Lecture Notes on Quantum Geometry

Contents

1 Adiabatic approximation

The adiabatic approximation is a technique used in quantum mechanics to solve the time-dependent Schrödinger equation. Its basic assumption is that the parameters of the hamiltonian change slowly enough that the wavefunction of the system can be assumed to remain in its instantaneous eigenstate. In other words, the evolution of the parameters of the hamiltonian occurs on a time scale, e.g., a period T_{ext}, that is much longer than the time scale of the evolution of its internal variables, e.g., a period T_{int}. $T_{ext} \gg T_{int}$ defines the condition of adiabatic evolution of the control parameters.

In this spirit, we search for solutions of the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = H\left|\Psi(t)\right\rangle \tag{1}$$

using the following ansatz:

$$\left|\Psi(t)\right\rangle = \sum_n \Psi_n(t) = \sum_n c_n(t)\left|\psi_n(t)\right\rangle \tag{2}$$

The wavefunctions $\psi_n(t)$ are defined as the instantaneous solutions of the equation

$$H(t)\psi_n(t) = E_n(t)\psi_n(t) \tag{3}$$

where we assume that $\psi_n(t)$ constitute an instantaneous orthonormal basis.

$$\langle\psi_k(t)|\psi_n(t)\rangle = \delta_{k,n}, \forall t \tag{4}$$

We plug our ansatz into the time-dependent Schrödinger equation, finding

$$i\hbar\sum_n\left(\dot{c_n}(t)\left|\psi_n(t)\right\rangle + c_n(t)\left|\dot{\psi_n}(t)\right\rangle\right) = \sum_n c_n(t)E_n(t)\left|\psi_n(t)\right\rangle \tag{5}$$

We project on the components $\langle\psi_k(t)|$, to obtain

$$i\hbar\dot{c_k}(t) = c_k(t)E_k(t) - i\hbar\sum_n\langle\psi_k(t)|\dot{\psi_n}(t)\rangle\, c_n(t) \tag{6}$$

$$= c_k(t)\left(E_k(t) - i\hbar\langle\psi_k(t)|\dot{\psi_k}(t)\rangle\right) - \underbrace{i\hbar\sum_{n\neq k}\langle\psi_k(t)|\dot{\psi_n}(t)\rangle\, c_n(t)}_{\text{coupling terms}} \tag{7}$$

In the adiabatic approximation, we neglect the coupling terms. This implements our assumption that the parameters of the hamiltonian vary slowly enough that the wavefunction

of the system can be assumed to stay in its instantaneous eigenstate. In this approximation, we assume that the products $\langle\psi_k(t)|\dot{\psi_n}(t)\rangle$ are negligible. Thus, our evolution is reduced to

$$i\hbar\dot{c_k}(t) \approx \left(E_k(t) - i\hbar\,\langle\psi_k(t)|\dot{\psi_k}(t)\rangle\right) c_k(t). \tag{8}$$

The solution is found as

$$c_k(t) = \exp\left\{\frac{1}{i\hbar}\int_0^t \left(E_k(t') - i\hbar\,\langle\psi_k(t')|\dot{\psi_k}(t')\rangle\right) \mathrm{d}t'\right\} \tag{9}$$

The evolution of the wavefunctions can be written in a compact form as

$$\Psi_n(t) \approx e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t) \tag{10}$$

where

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\mathrm{d}t' \tag{11}$$

is the standard phase evolution of an eigenstate, also known as the *dynamical phase*. The second factor contains the phase

$$\gamma_n(t) = \int_0^t i\,\langle\psi_n(t')|\dot{\psi_n}(t')\rangle\,\mathrm{d}t' \tag{12}$$

that is known as the *geometric phase* or Berry phase. The term *geometric phase* somehow suggests that this quantity is determined by the geometric properties of the wavefunctions. In the next section we will elaborate on this concept.

2 Geometric phase

As introduced earlier, we consider hamiltonians that are characterised by a set of parameters $k_1, \ldots, k_N$ that constitute a vector space $\mathbf{k} = (k_1, k_2, \ldots, k_N)$ (configuration space). We have a solution of the following equation for all values of the parameters:

$$H(\mathbf{k})\,|\psi_n(\mathbf{k})\rangle = E_n(\mathbf{k})\,|\psi_n(\mathbf{k})\rangle \tag{13}$$

where $\psi_n(\mathbf{k})$ constitute an orthonormal set. We consider a time-dependent evolution in the configuration space described by the path

$$\mathbf{k}(t) = (k_1(t), \ldots, k_N(t)) \tag{14}$$

This defines a time-dependent hamiltonian $H\left[\mathbf{k}(t)\right]$ that can be solved with the method of the adiabatic approximation. According to our previous analysis, an adiabatic evolution will be associated with the acquisition of a geometric phase given by

$$\gamma_n(t) = \int_0^t i\,\langle\psi_n\left(\mathbf{k}(t')\right)|\frac{\mathrm{d}}{\mathrm{d}t'}\psi_n\left(\mathbf{k}(t')\right)\rangle\,\mathrm{d}t' = \tag{15}$$

However, we recall that

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_n\left(\mathbf{k}(t)\right) = \frac{\mathrm{d}}{\mathrm{d}t}\psi_n\left(k_1(t), ..., k_N(t)\right) = \tag{16}$$

$$= \frac{\partial\psi_n}{\partial k_1}\frac{\mathrm{d}k_1}{\mathrm{d}t} + ... + \frac{\partial\psi_n}{\partial k_N}\frac{\mathrm{d}k_N}{\mathrm{d}t} = \nabla_{\mathbf{k}}\psi_n \cdot \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} \tag{17}$$

Therefore we can write

$$\gamma_n(t) = \int_0^t i\left\langle\psi_n\left(\mathbf{k}(t')\right)|\nabla_{\mathbf{k}}|\psi_n\left(\mathbf{k}(t')\right)\right\rangle \cdot \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t'}\mathrm{d}t' \tag{18}$$

By integrating around a closed loop $\mathcal{C}$, we find

$$\gamma_n(\mathbf{k}) = \oint_{\mathcal{C}} i\left\langle\psi_n(\mathbf{k})|\nabla_{\mathbf{k}}|\psi_n(\mathbf{k})\right\rangle \cdot \mathrm{d}\mathbf{k} \tag{19}$$

