to see that the CSCO forms an abelian group. (Note that these operators are neither symmetry operations nor unitary). Since the irreducible representations of an abelian group are all 1-dimensional, there must be a basis wrt which every member of the CSCO is diagonal.

Symmetry Operators

Yet another way to label the basis of $\mathcal{H}$ is in terms of the symmetry operations that leaves H invariant. Let G be the symmetry group, then every member of G commutes with H but not necessarily so among themselves.

To understand what this means, we need to know the condition required for 2 matrices to commute with each other. The simplest case is for 2×2 matrices:
Let

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad N = \begin{pmatrix} e & f \\ g & h \end{pmatrix}$$

then

$$M N = \begin{pmatrix} a e + b g & a f + b h \\ c e + d g & c f + d h \end{pmatrix}$$

$$N M = \begin{pmatrix} e a + f c & e b + f d \\ g a + h c & g b + h d \end{pmatrix}$$

Thus, $M N = N M$ requires

$$b g = f c \qquad a f + b h = e b + f d$$
$$c e + d g = g a + h c \qquad c f = g b$$

or

$$b g = f c \qquad (a - d) f = (e - h) b$$
$$c (e - h) = g (a - d)$$

For $a \neq d$ and $b \neq 0$, $c \neq 0$, we have

$$\frac{e - h}{a - d} = \frac{g}{c} = \frac{f}{b}$$

If M is diagonal ($b = c = 0$), then
i) if $a = d$, then $M N = N M$ for all N.
ii) if $a \neq d$, then $M N = N M$ only if N is also diagonal ($f = g = 0$)

Problems

4.1 Let $G = T^d$ be the discrete translational symmetry group, V be the vector space of one particle on the one- dimensional lattice of Chap. 1, and P_k be the projection operator to the irreducible representation described in this chapter. If $| x \rangle = | n b + y \rangle$, $n =$ integer and $-b/2 < y \leq b/2$, prove that $P_k | x \rangle = P_k | y \rangle e^{-i k n b}$ that $P_k | x \rangle e^{i k x} = P_k | y \rangle e^{i k y}$. Compare with Eq. (1.3-6).

4.2 Let $G = S_3$ and $V = V_2 \times V_2$ where V_2 is the two- dimensional vector space of Problem 3.1. Starting with basis vectors $\hat{e}_x \hat{e}_x$, $\hat{e}_x \hat{e}_y$, $\hat{e}_y \hat{e}_x$ and $\hat{e}_y \hat{e}_y$, construct four new basis vectors which transform irreducibly under S_3. Use the projection operator technique.

4.3 Prove that the operators $P^i{}_{\mu j}$ have the following property: ${P^j{}_{\mu i}}^\dagger = P^i{}_{\mu j}$.

4.4 Prove that:
(i) ${P^j{}_{\mu i}}^\dagger P^j{}_{\mu i} = P_{\mu i}$
(ii) $P_{\mu i} P^l{}_{\sigma k} P_{\nu j} = \delta_{\mu\sigma} \delta_{\sigma\nu} \delta^i{}_j \delta_{i k} P^l{}_{\sigma k}$

Use (ii) to interpret $P^l{}_{\sigma k}$ as the "transfer operator" from vectors of type $| \sigma l \rangle$ to the type $| \sigma k \rangle$.

4.5 Suppressing the irreducible label μ and matrix indices (i, j), Definition 4.3 for irreducible operators can be written as

$$U(g) O U(g)^{-1} = O D(g)$$

where $\{ D(g) ;\ g \in G \}$ form a representation of the group G. Consider replacing the right- hand side of this equation by the following alternatives, in turn:

(i)	$O\, D(g)^*$	**(ii)**	$O\, D(g^{-1})$	**(iii)**	$O\, D(g)^\dagger$
(iv)	$D(g)^T\, O$	**(v)**	$D(g^{-1})\, O$	**(vi)**	$D(g)^\dagger\, O$

where the order of appearance of the two factors is important because of the implied matrix multiplication. In which of the six cases do we get true representations of the group G on the space of the linear operators $\{ O^\mu{}_i \}$; thereby obtain viable alternatives to the original definition? Among the original definition and the alternatives, which ones are equivalent to each other if (a) $D(G)$ is unitary, (b) $D(G)$ is equivalent to $D(g)^*$, (c) $D(G)$ is both unitary and equivalent to $D(g)^*$?