# Electronic structure of solid matter

## MSc course 2019

### Problem set 1

**Exercise 1**

Consider the empty lattice bands of a simple cubic lattice along the $\Gamma X$ line in the Brillouin zone, where $\Gamma = (0,0,0)$ and $X = \frac{\pi}{a}(0,0,1)$. The bands $D, E, F$ and $G$ generated by $\mathbf{K}_D = \frac{2\pi}{a}(1,0,0)$, $\mathbf{K}_E = \frac{2\pi}{a}(0,1,0)$, $\mathbf{K}_F = \frac{2\pi}{a}(-1,0,0)$ and $\mathbf{K}_G = \frac{2\pi}{a}(0,-1,0)$, respectively, are degenerate:

$$\varepsilon_{D,E,F,G}(\mathbf{k}) = \varepsilon_0 \left(\kappa^2 + 4\right) ,$$

where $\varepsilon_0 = \frac{\hbar^2 \pi^2}{2ma^2}$ and $\mathbf{k} = \frac{\pi}{a}(0,0,\kappa)$ $(0 < \kappa < 1)$. The corresponding Bloch-states are

$$\varphi_D(\mathbf{r}) = e^{i\frac{\pi}{a}(\kappa z + 2x)}, \quad \varphi_E(\mathbf{r}) = e^{i\frac{\pi}{a}(\kappa z + 2y)}, \quad \varphi_F(\mathbf{r}) = e^{i\frac{\pi}{a}(\kappa z - 2x)}, \quad \varphi_G(\mathbf{r}) = e^{i\frac{\pi}{a}(\kappa z - 2y)} ,$$

where we dropped the normalization factor $V^{-1/2}$.

**a)** Using first order degenerate perturbation theory prove that in the presence of a weak potential these bands split into two nondegenerate and one twofold degenerate bands! What are the corresponding eigenstates!

**b)** Prove the above statement by using the decomposition of the four-dimensional reducible representation (basis) into irrreducible representation of the $C_{4v}$ point group (the little group of the $\mathbf{k}$ points)! Compare the symmetry of the eigenstates to those obtained from part a) !

**Exercise 2**

Consider now the empty lattice bands along the $\Gamma R$ line, where $R = \frac{\pi}{a}(1,1,1)$. Here the bands $B, F$ and $G$ generated by $\mathbf{K}_B = \frac{2\pi}{a}(0,0,-1)$, $\mathbf{K}_F = \frac{2\pi}{a}(-1,0,0)$ and $\mathbf{K}_G = \frac{2\pi}{a}(0,-1,0)$ are degenerate:

$$\varepsilon_{B,F,G}(\mathbf{k}) = \varepsilon_0 \left(2\kappa^2 + (2-\kappa)^2\right) ,$$

where $\mathbf{k} = \frac{\pi}{a}(\kappa,\kappa,\kappa)$ $(0 < \kappa < 1)$. Neglecting normalization, the corresponding Bloch-states are

$$\varphi_B(\mathbf{r}) = e^{i\frac{\pi}{a}(\kappa x + \kappa y + (\kappa-2)z)}, \quad \varphi_F(\mathbf{r}) = e^{i\frac{\pi}{a}((\kappa-2)x + \kappa y + \kappa z)}, \quad \varphi_G(\mathbf{r}) = e^{i\frac{\pi}{a}(\kappa x + (\kappa-2)y + \kappa z)} .$$

**a)** Using first order degenerate perturbation theory derive how these bands are lifted in the presence of a weak potential!

**b)** Obtain the above result by using group theory! (The little group of the $\mathbf{k}$ points is $C_{3v}$. It is worth to use a coordinate transformation that brings the (111) axis into the $z$ direction!)

**Exercise 3**

The empty lattice bands generated by the reciprocal vectors $\mathbf{K}_A = \frac{2\pi}{a}(0,0,0)$, $\mathbf{K}_F = \frac{2\pi}{a}(-1,0,0)$, $\mathbf{K}_G = \frac{2\pi}{a}(0,-1,0)$ and $\mathbf{K}_H = \frac{2\pi}{a}(-1,-1,0)$ are degenerate at the $M = \frac{\pi}{a}(1,1,0)$ point of the Brillouin zone of a simple cubic lattice:

$$\varepsilon_{A,F,G,H}(M) = 2\varepsilon_0 \,.$$

Determine the lifting of these energy bands at the $M$ point by using both methods as above!

**Exercise 4**

**a)** Prove that for $\psi \in \mathcal{L}^2(\mathbb{R}^3)$ (*spinless case*)

$$\langle C\psi | \mathbf{L}\psi \rangle = 0$$

and

$$\langle C\psi | \mathbf{L}C\psi \rangle = -\langle \psi | \mathbf{L}\psi \rangle \,,$$

where $\mathbf{L}$ is the angular momentum vector operator and $C$ means complex conjugation!