The quantity

$$\mathcal{A}_n(\mathbf{k}) = i\left\langle\psi_n(\mathbf{k})|\nabla_{\mathbf{k}}|\psi_n(\mathbf{k})\right\rangle \tag{20}$$

is called the Berry connection. It relates to the overlap between wavefunctions in configuration space separated by an infinitesimal distance, via the equation

$$\begin{aligned}\left\langle\psi_n(\mathbf{k})|\nabla_{\mathbf{k}}|\psi_n(\mathbf{k})\right\rangle &= \lim_{\delta\mathbf{k}\to 0}\frac{\langle\psi_{\mathbf{k}}|\psi_{\mathbf{k}+\delta\mathbf{k}}\rangle - \langle\psi_{\mathbf{k}}|\psi_{\mathbf{k}}\rangle}{\delta\mathbf{k}} \\ &= -i\mathcal{A}_{\mathbf{k}}.\end{aligned} \tag{21}$$

When studying systems characterised by a three-dimensional configuration space (e.g. the momentum space associated with the electronic wavefunctions of a periodic solid), we can make use of Stokes' theorem. In this case, the contour integral of the Berry connection can be written as a surface integral:

$$\oint_{\mathcal{C}} \mathcal{A}_n(\mathbf{k}) \cdot \mathrm{d}\mathbf{k} = \iint_{\mathcal{S}} \nabla_{\mathbf{k}} \times \mathcal{A}_n(\mathbf{k}) \cdot \mathrm{d}^2\mathbf{k}\,. \tag{22}$$

The quantity

$$\mathcal{B}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathcal{A}_n(\mathbf{k}) \tag{23}$$

is called the Berry curvature, and represents the flux that penetrates the surface area enclosed by the contour $\mathcal{C}$.

3 Example 1: spin 1/2 in a rotating magnetic field

As a first concrete example of the acquisition of a geometric phase in the adiabatic approximation, we consider a spin 1/2 system, immersed in an external time-dependent magnetic field $\vec{\mathbf{B}}$

$$\mathcal{H}(t) = -\frac{\mu}{2}\,\vec{\sigma}\cdot\vec{\mathbf{B}}(t) \tag{24}$$

where the magnetic field $\vec{\mathbf{B}}$ depends on time:

$$\vec{\mathbf{B}}(t) = B_0[\sin\theta\cos\omega t\ \hat{\mathbf{x}} + \sin\theta\sin\omega t\ \hat{\mathbf{y}} + \cos\theta\ \hat{\mathbf{z}}] \tag{25}$$

namely, it is periodic, such that $\vec{\mathbf{B}}\big(t+\frac{2\pi}{\omega}\big) = \vec{\mathbf{B}}(t)$. Upon a complete field rotation, we will show that in the adiabatic limit ($\omega \ll \mu B_0$) the wavefunctions acquires a geometric phase given by:

$$\langle\psi^{\pm}\left(t=\frac{2\pi}{\omega}\right)|\,|\psi^{\pm}\big(t=0\big)\rangle = \underbrace{e^{\pm i\frac{2\pi}{\omega}\mu B_0}}_{\text{dynamical phase}} \quad \underbrace{e^{-i\pi(1\pm\cos\theta)}}_{\text{geometric phase}} \tag{26}$$

We will now proceed with this important calculation using a direct diagonalisation of the hamiltonian and the application of the results of the adiabatic approximation. We calculated previously that the geometric phase can be found using:

$$\gamma_n = i\int_{\mathcal{C}}\langle n,\vec{\mathbf{B}}|\,\boldsymbol{\nabla}_B\,|n,\vec{\mathbf{B}}\rangle\cdot\mathrm{d}\vec{\mathbf{B}} \tag{27}$$

The integral being performed over a contour $\mathcal{C}$ defined by the closed path of the magnetic field. The wavefunction then reads:

$$|\psi(t)\rangle = \underbrace{\exp\left\{-\frac{i}{\hbar}\int_0^{\frac{2\pi}{\omega}}E(t')\mathrm{d}t'\right\}}_{\text{dynamical phase}} \quad \underbrace{e^{i\gamma_n(t)}}_{\text{geometric phase}}\ |n,\vec{\mathbf{B}}\rangle \tag{28}$$

The "instantaneous" eigenvalues of the hamiltonian $\mathcal{H}$ can be found solving the equation:

$$\det\{E\mathbb{1} - \mathcal{H}(t)\} = 0 \tag{29}$$

The hamiltonian can be written as a matrix operator in the spin space as:

$$\mathcal{H}(t) = -\frac{\mu B}{2}(\sigma_x B_x + \sigma_y B_y + \sigma_z B_z) = \tag{30}$$

$$-\frac{\mu B}{2}\left[\begin{pmatrix}0&1\\1&0\end{pmatrix}\sin\theta\cos\omega t\hat{\mathbf{x}} + \begin{pmatrix}0&-i\\i&0\end{pmatrix}\sin\theta\sin\omega t\hat{\mathbf{y}} + \begin{pmatrix}1&0\\0&-1\end{pmatrix}\cos\theta\hat{\mathbf{z}}\right] \tag{31}$$

where σ_i are the Pauli matrices. The basis in the spin space is represented by the two vectors spin up and spin down states:

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{32}$$

$$|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{33}$$

Therefore, the matrix form of the $\mathcal{H}(t)$ in this basis following from eq.31:

$$\mathcal{H}(t) = \frac{\mu B}{2} \begin{pmatrix} -\cos\theta & -\sin\theta\cos\omega t + i\sin\theta\sin\omega t \\ -\sin\theta\cos\omega t - i\sin\theta\sin\omega t & \cos\theta \end{pmatrix} = \tag{34}$$

$$= -\frac{\mu B}{2} \begin{pmatrix} \cos\theta & \sin\theta e^{-i\omega t} \\ \sin\theta e^{i\omega t} & -\cos\theta \end{pmatrix} \tag{35}$$

