1. Consider the second free-electron band of a simple cubic lattice along the ΓL line in the Brilloiun zone, i.e., for $\mathbf{k} = \frac{\pi}{a}\xi\,(1,1,1) \quad \xi \in (0,1)$. This three-fold degenerate band is related to the translation vectors of the reciprocal lattice, $\mathbf{K}_1 = \frac{2\pi}{a}\,(-1,0,0)$, $\mathbf{K}_2 = \frac{2\pi}{a}\,(0,-1,0)$, and $\mathbf{K}_3 = \frac{2\pi}{a}\,(0,0,-1)$. How will be the degeneracy lifted in the presence of a crystal potential? Describe the symmetry of the corresponding Bloch-functions!

2. Prove that the time-inversion can be represented by $T = e^{i\theta}\sigma_y C$, where $\theta \in \mathbb{R}$ and C stands for the complex conjugation.

3. 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,

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

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

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

$$\left\langle \psi_{\mathbf{k}}^{(+/-)} \left|\sigma_x\right| \psi_{\mathbf{k}}^{(+/-)} \right\rangle = \left\langle \psi_{\mathbf{k}}^{(+/-)} \left|\sigma_y\right| \psi_{\mathbf{k}}^{(+/-)} \right\rangle = 0\ . \tag{3}$$

Give the expressions for c_1 and c_2 and show that

$$\left\langle \psi_{\mathbf{k}}^{(+/-)} \left|\sigma_z\right| \psi_{\mathbf{k}}^{(+/-)} \right\rangle = \pm P_{\mathbf{k}} \tag{4}$$

$$0 \le P_{\mathbf{k}} \le 1 \tag{5}$$

4. 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,

$$H_{ij}^{\alpha\beta} = \varepsilon_\alpha \delta_{\alpha\beta}\delta_{ij} + t_1\,(1-\delta_{\alpha\beta})\,\delta_{ij} + t_2\,(\delta_{\alpha A}\delta_{\beta B}\delta_{i,j+1} + \delta_{\alpha B}\delta_{\beta A}\delta_{i+1,j}) \tag{6}$$

where i and j denote lattice vectors (cells), $\alpha, \beta = A$ or B label atoms within a cell, ε_α are on-site energies, while t_1 and t_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

$$\sum_{\beta j} H_{ij}^{\alpha\beta}\varphi_{\beta j} = \varepsilon\varphi_{\alpha i} \tag{7}$$

can be written as

$$\varepsilon\varphi_{Ai} - t_1\varphi_{Bi} - t_2\varphi_{B,i-1} = 0 \tag{8}$$

$$\varepsilon\varphi_{Bi} - t_1\varphi_{Ai} - t_2\varphi_{A,i+1} = 0 \tag{9}$$

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

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

$$\varepsilon\varphi_{Ai} - t_1\varphi_{Bi} - t_2\varphi_{B,i-1} = 0 \tag{10}$$
$$\varepsilon\varphi_{Bi} - t_1\varphi_{Ai} - t_2\varphi_{A,i+1} = 0 \tag{11}$$

for $i < 0$ and

$$\varepsilon\varphi_{A0} - t_1\varphi_{B0} - t_2\varphi_{B,-1} = 0 \tag{12}$$
$$\varepsilon\varphi_{B0} - t_1\varphi_{A0} = 0 \tag{13}$$

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

6. Let H^0 denote the non-relativistic Hamilton operator of a non-spinpolarized system that has a twofold degenerate band with the dispersion relation, $\varepsilon_0(\mathbf{k})$. (We know that $\varepsilon_0(\mathbf{k})$ is an even function of $\mathbf{k}$.) Treating the spin-orbit coupling,

$$H_{SO} = \frac{\hbar}{4m^2c^2}(\nabla V \times \mathbf{p})\,\boldsymbol{\sigma}\,, \tag{14}$$

within first-order perturbation theory, the matrix of perturbation can be written as

$$H_{SO}(\mathbf{k}) = \boldsymbol{\alpha}(\mathbf{k})\,\boldsymbol{\sigma}\,. \tag{15}$$

Give the expression of $\boldsymbol{\alpha}(\mathbf{k})$ and prove that it is an odd function of $\mathbf{k}$!

7. Up to first order in $\mathbf{k}$, a general expression of the Rashba Hamiltonian of a non-magnetic surface is given by

$$H_R(\mathbf{k}) = \sum_{i,j=x,y} \alpha_{ij}k_i\sigma_j\,. \tag{16}$$

Which of the parameters α_{ij} must vanish in case of C_{2v} point-group symmetry? Solve the eigenvalue problem,

$$\left[\varepsilon_0 + \frac{\hbar^2 {k_x}^2}{2m_x^*} + \frac{\hbar^2 {k_y}^2}{2m_y^*} + H_R(\mathbf{k})\right]\psi_{\mathbf{k}} = \varepsilon_{\mathbf{k}}\psi_{\mathbf{k}}\,, \tag{17}$$

and calculate the spin-polarization, $\mathbf{P}_{\mathbf{k}} = \langle\psi_{\mathbf{k}}|\,\boldsymbol{\sigma}\,|\psi_{\mathbf{k}}\rangle$!