**b)** Let $\psi_\alpha \in \mathcal{L}^2(\mathbb{R}^3)$ $(\alpha = 1, \ldots, n)$ be degenerate eigenfunctions of a time-reversal invariant Hamilton operator $H$, $CHC = H$. Prove that the expectation value of $\mathbf{L}$ vanishes on this subspace,

$$\sum_{\alpha=1}^{n} \langle \psi_\alpha | \mathbf{L}\psi_\alpha \rangle = 0 \,.$$

**Exercise 5**

Let us denote the two degenerate (orthonormal) Bloch-functions of a crystal with both time- and space-inversion symmetry by $\psi_{\mathbf{k}}^{(\mu)}$ $(\mu = 1, 2)$. Let us construct the orthonormal linear combinations,

$$\psi_{\mathbf{k}}^{(+)} = c_1 \psi_{\mathbf{k}}^{(1)} + c_2 \psi_{\mathbf{k}}^{(2)}$$
$$\psi_{\mathbf{k}}^{(-)} = -c_2^* \psi_{\mathbf{k}}^{(1)} + c_1^* \psi_{\mathbf{k}}^{(2)}$$

$c_1, c_2 \in \mathbb{C}$, $|c_1|^2 + |c_2|^2 = 1$, such that

$$\left\langle \psi_{\mathbf{k}}^{(+/-)} \right| \sigma_x \left| \psi_{\mathbf{k}}^{(+/-)} \right\rangle = \left\langle \psi_{\mathbf{k}}^{(+/-)} \right| \sigma_y \left| \psi_{\mathbf{k}}^{(+/-)} \right\rangle = 0 \,.$$

Give the expressions for $c_1$ and $c_2$ and show that

$$P_{\mathbf{k}} = \left\langle \psi_{\mathbf{k}}^{(+)} \right| \sigma_z \left| \psi_{\mathbf{k}}^{(+)} \right\rangle = -\left\langle \psi_{\mathbf{k}}^{(-)} \right| \sigma_z \left| \psi_{\mathbf{k}}^{(-)} \right\rangle \,!$$
$$(0 \le P_{\mathbf{k}} \le 1)$$

**Exercise 6**

Consider a one-dimensional lattice with two atoms $(A, B)$ per unit cell and lattice constant, $a$. The simplest two-band model of this system is described by the following tight-binding Hamiltonian,

$$H_{ij}^{\alpha\beta} = \varepsilon_\alpha \delta_{\alpha\beta}\delta_{ij} + \gamma_1 (1 - \delta_{\alpha\beta})\,\delta_{ij} + \gamma_2 \left(\delta_{\alpha A}\delta_{\beta B}\delta_{i,j+1} + \delta_{\alpha B}\delta_{\beta A}\delta_{i+1,j}\right)$$

where $i$ and $j$ denote lattice vectors (cells), $\alpha, \beta = A$ or $B$ label atoms within a cell, $\varepsilon_\alpha$ are on-site energies, while $\gamma_1$ and $\gamma_2$ are the intracell and intercell hopping parameters, respectively. For simplicity, let's take $\varepsilon_A = \varepsilon_B = 0$. Determine the dispersion relation of this model and give the condition for a gap in the spectrum!

Hint: The eigenvalue equation of the Hamiltonian

$$\sum_{\beta j} H_{ij}^{\alpha\beta}\varphi_{\beta j} = \varepsilon\varphi_{\alpha i}$$

can be written as

$$\begin{aligned} \varepsilon\varphi_{Ai} - \gamma_1\varphi_{Bi} - \gamma_2\varphi_{B,i-1} &= 0 \\ \varepsilon\varphi_{Bi} - \gamma_1\varphi_{Ai} - \gamma_2\varphi_{A,i+1} &= 0 \end{aligned}$$

for $i \in \mathbb{Z}$. Use the Bloch-theorem for the eigenvectors $\varphi_{\alpha i}$!

**Exercise 7**

Let's consider a semi-infinite chain in the above model,

$$\begin{aligned} \varepsilon\varphi_{Ai} - \gamma_1\varphi_{Bi} - \gamma_2\varphi_{B,i-1} &= 0 \\ \varepsilon\varphi_{Bi} - \gamma_1\varphi_{Ai} - \gamma_2\varphi_{A,i+1} &= 0 \end{aligned}$$

for $i < 0$ and

$$\begin{aligned} \varepsilon\varphi_{A0} - \gamma_1\varphi_{B0} - \gamma_2\varphi_{B,-1} &= 0 \\ \varepsilon\varphi_{B0} - \gamma_1\varphi_{A0} &= 0 \end{aligned}$$

Derive the condition for which a localized surface state, $\varphi_{\alpha,i-1} = e^{-ika-\mu a}\varphi_{\alpha,i}$ $(\mu > 0)$, exists! Note that the energy of this state lies in the gap as above.

**Exercise 8**

Consider the general expression of the Bychkov-Rashba Hamiltonian of surface states around a high-symmetry point $\mathbf{Q}$ of the surface Brillouin zone of a non-magnetic metal up to third order in $k$,

$$\begin{aligned} H_{\mathrm{BR}}(\mathbf{k}) = \varepsilon_0 &+ \sum_{n+m=2} b_{nm}\, k_x^n k_y^m \\ &+ \sum_{n+m=1,3} \left(c_{nm}\, k_x^n k_y^m\, \sigma_x + d_{nm}\, k_x^n k_y^m\, \sigma_y + e_{nm}\, k_x^n k_y^m\, \sigma_y\right) . \end{aligned}$$

Which of the parameters must vanish for **a)** $C_{2v}$ **b)** $C_{3v}$ and **c)** $C_{4v}$ point-group symmetry (little group of $\mathbf{Q}$)?