For this problem, the eigenvalues are:

$$E_\pm = \pm\frac{\mu B}{2} \tag{36}$$

This can be readily seen by working out the determinant $\det\{\mathcal{H}(t)\} = -\frac{\mu^2 B^2}{4}$ and the trace $Tr\{\mathcal{H}(t)\} = 0$ of the matrix seen above [1]. The eigenvectors are:

$$\vec{\mathbf{v}}_+ = \begin{pmatrix} -\sin(\theta/2) \\ \cos(\theta/2)e^{i\omega t} \end{pmatrix} \qquad \vec{\mathbf{v}}_- = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\omega t} \end{pmatrix}$$

To find these we have to solve the matrix equation:

$$(\mathcal{H}(t) - E_\pm \mathbb{1}) \cdot \vec{\mathbf{v}}_\pm = 0 \tag{37}$$

We look for eigenvectors in the form:

$$\vec{\mathbf{v}}_+ = \begin{pmatrix} x_+ \\ y_+ \end{pmatrix} \qquad \vec{\mathbf{v}}_- = \begin{pmatrix} x_- \\ y_- \end{pmatrix}$$

where $x_\pm, y_\pm \in \mathbb{C}$ are complex numbers. For the positive eigenvalue the matrix problem to solve is thus:

$$\begin{pmatrix} 2\cos^2\frac{\theta}{2} & 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\omega t} \\ 2\cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{i\omega t} & 2\sin^2\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} x_+ \\ y_+ \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{38}$$

[1] We remind the reader that since every hermitian matrix can be expressed in an orthonormal basis of its eigenstates, and determinants are traces are invariant under similarity transformations, the determinant of the matrix found is the product of the two eigenvalues, the trace being their sum instead.

This leads to the two coupled equations:

$$\begin{cases} \cos^2\frac{\theta}{2}x_+ = -\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\omega t}y_+ \\ \cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{i\omega t}x_+ = -\sin^2\frac{\theta}{2}y_+ \end{cases} \tag{39}$$

To solve the system we can use polar notation for the complex variables:

$$x_+ = R_{x_+}e^{i\phi_{x_+}}$$
$$y_+ = R_{y_+}e^{i\phi_{y_+}}$$

So the two complex equations written above can be recast as:

$$\begin{cases} R_{x_+}\frac{\cos\frac{\theta}{2}}{\sin\frac{\theta}{2}} = R_{y_+} \\ \phi_{x_+} + \omega t = \phi_{y_+} + \pi \end{cases} \tag{40}$$

Imposing the normalisation condition gives:

$$R_{x_+}^2 + R_{y_+}^2 = R_{x_+}^2\left(1 + \frac{\cos^2\frac{\theta}{2}}{\sin^2\frac{\theta}{2}}\right) = 1 \tag{41}$$

This in turn gives:

$$R_{x_+} = \sin\frac{\theta}{2}$$
$$R_{y_+} = \cos\frac{\theta}{2}$$

We can arbitrarily choose $\phi_{x_+} = \pi$ (a common phase factor between x_+ and y_+ could easily be factored out of the vector, and it would not affect the result), so the phases result:

$$\phi_{x_+} = \pi$$
$$\phi_{y_+} = \omega t$$

Whence:

$$\vec{\mathbf{v}}_+ = \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2}e^{i\omega t} \end{pmatrix} \tag{42}$$

The case for the negative eigenvalue is completely analogous, the matrix problem to solve in this case is:

$$\begin{pmatrix} -2\sin^2\frac{\theta}{2} & 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\omega t} \\ 2\cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{i\omega t} & -2\cos^2\frac{\theta}{2} \end{pmatrix}\begin{pmatrix} x_- \\ y_- \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{43}$$

which leads to the following radius/phases relations:

$$\begin{cases} R_{x_-} = \frac{\cos\frac{\theta}{2}}{\sin\frac{\theta}{2}}R_{y_-} \\ \phi_{x_-} = \phi_{y_-} - \omega t \end{cases} \tag{44}$$

In this case applying the normalisation condition and imposing $\phi_{x_-} = 0$ we find:

$$\vec{\mathbf{v}}_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} e^{-i\omega t} \end{pmatrix} \tag{45}$$

Let's now return to the original problem of calculating the contributions to the phase of the wavefunction $|\psi\rangle$. The dynamical phase is simply given by:

$$\frac{i}{\hbar}\int_0^{\frac{2\pi}{\omega}} E_\pm(t')\mathrm{d}t' = \frac{i}{\hbar}\int_0^{\frac{2\pi}{\omega}} \pm\frac{\mu B_0}{2}\mathrm{d}t' = \pm\frac{i\pi\mu B_0}{\hbar\omega} \tag{46}$$

Now let us turn to the geometric phase:

$$\gamma_n = i\int_{\mathcal{C}} \langle n, \vec{\mathbf{B}}|\, \boldsymbol{\nabla}_B\, |n, \vec{\mathbf{B}}\rangle \cdot \mathrm{d}\vec{\mathbf{B}} \tag{47}$$

This calculation is best carried out in spherical coordinates, the gradient operator thus takes the form:

$$\boldsymbol{\nabla} = \hat{\mathbf{r}}\frac{\partial}{\partial r} + \frac{1}{r}\hat{\boldsymbol{\theta}}\frac{\partial}{\partial\theta} + \frac{1}{r\sin\theta}\hat{\boldsymbol{\phi}}\frac{\partial}{\partial\phi} \tag{48}$$

Since the coordinates are the component of the magnetic field, it follows that $\phi = \omega t$ and $r = B_0$. So the eigenvectors gradient with respect to the field can be written as:

$$\boldsymbol{\nabla}_B\, \vec{\mathbf{v}}_\pm = \begin{pmatrix} \frac{\partial}{\partial B_0} & \frac{1}{B_0}\frac{\partial}{\partial\theta} & \frac{1}{B_0\sin\theta}\frac{\partial}{\partial\omega t} \end{pmatrix} \vec{\mathbf{v}}_\pm \tag{49}$$

