Problem 10: Spin-orbit coupling (4 points)

Consider a quadratic lattice in the x-y-plane with one atom per unit cell and lattice constant a. Use the empirical tight-binding method to calculate the band structure. Employ s, p_x and p_y orbitals for spin-up and spin-down electrons. Take interactions between nearest neighbors into account and use the spin-orbit coupling within the on-site approximation. For simplicity, set

$$V_1 = -V_{ss} = +V_{pp\sigma} = +V_{pp\pi} \quad \text{and} \quad V_2 = V_{sp} \; .$$

Use the abbreviation

$$f(\vec{k}) = 2\,V_1 \left(\cos(k_x\,a) + \cos(k_y\,a)\right) \; .$$

a) Set up the (6×6) Hamilton matrix

$$\bar{\bar{H}}(\vec{k}) = \begin{pmatrix} H^{\uparrow\uparrow} & H^{\uparrow\downarrow} \\ H^{\downarrow\uparrow} & H^{\downarrow\downarrow} \end{pmatrix} \; .$$

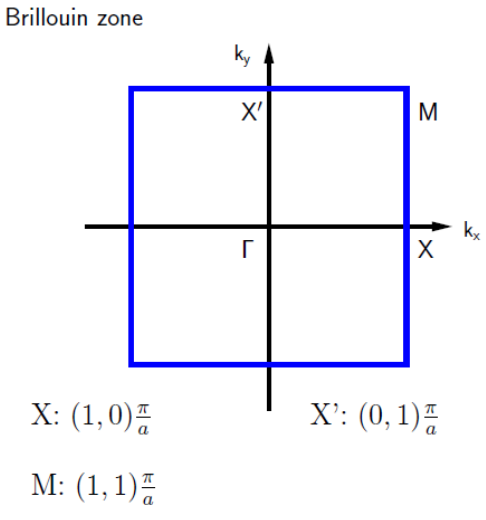
b) Calculate the eigenvalues and eigenvectors of $H^{\uparrow\uparrow}$ at the Γ point.

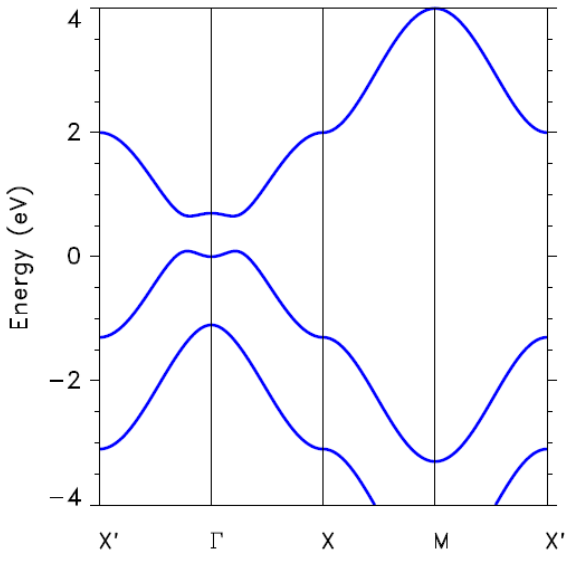
c) Calculate the band structure $E_{n\,\vec{k}}$ for the special case $V_2 = 0$. Plot the bands along $X' - \Gamma - X - M - X'$ for

i) $E_s = 2.0$ eV, $E_p = -2.2$ eV, $V_1 = 0.5$ eV, $V_2 = 0.0$ eV and $\lambda = 0.0$ eV

ii) $E_s = 2.0$ eV, $E_p = -2.2$ eV, $V_1 = 0.5$ eV, $V_2 = 0.0$ eV and $\lambda = 0.9$ eV

d) The figure below shows the band structure for the parameters of c) ii), but with $V = 0.4$ eV. There is a gap at Γ between 0.0 and 0.7 eV. Use your results from b) to compare the corresponding eigenvectors *of the energetically highest state* with those from c) i) at Γ.





Problem 11: Rashba effect in a two-dimensional electron gas (4 points)

An electron is moving in the x-y plane at $z = 0$ under the influence of spin-orbit coupling. The movement in the z direction is confined due to a potential $V(z)$. Therefore, the kinetic enery with respect to the z direction is neglected in the following. The Hamilton operator of the system has the form

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2\,m} + \frac{\hbar}{4\,m^2\,c^2}\left(\vec{\nabla}\,V \times \hat{\vec{p}}\right) \cdot \hat{\vec{\sigma}}$$

with

$$\frac{\hbar}{4\,m^2\,c^2}\,\vec{\nabla}\,V = \left(0,\,0,\,\frac{\hbar}{4\,m^2\,c^2}\,\frac{\partial\,V}{\partial\,z}\Big|_{z\,=\,0}\right) := (0,\,0,\,\gamma)\;.$$

a) Calculate the eigenstates of $\hat{H}$. To this end, employ a wave function of the form

$$\psi_{n,\,\vec{k}}\,(x,\,y,\,0) = \begin{pmatrix} a_{n,\,\vec{k}} \\ b_{n,\,\vec{k}} \end{pmatrix} \mathrm{e}^{i\,\vec{k}\,\cdot\,\vec{r}} \qquad \text{with} \qquad \vec{k} = (k_x,\,k_y,\,0) \qquad \text{and} \qquad n = 1,\,2\;.$$

This ansatz leads to a (2×2) linear system of equations which gives you $E_{n,\,\vec{k}}$, $a_{n,\,\vec{k}}$ and $b_{n,\,\vec{k}}$. Choose $a_{1,\,\vec{k}} = a_{2,\,\vec{k}} = 1/\sqrt{2}$ in the calculation. Plot the eigenvalues $E_{n,\,\vec{k}}$ as a function of k_x for $k_y = 0$.

b) Use $a_{n,\,\vec{k}}$ and $b_{n,\,\vec{k}}$ to calculate the spin expectation values $\langle\hat{S}_x\rangle$, $\langle\hat{S}_y\rangle$ and $\langle\hat{S}_z\rangle$. Which direction has the vector $\langle\hat{\vec{S}}\rangle$ for $\gamma > 0$ at

i) $\vec{k} = (k_x,\,0,\,0)$ and ii) $\vec{k} = (0,\,k_y,\,0)$?

Consider the two cases $k_x > 0$ and $k_x < 0$ for i) and the cases $k_y > 0$ and $k_y < 0$ for ii).

Problem 12: Density of states for a linear chain (2 points)

The band structure of a linear chain with one s-like orbital per atom is given within the framework of the empirical tight-binding method by

$$E_k = E_s + 2\,V_{ss}\,\cos(k\,a)\;.$$

Calculate the density of states

$$N(E) = 2 \cdot \sum_k \delta\,(E - E_k)$$

of the chain. The factor 2 results from the spin and the sum runs over all k within the first Brillouin zone.

Hint: Substitute the sum by an integral.