Summary of lectures on translational symmetry

- wavefunction for electrons in a periodic potential has Bloch form

$$\psi_{\vec{k}}(\vec{r} + \underbrace{\vec{R}}_{\text{a lattice vector}}) = e^{i\vec{k}\cdot\vec{R}}\,\psi_{\vec{k}}(\vec{r})$$

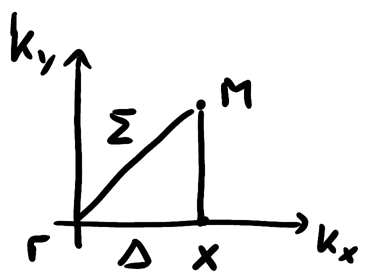
- define little group $G_{\vec{k}}$ = all symmetry operations of the point group that leave $\vec{k}$ invariant

$$R\vec{k} = \vec{k} + \underbrace{\vec{G}}_{\text{a reciprocal lattice vector}}$$

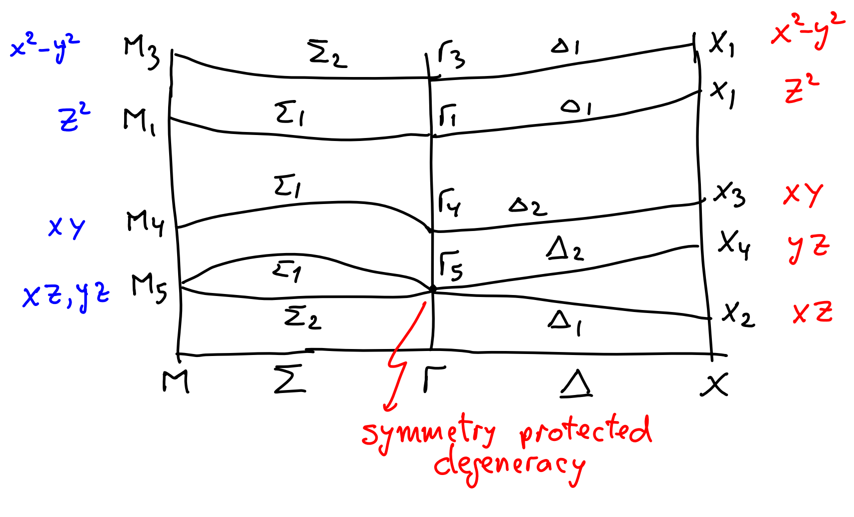
- wavefunctions transform as representation D of the lattice point group

- decompose D into i.r.r. of the little groups
  => get symmetry of eigenstates and degeneracies of bands at each $\vec{k}$

Ex: dispersion of *d*-orbitals in a square lattice



- decompose $D^{(l=2)}$ into i.r.r. of the little groups for each $\vec{k}$



Ex: Phonon dispersions

- atomic displacements $\{\vec{\boldsymbol{u}}_i\}$ form a $3n$-dimensional representation D of the symmetry point group (n atoms/unit cell)

- for each atom type: character

$$\chi(\alpha) = (1 + 2\cos\alpha) \times \text{phase factor}$$

- decompose D into i.r.r of the little groups for each $\vec{\boldsymbol{k}}$

Little Groups and Small Representations for Special Points of the Square Lattice

Consider symmetry direction in k-space $\Gamma \rightarrow \Delta \rightarrow X$

1. Γ-point, $\mathbf{k} = (0, 0)$, little group $= 4mm$

$4mm$ (C_{4v})		E	2_z	4_z [2]	m_x [2]	m_d [2]	
Γ_1	A_1	1	1	1	1	1	z, x^2+y^2, z^2
Γ_2	A_2	1	1	1	−1	−1	R_z
Γ_3	B_1	1	1	−1	1	−1	x^2-y^2
Γ_4	B_2	1	1	−1	−1	1	xy
Γ_5	E	2	−2	0	0	0	(x, y), (xz, yz), (R_x, R_y)

2. Δ-point, $\mathbf{k} = (k_x, 0)$, little group $= m$

relabel from tables
$x, y, z \rightarrow z, x, y$

m (C_{1h}/C_s)		E	$\cancel{m_z}$ m_y	
Δ_1	A'	1	1	x, $\cancel{y}$ z, x^2, y^2, z^2, $\cancel{xy}$ xz, $\cancel{R_z}$ R_y
Δ_2	A''	1	−1	$\cancel{z}$ y, yz, $\cancel{xz}$ xy, R_x, $\cancel{R_y}$ R_z

3. X-point, $\mathbf{k} = (\pi/a, 0)$, little group $= 2mm$

$2mm$ (C_{2v})		E	2_z	m_y	m_x	
X_1	A_1	1	1	1	1	z, x^2, y^2, z^2
X_3	A_2	1	1	−1	−1	xy, R_z
X_2	B_1	1	−1	1	−1	x, xz, R_y
X_4	B_2	1	−1	−1	1	y, yz, R_x