The gradient must be performed for each spin component of the eigenvectors:

$$\boldsymbol{\nabla}_B\, \vec{\mathbf{v}}_+ = \frac{1}{2B_0}\begin{pmatrix} -\cos\frac{\theta}{2}\hat{\boldsymbol{\theta}} \\ -\sin\frac{\theta}{2}e^{i\omega t}\hat{\boldsymbol{\theta}} + \frac{i}{\sin\frac{\theta}{2}}e^{i\omega t}\hat{\boldsymbol{\phi}} \end{pmatrix} \tag{50}$$

$$\boldsymbol{\nabla}_B\, \vec{\mathbf{v}}_- = \frac{1}{2B_0}\begin{pmatrix} -\sin\frac{\theta}{2}\hat{\boldsymbol{\theta}} \\ \cos\frac{\theta}{2}e^{i\omega t}\hat{\boldsymbol{\theta}} + \frac{i}{\cos\frac{\theta}{2}}e^{i\omega t}\hat{\boldsymbol{\phi}} \end{pmatrix} \tag{51}$$

The diagonal matrix elements of the gradient operator are then:

$$\langle\vec{\mathbf{v}}_+|\, \boldsymbol{\nabla}_B\, |\vec{\mathbf{v}}_+\rangle = \frac{1}{2B_0}\begin{pmatrix} -\sin\frac{\theta}{2} & \cos\frac{\theta}{2}e^{-i\omega t} \end{pmatrix}\begin{pmatrix} -\cos\frac{\theta}{2}\hat{\boldsymbol{\theta}} \\ -\sin\frac{\theta}{2}e^{i\omega t}\hat{\boldsymbol{\theta}} + \frac{i}{\sin\frac{\theta}{2}}e^{i\omega t}\hat{\boldsymbol{\phi}} \end{pmatrix} = \tag{52}$$

$$= \frac{1}{2B_0}\cot\frac{\theta}{2}\hat{\boldsymbol{\phi}} = \begin{pmatrix} 0 & 0 & \frac{i}{2B_0}\cot\frac{\theta}{2} \end{pmatrix} \tag{53}$$

and:

$$\langle\vec{\mathbf{v}}_-|\, \boldsymbol{\nabla}_B\, |\vec{\mathbf{v}}_-\rangle = \frac{1}{2B_0}\begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2}e^{-i\omega t} \end{pmatrix}\begin{pmatrix} -\sin\frac{\theta}{2}\hat{\boldsymbol{\theta}} \\ \cos\frac{\theta}{2}e^{i\omega t}\hat{\boldsymbol{\theta}} + \frac{i}{\cos\frac{\theta}{2}}e^{i\omega t}\hat{\boldsymbol{\phi}} \end{pmatrix} = \tag{54}$$

$$= \frac{1}{2B_0}\tan\frac{\theta}{2}\hat{\boldsymbol{\phi}} = \begin{pmatrix} 0 & 0 & \frac{i}{2B_0}\tan\frac{\theta}{2} \end{pmatrix} \tag{55}$$

The integral in eq.27 can be carried out by means of a variable change. The gradient operator expectation value only depends on ϕ, which in turn in proportional to time. For this reason $\mathcal{C}$ can be chosen as a circle (radius B_0) revolving around the ϕ coordinate. So we can make a variable substitution from ϕ to time t. The time derivative of the magnetic field is:

$$\mathrm{d}\vec{\mathbf{B}}\Big/\mathrm{d}t = B_0\omega\sin\theta(-\sin\omega t\,\hat{\mathbf{x}} + \cos\omega t\,\hat{\mathbf{y}}) = B_0\omega\sin\theta\,\hat{\boldsymbol{\phi}} \tag{56}$$

This latter is also oriented along $\hat{\boldsymbol{\phi}}$, so the integral gets even simpler:

$$\gamma_{v_+} = \int_{\phi=0,B=B_0}^{\phi=2\pi,B=B_0} \frac{1}{2B_0}\cot\frac{\theta}{2}\,\hat{\boldsymbol{\phi}}\cdot d\vec{\mathbf{B}} = \int_{t=0}^{t=\frac{2\pi}{\omega}} \frac{1}{2B_0}\cot\frac{\theta}{2}\,\hat{\boldsymbol{\phi}}\cdot\frac{\mathrm{d}\vec{\mathbf{B}}}{\mathrm{d}t}\,dt = \tag{57}$$

$$\gamma_{v_+} = i\int_0^{\frac{2\pi}{\omega}} \frac{i}{2B_0}\cot\frac{\theta}{2}\,B_0\omega\sin\theta dt = -\pi\cot(\theta/2)\sin\theta = -\pi(1+\cos\theta) \tag{58}$$

and similarly:

$$\gamma_{v_-} = i\int_0^{\frac{2\pi}{\omega}} \frac{i}{2B_0}\tan\frac{\theta}{2}\,B_0\omega\sin\theta dt = -\pi\tan(\theta/2)\sin\theta = -\pi(1-\cos\theta) \tag{59}$$

4 Anomalous transport

We will now give a brief account of the basic description of transport phenomena associated with a geometric structure of the electronic wavefunctions. In a curved space, the traditional derivative operation is not gauge-invariant. Consequently, a gauge-covariant derivative must be introduced:

$$\nabla_{\mathbf{k}} \to \nabla_{\mathbf{k}} - i\mathcal{A}_{\mathbf{k}}. \tag{60}$$

On a momentum-space basis, the gauge-covariant position operators are expressed as

$$\begin{aligned}\hat{x} &= \nabla_{k_x} - i\mathcal{A}_{k_x}\\ \hat{y} &= \nabla_{k_y} - i\mathcal{A}_{k_y}.\end{aligned} \tag{61}$$

We can characterise electronic transport by taking into account the effects of an electric field $\hat{H}' = -e\mathcal{E}_x\hat{x}$ within the adiabatic approximation. This leads to an additional contribution to the time evolution of the position operators:

$$\begin{aligned}\left\langle\frac{\mathrm{d}\hat{y}}{\mathrm{d}t}\right\rangle &= \frac{i}{\hbar}\left[\hat{H}',\hat{y}\right]\\ &= -\frac{ie\mathcal{E}_x}{\hbar}[\hat{x},\hat{y}]\\ &= \frac{e\mathcal{E}_x}{\hbar}\left(\frac{\partial\mathcal{A}_{k_y}}{\partial k_x} - \frac{\partial\mathcal{A}_{k_x}}{\partial k_y}\right)\\ &= \frac{e}{\hbar}\mathcal{E}_x\mathcal{B}^z_{\mathbf{k}} = v_y^{\mathrm{AH}}\end{aligned} \tag{62}$$

