Crystal and Symmetries

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1 Introduction

Take a lattice with point group symmetry operations {G} leaving it invariant. The group elements are 3×3 unitary matrices. Unlike Bloch translation symmetry which simplifies our problem significantly, these point group symmetries can reduce computations by a factor of 3 or 24. Major significance is in getting the selection rules, as in which transitions are allowed in presence of external potentials (which can cause transition between electron states).

2 Mathematics Preliminary

What we want to study is how functions (can be wavefunctions) transform under action of the group, i.e.,

$$\psi_i(G\mathbf{r}) = \sum_j A(G)_{ij}\psi_j(\mathbf{r}). \tag{1}$$

This way we can find the matrices A(G). The set of matrices {A} is called a **representation of the group**. The matrices A and the group elements can all be taken to be unitary ($A^\dagger = A^{-1}$ and $G^\dagger = G^{-1}$).
Two representations $\{A^{(n)}\}$ and $\{A^{(m)}\}$ are **equivalent** if there exists a single matrix M such that the below holds for all elements of the group.

$$M^{-1}A^{(n)}(G)M = A^{(m)}(G) \tag{2}$$

Also, if we can decompose all matrices of our representation in some basis to Block diagonal form, then our representation is called **reducible**. To derive the main results like the great orthogonality theorem, we consider a matrix M, which is defined by a matrix X (choice of X could be arbitrary)

$$M = \sum_G A^{(m)}(G)XA^{(n)}(G^\dagger). \tag{3}$$

Then we see that

$$
\begin{aligned}
A^{(m)}(G)M &= \sum_{G'} A^{(m)}(G)A^{(m)}(G')XA^{(n)}(G'^{\dagger}) \\
&= \sum_{G'} A^{(m)}(GG')XA^{(n)}(G'^{\dagger}) \\
&= \sum_{G'} A^{(m)}(G')XA^{(n)}(G'^{\dagger}G) \quad (\text{replace } G' \to G^{\dagger}G') \\
&= \sum_{G'} A^{(m)}(G')XA^{(n)}(G'^{\dagger})A^{(n)}(G) = MA^{(n)}.
\end{aligned}
\tag{4}
$$

So, for $\{A^{(n)}\}$ and $\{A^{(m)}\}$ representations to not be equivalent; the matrix M must be non-invertible. In the same way we can take a conjugate transpose of this to get a relation for matrix $M^{\dagger}$. We define a matrix, now $P = M + M^{\dagger}$, this matrix P now also satisfies

$$A^{(m)}(G)P = PA^{(n)}(G) \tag{5}$$

where P is now a hermitian matrix (as $P^{\dagger} = P$). Since, P is Hermitian, we can now diagonalize it and find the orthonormal basis. Then we write all the matrices $\{A^{(n)}\}, \{A^{(m)}\}$ and P in this basis.

Q. How do we know if our representations are irreducible?
If even a single off diagonal term in our representation is 0, then it's reducible. We can see that by taking $n = m$ in the equation above in our diagonal basis, that implies

$$A(G)_{ij}P_{jj} = P_{ii}A(G)_{ij}, \tag{6}$$

so, either $P_{ii} = P_{jj}$ or $A(G)_{ij} = 0$. If for any ij, let's say $A(G)_{12}$ is 0, then that means no transformation can take $G\psi_1$ to ψ_2 and vice versa. Hence, the wavefunctions generated by $G\psi_1$ and $G\psi_2$ are disjoint. So, if our **representation is irreducible then all the eigenvalues of P must be same**.