ETH
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Solid State Theory
Exercise 2

SS 08
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Point groups and their representations

Exercise 2.1 Energy bands of almost free electrons on the fcc lattice

Let us consider almost free electrons on a face-centered cubic (fcc) lattice. The goal of this exercise is to compute the lowest energy bands along the Δ-line using degenerate perturbation theory and the machinery of the *group theory*. Remember that in reciprocal space, the fcc lattice transforms into a body-centered cubic (bcc) lattice. The point group of the cubic Bravais lattices (simple cubic, fcc, bcc) is denoted by O_h (symmetry group of a cube). Its character table is given in Tab. 1.

a) We first study the Γ point ($\vec{k} = 0$). For *free* electrons ($V = 0$) the lowest energy level is non-degenerate and the second one has a eight fold degeneracy. We focus on the second level and denote the eight-dimensional representation of O_h defined on this subspace by Γ. Find the irreducible representations contained in Γ. Compute the group character χ_Γ and use the character table of O_h to show that

$$\Gamma = \Gamma_1^+ \oplus \Gamma_2^- \oplus \Gamma_4^- \oplus \Gamma_5^+ . \tag{1}$$

O_h	E $[xyz]$	$C_3(8)$ $[zxy]$	$C_4^2(3)$ $[\bar{x}\bar{y}z]$	$C_2(6)$ $[yx\bar{z}]$	$C_4(6)$ $[\bar{y}xz]$	J $[\bar{x}\bar{y}\bar{z}]$	$JC_3(8)$ $[\bar{z}\bar{x}\bar{y}]$	$JC_4^2(3)$ $[xy\bar{z}]$	$JC_2(6)$ $[\bar{y}\bar{x}z]$	$JC_4(6)$ $[z\bar{x}\bar{z}]$
$\chi_{\Gamma_1^+}$	1	1	1	1	1	1	1	1	1	1
$\chi_{\Gamma_1^-}$	1	1	1	1	1	-1	-1	-1	-1	-1
$\chi_{\Gamma_2^+}$	1	1	1	-1	-1	1	1	1	-1	-1
$\chi_{\Gamma_2^-}$	1	1	1	-1	-1	-1	-1	-1	1	1
$\chi_{\Gamma_3^+}$	2	-1	2	0	0	2	-1	2	0	0
$\chi_{\Gamma_3^-}$	2	-1	2	0	0	2	1	-2	0	0
$\chi_{\Gamma_4^+}$	3	0	-1	-1	1	3	0	-1	-1	1
$\chi_{\Gamma_4^-}$	3	0	-1	-1	1	-3	0	1	1	-1
$\chi_{\Gamma_5^+}$	3	0	-1	1	-1	3	0	-1	1	-1
$\chi_{\Gamma_5^-}$	3	0	-1	1	-1	-3	0	1	-1	1

Table 1: The character table of the cubic point group O_h.

b) A finite periodic potential will in general split the second energy level at the Γ point. Applying degenerate perturbation theory to the Bloch equation [Eq. (1.20) in the lecture notes] leads to a 8×8 matrix with off-diagonal elements $u = V_{\frac{4\pi}{a}(1,1,1)}$, $v = V_{\frac{4\pi}{a}(1,0,0)}$ and $w = V_{\frac{4\pi}{a}(1,1,0)}$ (we basically follow chapter 1.3 of the lecture notes). This matrix can be diagonalized by going into the symmetry subspaces.

Show that for the energies and the wave functions one finds

$$\begin{array}{lll}
\Gamma_1^+ : & E_0 + u + 3v + 3w & \cos\left(\frac{2\pi}{a}x\right)\cos\left(\frac{2\pi}{a}y\right)\cos\left(\frac{2\pi}{a}z\right); \\
\Gamma_2^- : & E_0 - u - 3v + 3w & \sin\left(\frac{2\pi}{a}x\right)\sin\left(\frac{2\pi}{a}y\right)\sin\left(\frac{2\pi}{a}z\right); \\
\Gamma_4^- : & E_0 - u + v - w & \left\{\sin\left(\frac{2\pi}{a}x\right)\cos\left(\frac{2\pi}{a}y\right)\cos\left(\frac{2\pi}{a}z\right), \text{cyclic}\right\}; \\
\Gamma_5^+ : & E_0 + u - v - w & \left\{\cos\left(\frac{2\pi}{a}x\right)\sin\left(\frac{2\pi}{a}y\right)\sin\left(\frac{2\pi}{a}z\right), \text{cyclic}\right\};
\end{array} \tag{2}$$

where $E_0 = \frac{\hbar^2}{2m}3(\frac{2\pi}{a})^2$.

c) How do the irreducible representations split on the Δ-line? The Δ-line is defined by the points $\vec{k} = \frac{\pi}{a}(0, 0, \delta)$, $0 \leq \delta \leq 1$. Use the character table of C_{4v}.

C_{4v}	E $[xyz]$	$C_2(1)$ $[\bar{x}\bar{y}z]$	$C_4(2)$ $[y\bar{x}z]$	$\sigma_v(2)$ $[\bar{x}yz]$	$\sigma_d(2)$ $[yxz]$
χ_{Δ_1}	1	1	1	1	1
χ_{Δ_2}	1	1	1	-1	-1
χ_{Δ_3}	1	1	-1	1	-1
χ_{Δ_4}	1	1	-1	-1	1
χ_{Δ_5}	2	-2	0	0	0

Table 2: The character table of C_{4v}.

d) Let us now consider the point $X = \frac{2\pi}{a}(0, 0, 1)$. The lowest level is two fold and the second four fold degenerate for $V = 0$. Compute the energies and the wave functions for these two levels.

e) Finally, sketch the energy bands between the Γ and the X point. For an actual numerical calculation use the values $u = -0.05$, $v = 0.05$ and $w = 0.1$ (in units of $\frac{(2\pi\hbar)^2}{2ma^2}$).

Exercise 2.2 Lifting the degeneracy of the atomic states

Determine how the energy levels of the p, d and f orbitals of an atom lift due to a crystal field with cubic symmetry. Compute the corresponding eigenstates for the d orbitals. For this, consider the homogeneous harmonic polynomials of order 2. Alternatively, have a look at the basis functions given on page 11 of the lecture notes.