This additional contribution is called the anomalous velocity and it is responsible for a number of unconventional transport and spin dynamics phenomena. Importantly, these transport phenomena manifest in a perpendicular direction with respect to the external electric field. Therefore, we define the anomalous transverse conductance as

$$\sigma_{xy}^{\mathrm{AH}} = -v_y^{\mathrm{AH}} e/\mathcal{E}_x. \tag{63}$$

We can calculate it by integrating over all occupied states throughout the Brillouin zone (BZ) and summing over all electronic bands n the Berry curvature $\mathcal{B}_n^z$, weighted by the Fermi-Dirac distribution: $f(\epsilon_{\mathbf{k}}^n)$

$$\sigma_{xy}^{\mathrm{AH}} = -\frac{e^2}{2\pi h} \sum_n \iint_{\mathrm{BZ}} f(\epsilon_{\mathbf{k}}^n) \mathcal{B}_n^z \, \mathrm{d}^2\mathbf{k} \,. \tag{64}$$

The dispersion relation $\epsilon_{\mathbf{k}}$ of band n enters this expression via the Fermi-Dirac distribution.

We can now recognise that the observation of transport phenomena related to the geometric structure of electronic wavefunctions necessitates the existence of a finite Berry curvature integration over the Brillouin zone. This requirement is subject to stringent symmetry restrictions. Systems with time-reversal symmetry have a Berry curvature that is an odd function of $\mathbf{k}$, resulting in a zero integration throughout the Brillouin zone. In systems with time-reversal symmetry, anomalous transport in the sense described here is only possible in solids with very low crystal symmetries.

At zero temperature and for a single fully occupied band n, equation (64) simplifies to

$$\begin{aligned} \sigma_{xy,n}^{\mathrm{AH}} &= -\frac{e^2}{2\pi h} \iint_{\mathrm{BZ}} \mathcal{B}_n^z \, \mathrm{d}^2\mathbf{k} \\ &= -\frac{e^2}{h} C_n. \end{aligned} \tag{65}$$

The Chern number of band n, denoted as C_n, is a topological quantity that gives a quantised contribution to the anomalous Hall conductance. For a fully occupied band (Chern insulator), the anomalous Hall conductance is quantised. In the case of partially occupied bands i.e., Fermi liquids, the conductance is not quantised as a result of contributions from states at the Fermi energy.

In two dimensions, for a given (Bloch) wavefunction ψ, the Berry curvature can be written as

$$\begin{aligned} \mathcal{B}_z = \nabla_{k_x} \mathcal{A}_{k_y} - \nabla_{k_y} \mathcal{A}_{k_x} &= i \langle \nabla_{k_x} \psi | \nabla_{k_y} \psi \rangle - i \langle \nabla_{k_y} \psi | \nabla_{k_x} \psi \rangle \\ &= -i \big[\, |\nabla_{\mathbf{k}} \psi\rangle \times \langle \nabla_{\mathbf{k}} \psi| \, \big]_z. \end{aligned} \tag{66}$$

For two wavefunctions ψ_m and ψ_n, we can write

$$\begin{aligned}\left\langle \psi_m \middle| \nabla \middle| \hat{H}\psi_n \right\rangle &= \epsilon_n \langle \psi_m | \nabla \psi_n \rangle + \langle \psi_m | \psi_n \rangle \nabla \epsilon_n \\ &= \langle \psi_m | \nabla \hat{H} | \psi_n \rangle + \langle \psi_m | \hat{H} | \nabla \psi_n \rangle \\ &= \langle \psi_m | \nabla \hat{H} | \psi_n \rangle + \epsilon_m \langle \psi_m | \nabla \psi_n \rangle , \end{aligned} \tag{67}$$

which gives

$$\langle \psi_m | \nabla \psi_n \rangle = \frac{\langle \psi_m | \nabla \hat{H} | \psi_n \rangle}{\epsilon_n - \epsilon_m}. \tag{68}$$

Then the total Berry curvature of band n is given by

$$\begin{aligned}\mathcal{B}^n_{\mathbf{k}} &= -i \sum_{m \neq n} \left[\langle \psi_m | \nabla_{\mathbf{k}} \psi_n \rangle \times \langle \nabla_{\mathbf{k}} \psi_n | \psi_m \rangle \right]_z \\ &= -i \sum_{m \neq n} \frac{\left[\langle \psi_m | \nabla_{\mathbf{k}} \hat{H} | \psi_n \rangle \times \langle \psi_n | \nabla_{\mathbf{k}} \hat{H} | \psi_m \rangle \right]_z}{(\epsilon_m - \epsilon_n)^2} \\ &= -2 \sum_{m \neq n} \mathrm{Im} \frac{\langle \psi_m | \nabla_{k_x} \hat{H} | \psi_n \rangle \langle \psi_n | \nabla_{k_y} \hat{H} | \psi_m \rangle}{(\epsilon_m - \epsilon_n)^2} \end{aligned} \tag{69}$$

which illustrates that when two bands m and n are nearly degenerate, the Berry curvature is enhanced. Additionally, since equation (69) is odd with respect to permuting m and n, the sum over all bands $\sum_n \mathcal{B}^n_{\mathbf{k}}$, as well as the sum over all Chern numbers $\sum_n C_n$, returns zero.

5 Berry curvature of a two-level system

We will now consider a case of a two-level system with a k-dependent spin texture.

