

Matrix representations form an irreducible or reducible group representation.

Let $\{\Phi_s\} \equiv$ set of n-degenerate eigenfunctions of **H** corresponding to a particular eigenvalue E

$$\Rightarrow \hat{H}\phi_s = E\phi_s \quad s = 1,...,n$$

$$\because [\hat{T}, \hat{H}] = 0 \Rightarrow \hat{H}\hat{T}\phi_s = \hat{T}\hat{H}\phi_s = \hat{T}E\phi_s = E\hat{T}\phi_s$$

$$\Rightarrow \hat{T}\phi_s \text{ is an eigenfunction of } \mathbf{H} \text{ with the same eigenvalue E}$$

$$\hat{T}\phi_s = \text{linear combination of } \{\varphi_s\}; \text{ that is, } \hat{T}\phi_s = \sum_{i=1}^n \phi_i \Gamma(T)_{is}, s = 1,...,n$$

In matrix form: $\hat{T}\langle\phi_1,...,\phi_s,...| = \langle\phi_1',...,\phi_s',...| = \langle\phi_1,...,\phi_s,...|\Gamma(T)$
or $\hat{T}\langle\phi| = \langle\phi'| = \langle\phi|\Gamma(T) = 1.\rangle$
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Thus, $\{\phi_s\}$ can be regarded as a set of basis functions in an n-dimensional vector space called **function space**.

• can interchange "eigenfunction" and "eigenvector".

Eq. 1.) implies that every set $\{\phi_s\}$ that corresponds to eigenvalue E forms a basis for one of the IRs of the symmetry group $G = \{T\}$.

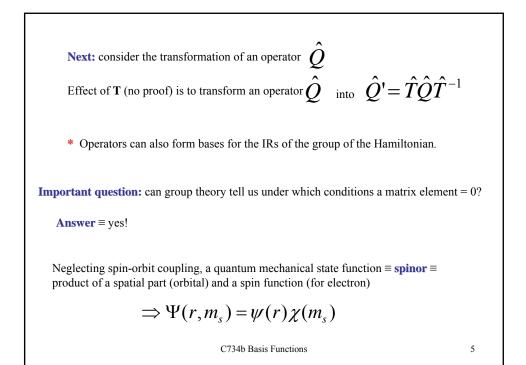
> every energy level may be labeled according to its IR in G.

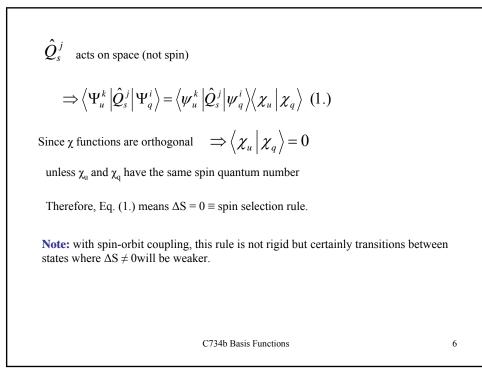
Question: How to construct basis function sets which form bases for particular IRs?

Answer: Use projection operators (later).

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Now consider what happens to
$$\langle Q \rangle$$
 under a symmetry operator T.
It's value is unchanged.

$$\therefore \langle Q \rangle = \langle \Psi_u^k | \hat{Q}_s^j | \Psi_q^i \rangle = \langle \hat{T} \Psi_u^k | \hat{T} \hat{Q}_s^j \hat{T}^{-1} | \hat{T} \Psi_q^i \rangle \quad (2.)$$
Left-hand side of Eq. (2.) is invariant and therefore belongs to the totally symmetric representation Γ^1 : A_1 or equivalent.

$$\hat{Q}_s^j | \Psi_q^i \rangle \text{ is a function that transforms according to the direct product } \Gamma^j \otimes \Gamma^i$$
The integrand in Eq. (2.) is the product of two functions: $\Psi_u^{k^*}$ and $\hat{Q}_s^j | \Psi_q^i \rangle$
It transforms as the direct product: $\Gamma^{k^*} \otimes \Gamma^j \otimes \Gamma^i$

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Question: What is the condition that
$$\Gamma^{a^*} \otimes \Gamma^b$$
 contains Γ^1 ?
Condition is:

$$a_1 = \frac{1}{h} \sum_{T} \chi_1(T) \chi^{a^*b}(T) = \frac{1}{h} \sum_{T} \chi^a(T) \chi^b(T) \neq 0$$

$$IR \quad \text{reducible}$$
This will be true if $a = b$ (orthogonality theorem for characters)

$$\Rightarrow \quad \text{Eq.} (2) = 0 \text{ unless } \Gamma^j \otimes \Gamma^i \text{ contains } \Gamma^k \text{ (by orthogonality)}$$
or $\Gamma^i \otimes \Gamma^j \otimes \Gamma^k \subset \Gamma^1$
Conclusion: a matrix element is zero unless the direct product of any two of the representations contains the third one.

