Appendix C

Free-Electron Model

The free-electron model permits a visual demonstration of the influence that Rashba spin-orbit interaction has on the electron energy and the spin. In particular, it shows that electrons with the same wave vector and different spins will have different energies, and that Rashba spin-orbit interaction leads to ordered spins that point perpendicular to the direction of electron propagation. The one-electron Hamiltonian is written as

$$H = \frac{p^2}{2m} + H_R \ , \tag{C.1}$$

with the Rashba Hamiltonian

$$H_R = \alpha\,(\vec{e}_z \times \vec{k})\,\vec{\sigma} \ . \tag{C.2}$$

Here α denotes the effective SOC strength of an electron propagating with momentum $\vec{p} = h\vec{k}$ in an electric field (pointing towards the z-axis). $\vec{\sigma}$ denotes the Pauli matrix vector, commonly used to describe the electron spin. We rewrite the Rashba Hamiltonian in the form:

$$H_R = \alpha\,(\vec{e}_z \times \vec{k})\,\vec{\sigma} = \begin{vmatrix} 0 & 0 & e_z \\ k_x & k_y & k_z \\ \sigma_x & \sigma_y & \sigma_z \end{vmatrix} = \alpha(k_x\sigma_y - \sigma_x k_y), \tag{C.3}$$

with

$$\vec{\mathbf{p}} = -i\hbar\vec{\nabla} \ , \tag{C.4}$$

and

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{C.5}$$

We obtain a 2×2 Hamiltonian matrix for the 2D problem

$$H = \begin{pmatrix} -\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}) & -\alpha\hbar\frac{\partial}{\partial x} + i\alpha\hbar\frac{\partial}{\partial y} \\ \alpha\hbar\frac{\partial}{\partial x} + i\alpha\hbar\frac{\partial}{\partial y} & -\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}) \end{pmatrix} \ . \tag{C.6}$$

We choose spherical coordinates with the z-axis perpendicular to the 2D electron plane, so that the components of the unit vector $\vec{e} = (e_x, e_y, e_z)$ become

$$e_x = \sin\vartheta\cos\varphi, \quad e_y = \sin\vartheta\sin\varphi, \quad e_z = \cos\vartheta. \tag{C.7}$$

The function $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ are the eigenfunctions of σ_z of the spin operator.

It is important to note that superposition of spin states in opposite directions with equal amplitudes and with fixed phase relation, such as

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \tag{C.8}$$

does not result in a cancellation of spins, but a spin in another direction [80]. Similar to a coherent superposition of right- and left-circularly polarized light waves, which also does not result in an unpolarized wave, but in rather a linear polarisation.

The spin part of an electron wave function χ, describing an electron with an arbitrary spin direction, can be written (in the non-relativistic limit) as linear combination of spin-up, $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, and spin-down $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ functions with a fixed phase relation [80].

$$\chi = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a_1\begin{pmatrix} 1 \\ 0 \end{pmatrix} + a_2\begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{C.9}$$

For a spin function that describes a spin in the direction ϑ, φ, we have

$$\frac{a_2}{a_1} = \tan\frac{\vartheta}{2}e^{i\varphi} , \tag{C.10}$$

with the common phase factors

$$a_1 = \cos\frac{\vartheta}{2}, \quad a_2 = \sin\frac{\vartheta}{2}e^{i\varphi}. \tag{C.11}$$

The full wave function of an electron can hence be written as:

$$\psi = e^{i(k_x x + k_y y)}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} . \tag{C.12}$$

To determine the eigenvalues of the Hamiltonian, one has to solve the system of homogeneous equations. For non-trivial solutions, the determinant of the coefficients has to be zero:

$$det(\mathbf{H}\psi - E\mathbf{I}) = 0, \quad or \tag{C.13}$$

$$\begin{vmatrix} \frac{\hbar^2}{2m}(k_x^2 + k_y^2) - E & -\alpha\hbar(ik_x + k_y) \\ \alpha\hbar(ik_x - k_y) & \frac{\hbar^2}{2m}(k_x^2 + k_y^2) - E \end{vmatrix} = 0 . \tag{C.14}$$

Hence, the eigenvalues are

$$E_{1,2} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2) \pm \alpha\hbar\sqrt{k_x^2 + k_y^2}\ . \tag{C.15}$$

With there eigenvalues, we can now find the phase ratio of the spin function $\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$, which actually defines the spin orientation direction, by substituting the eigenvalues in e.g. the first system of equations. We then obtain

$$for\ E_1:\quad \frac{a_2}{a_1} = -\frac{\sqrt{k_x^2 + k_y^2}}{ik_x + k_y} = \frac{i(k_x + ik_y)}{\sqrt{k_x^2 + k_y^2}} = i(\cos\theta_k + i\sin\theta_k) = ie^{i\theta_k} \tag{C.16}$$

$$for\ E_2:\quad \frac{a_2}{a_1} = -\frac{i(k_x + ik_y)}{\sqrt{k_x^2 + k_y^2}} = -ie^{i\theta_k} = \frac{1}{ie^{-i\theta_k}}\ ,$$

where θ_k is the angle between the x axis and the vector $\vec{k}$. The wave function is then like [83]:

$$\psi_1(r) = e^{i\vec{k}\vec{r}}(|\uparrow\rangle + ie^{i\theta_k}|\downarrow\rangle)\ , \tag{C.17}$$

$$\psi_2(r) = e^{i\vec{k}\vec{r}}(ie^{-i\theta_k}|\uparrow\rangle + |\downarrow\rangle).$$

Finally, we found that a parabolic dispersion, typical for the free-electron Hamiltonian, splits into two branches with energies E_1 and E_2 when the as Rashba Hamiltonian is added to the free-electron Hamiltonian. Spin functions of corresponding eigenfunctions correspond to electrons with spins oriented in two opposite directions perpendicular to the vector $\vec{k}$.