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} = d_1 \sigma_x + d_2 \sigma_y + d_3 \sigma_z \tag{70}$$

with

$$d = |\mathbf{d}| = \sqrt{d_1^2 + d_2^2 + d_3^2} \tag{71}$$

and

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{72}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{73}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{74}$$

As derived above, the eigenvalues are

$$E_{\pm} = \pm|\mathbf{d}|. \tag{75}$$

The eigenvectors $\psi^{\pm}$, are found by solving the equation

$$\begin{bmatrix} d_3 + d & d_1 - id_2 \\ d_1 + id_2 & -d_3 + d \end{bmatrix} \begin{bmatrix} \psi_a^- \\ \psi_b^- \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{76}$$

We make the ansatz

$$\psi^- = \begin{bmatrix} \psi_a^- \\ \psi_b^- \end{bmatrix} = N \begin{bmatrix} d_3 - d \\ d_1 + id_2 \end{bmatrix} \tag{77}$$

The validity of this choice can be verified by direct computation:

$$(d_3 - d)(d_3 + d) + (d_1 - id_2)(d_1 + id_2) = d_3^2 - d^2 + d_1^2 + d_2^2 = 0 \tag{78}$$

$$(d_1 + id_2)(d_3 - d) + (-d_3 + d)(d_1 + id_2) = (d_1 + id_2)(d_3 - d) - (d_3 - d)(d_1 + id_2) = 0 \tag{79}$$

The normalisation coefficient N is found such as $|\langle\psi^-|\psi^-\rangle|^2 = 1$

$$N^2[(d_3 - d)^2 + d_1^2 + d_2^2] = 1 \tag{80}$$

$$N^2[d_3^2 + d^2 - 2d_3 d + d_1^2 + d_2^2] = N^2[2d^2 - 2d_3 d] = 1 \tag{81}$$

$$N = \frac{1}{\sqrt{2d(d - d_3)}} \tag{82}$$

$$\psi^- = \frac{1}{\sqrt{2d(d - d_3)}} \begin{bmatrix} d_3 - d \\ d_1 + id_2 \end{bmatrix} \tag{83}$$

Similarly, we find

$$\psi^+ = \frac{1}{\sqrt{2d(d + d_3)}} \begin{bmatrix} d_3 + d \\ d_1 + id_2 \end{bmatrix} \tag{84}$$

We compute the Berry connection, using

$$\mathcal{A}^{\pm}(\mathbf{k}) = i\langle\psi^{\pm}(\mathbf{k})|\nabla_{\mathbf{k}}|\psi^{\pm}(\mathbf{k})\rangle \tag{85}$$

We start with

$$\nabla_{\mathbf{k}}|\psi^{\pm}\rangle = \nabla_{\mathbf{k}} \frac{1}{\sqrt{2d(d \pm d_3)}} \begin{bmatrix} d_3 \pm d \\ d_1 + id_2 \end{bmatrix} = \tag{86}$$

$$= \frac{1}{\sqrt{2d(d \pm d_3)}} \begin{bmatrix} \nabla_{\mathbf{k}}(d_3 \pm d) \\ \nabla_{\mathbf{k}}(d_1 + id_2) \end{bmatrix} - \frac{\nabla_{\mathbf{k}} d(d \pm d_3)}{[2d(d \pm d_3)]^{3/2}} \begin{bmatrix} d_3 \pm d \\ d_1 + id_2 \end{bmatrix} \tag{87}$$

$$\langle\psi^{\pm}(\mathbf{k})|\nabla_{\mathbf{k}}|\psi^{\pm}(\mathbf{k})\rangle = \frac{1}{2d(d\pm d_3)}[(d\pm d_3)\nabla_{\mathbf{k}}(d\pm d_3)+(d_1-id_2)\nabla_{\mathbf{k}}(d_1+id_2)] \\ -\frac{1}{[2d(d\pm d_3)]^2}\nabla_{\mathbf{k}}d(d\pm d_3)[(d\pm d_3)^2+d_1^2+d_2^2]$$

We simplify the first term

$$\begin{aligned}
&[(d\pm d_3)\nabla_{\mathbf{k}}(d\pm d_3)+(d_1-id_2)\nabla_{\mathbf{k}}(d_1+id_2)] = \\
&= d_3\nabla_{\mathbf{k}}d_3 + d\nabla_{\mathbf{k}}d \pm d\nabla_{\mathbf{k}}d_3 \pm d_3\nabla_{\mathbf{k}}d + d_1\nabla_{\mathbf{k}}d_1 + d_2\nabla_{\mathbf{k}}d_2 - id_2\nabla_{\mathbf{k}}d_1 + id_1\nabla_{\mathbf{k}}d_2 \\
&= \frac{1}{2}\nabla_{\mathbf{k}}d_3^2 + \frac{1}{2}\nabla_{\mathbf{k}}d^2 \pm \nabla_{\mathbf{k}}(d_3 d) + \frac{1}{2}\nabla_{\mathbf{k}}^2 d_1^2 + \frac{1}{2}\nabla_{\mathbf{k}}d_2^2 - id_2\nabla_{\mathbf{k}}d_1 + id_1\nabla_{\mathbf{k}}d_2 \\
&= \nabla_{\mathbf{k}}d^2 \pm \nabla_{\mathbf{k}}(d_3 d) - id_2\nabla_{\mathbf{k}}d_1 + id_1\nabla_{\mathbf{k}}d_2 \\
&= \nabla_{\mathbf{k}}d(d\pm d_3) - id_2\nabla_{\mathbf{k}}d_1 + id_1\nabla_{\mathbf{k}}d_2
\end{aligned}$$

We can then write the simplified expression

$$\langle\psi^{\pm}(\mathbf{k})|\nabla_{\mathbf{k}}|\psi^{\pm}(\mathbf{k})\rangle = \frac{1}{2d(d\pm d_3)}[\nabla_{\mathbf{k}}d(d\pm d_3) - id_2\nabla_{\mathbf{k}}d_1 + id_1\nabla_{\mathbf{k}}d_2] \\ -\frac{1}{[2d(d\pm d_3)]^2}\nabla_{\mathbf{k}}d(d\pm d_3)[2d^2\pm 2d_3 d] \\ = \frac{1}{2d(d\pm d_3)}(-id_2\nabla_{\mathbf{k}}d_1 + id_1\nabla_{\mathbf{k}}d_2)$$

Therefore, the Berry connection is

$$\mathcal{A}^{\pm}(\mathbf{k}) = \frac{d_2\nabla_{\mathbf{k}}d_1 - d_1\nabla_{\mathbf{k}}d_2}{2d(d\pm d_3)} \tag{88}$$

For a two-dimensional system we can write the (z component) Berry curvature as

$$\mathcal{B}_z^{\pm} = \nabla_{k_x}\mathcal{A}_{k_y}^{\pm} - \nabla_{k_y}\mathcal{A}_{k_x}^{\pm} \tag{89}$$

leading to[2]

$$\begin{aligned}
\mathcal{B}_z^{+} = \frac{1}{2d^3}[&-d_1(\nabla_{k_x}d_2\nabla_{k_y}d_3 - \nabla_{k_x}d_3\nabla_{k_y}d_2) \\
&+d_2(\nabla_{k_x}d_1\nabla_{k_y}d_3 - \nabla_{k_x}d_3\nabla_{k_y}d_1) \\
&-d_3(\nabla_{k_x}d_1\nabla_{k_y}d_2 - \nabla_{k_x}d_2\nabla_{k_y}d_1)] \\
&= -\frac{1}{2d^3}\mathbf{d}\cdot(\nabla_{k_x}\mathbf{d}\times\nabla_{k_y}\mathbf{d}) \\
&= -\frac{1}{2}\hat{\mathbf{d}}\cdot(\nabla_{k_x}\hat{\mathbf{d}}\times\nabla_{k_y}\hat{\mathbf{d}})
\end{aligned} \tag{90}$$

[2] see Mathematica file

and

$$\mathcal{B}_z^- = \frac{1}{2}\hat{\mathbf{d}} \cdot (\nabla_{k_x}\hat{\mathbf{d}} \times \nabla_{k_y}\hat{\mathbf{d}}) \tag{91}$$

In a compact form, we have the very useful relation

$$\boxed{\mathcal{B}_z^{\pm} = \mp\frac{1}{2}\hat{\mathbf{d}} \cdot (\nabla_{k_x}\hat{\mathbf{d}} \times \nabla_{k_y}\hat{\mathbf{d}})} \tag{92}$$

The prefactor $\mp$ is related to the our definition of the Berry connection as $\mathcal{A}_n(\mathbf{k}) = i\,\langle\psi_n(\mathbf{k})|\nabla_{\mathbf{k}}|\psi_n(\mathbf{k})\rangle$. In the literature, some authors use the definition $\mathcal{A}_n(\mathbf{k}) = -i\,\langle\psi_n(\mathbf{k})|\nabla_{\mathbf{k}}|\psi_n(\mathbf{k})\rangle$, resulting in a $\pm$ prefactor.

6 Example 2. Rashba 2DEG

Let us now consider an ideal model of a two-dimensional electron gas (2DEG) confined in a x, y plane with a Rashba coupling

$$\mathcal{H}_{\mathrm{R}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\sigma_0 - \alpha_{\mathrm{R}}\,\boldsymbol{\sigma}\cdot\mathbf{k}\times\hat{\mathbf{z}}\,, \tag{93}$$

where α_{R} is a coupling constant, $\hat{\mathbf{z}}$ a unit vector in the z direction and σ_0 is the identity matrix. The full hamiltionian is therefore

$$H = \frac{\mathbf{k}^2}{2m}\sigma_0 + \alpha_{\mathrm{R}}(k_y\sigma_x - k_x\sigma_y) \tag{94}$$

Since crystal momentum is a good quantum number we can look for solutions of the kind $|\Psi\rangle = |\mathbf{k}\rangle|\psi\rangle$, where $\langle\mathbf{x}|\mathbf{k}\rangle \propto e^{i\mathbf{k}\cdot\mathbf{x}}$ is a plane wave and $|\psi\rangle$ is a spin state. Using explicitly the Pauli matrices previously defined and expressing the wave-vector as $\mathbf{k} = k(\cos\phi, \sin\phi, 0)$, we can write down the hamiltonian in the form

$$H = \frac{\hbar^2k^2}{2m}\begin{pmatrix} 1 & i\eta e^{-i\phi} \\ -i\eta e^{i\phi} & 1 \end{pmatrix}$$

where $\eta = 2m\alpha/(\hbar^2 k)$. We can find its eigenvalues by solving the quadratic equation

$$\det\begin{pmatrix} 1-\lambda & i\eta e^{-i\phi} \\ -i\eta e^{i\phi} & 1-\lambda \end{pmatrix} = (1-\lambda)^2 - \eta^2 = 0$$

which has the ϕ-independent solutions $\lambda^{\pm} = 1 \pm \eta$. Therefore the energy eigenstates are given by (see Figure 1)

$$E^{\pm} = \frac{\hbar^2k^2}{2m} \pm \alpha k \tag{95}$$

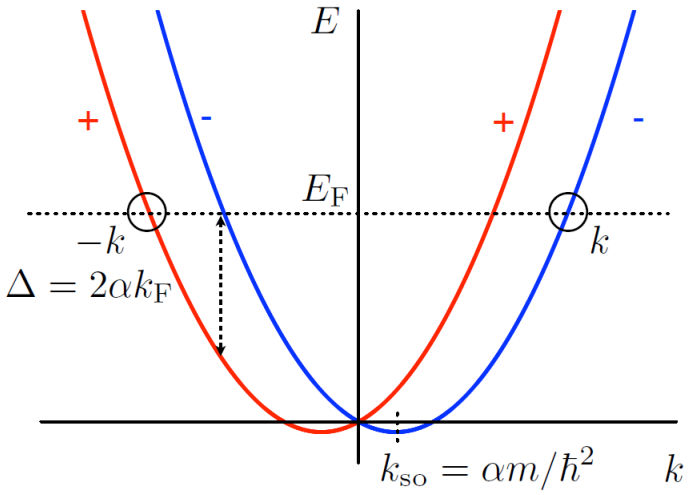

Figure 1: Section of the dispersion relation of a Rashba 2DEG

It is important to note that the energy depends on the spin state (here indicated as + or −). The normalised spin eigenvectors are

$$|\psi^+\rangle = \frac{1}{\sqrt{2}}(ie^{-i\phi}, 1) \tag{96}$$

$$|\psi^-\rangle = \frac{1}{\sqrt{2}}(-ie^{-i\phi}, 1) \tag{97}$$

One important result is that the spin direction is tied to the electron momentum, since it depends on the parameter ϕ. We can learn more about the spin direction by applying the Pauli matrices to these states. This allows us to track the spin direction in momentum space. By direct computation we find

$$\vec{S}^+ = (\langle\psi^+|\sigma_x|\psi^+\rangle, \langle\psi^+|\sigma_y|\psi^+\rangle, \langle\psi^+|\sigma_z|\psi^+\rangle) = \frac{2}{\sqrt{2}}(\sin\phi, -\cos\phi, 0) \tag{98}$$

$$\vec{S}^- = (\langle\psi^-|\sigma_x|\psi^-\rangle, \langle\psi^-|\sigma_y|\psi^-\rangle, \langle\psi^-|\sigma_z|\psi^-\rangle) = \frac{2}{\sqrt{2}}(-\sin\phi, \cos\phi, 0) \tag{99}$$

From these equations we can see that the spin is always perpendicular to the momentum and its direction is given by

$$\widehat{S}^{\pm} = \pm\widehat{\mathbf{k}} \times \widehat{z} \tag{100}$$

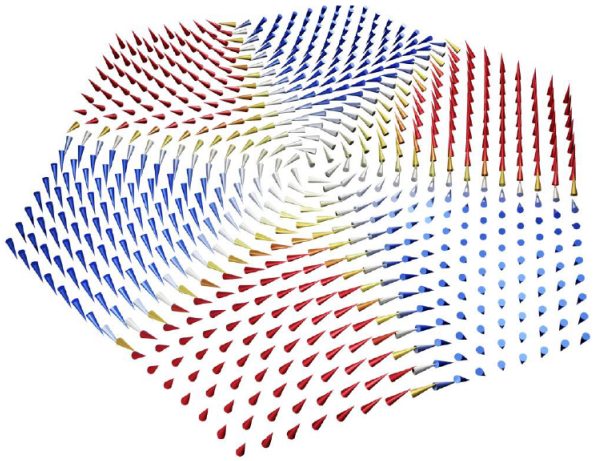

Figure 2: In the trigonal Rashba 2DEG, each spin band is characterised by a non-trivial spin texture with an out-of-plane spin components induced by the effect of trigonal warping.

We remark that the spin texture of a Rashba 2DEG lies fully on a two-dimensional plane. The relationship

$$\mathcal{B}_z^{\pm} = \mp \frac{1}{2} \hat{\mathbf{d}} \cdot (\nabla_{k_x} \hat{\mathbf{d}} \times \nabla_{k_y} \hat{\mathbf{d}}) \tag{101}$$

shows us that the absence of an out-of-plane component of the spin texture ensures a vanishing Berry curvature. The Berry curvature is not well defined at the origin, where the bands are degenerate.

7 Example 3. Rashba 2DEG with a trigonal crystal field

We now consider a Rashba 2DEG with a trigonal crystal field. At linear order in the momentum $\mathbf{k}$, the minimal two-band Hamiltonian for a Kramers' related pair of bands reads:

$$\mathcal{H}_{\mathrm{R}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m} \sigma_0 - \alpha_{\mathrm{R}} \boldsymbol{\sigma} \cdot \mathbf{k} \times \hat{\mathbf{z}} \,, \tag{102}$$

where $\boldsymbol{\sigma}$ is a vector of Pauli matrices, σ_0 is the identity matrix, α_{R} is the "Rashba" spin-orbit coupling strength, while m is the effective electron mass.

The Hamiltonian in Eq. (102) does not take into account crystalline anisotropy effects. Moreover, as we have demonstrated, the Berry curvature related to this minimal model is

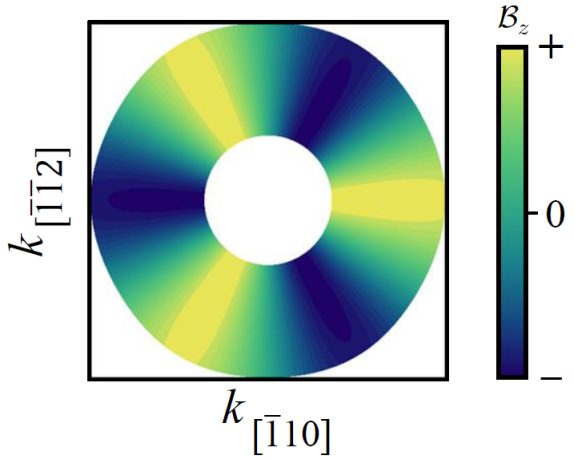

Figure 3: Exclusion plot of the Berry curvature $\mathcal{B}_z$ over the Fermi surfaces of the two spin sub-bands.

zero, since there is no term proportional to σ_z. Nevertheless, higher order momentum terms alter this result.

The first symmetry allowed term accounting for crystalline anisotropy is third order in momentum and takes the form

$$\mathcal{H}_w(\mathbf{k}) = \frac{\lambda}{2}(k_+^3 + k_-^3)\sigma_z \,. \tag{103}$$

where $k_\pm = k_x \pm ik_y$. This Hamiltonian is proportional to the Pauli matrix σ_z, which leads to an out-of-plane spin texture (see Figure 2) and a non-zero Berry curvature. To show the presence of a finite Berry curvature induced by warping, we use the relationship

$$\mathcal{B}_z^\pm = \mp\frac{1}{2}\hat{\mathbf{d}} \cdot (\nabla_{k_x}\hat{\mathbf{d}} \times \nabla_{k_y}\hat{\mathbf{d}}) \tag{104}$$

For this specific model the vector $\mathbf{d}$ has components

$$\mathbf{d} = \left\{-k_y, k_x, \lambda\left(k_+^3 + k_-^3\right)/2\right\}. \tag{105}$$

The $\mathbf{d}$ vector is independent of terms $\propto \sigma_0$, and thus of the momentum dependent effective electron mass. For the Berry curvature we find [3]

$$\mathcal{B}_z^\pm(k,\theta) = \pm\frac{2\sqrt{2}\lambda\alpha_{\mathrm{R}}^2 k^3\cos(3\theta)}{\left[2\alpha_{\mathrm{R}}^2 k^2 + \lambda^2 k^6\cos(6\theta) + \lambda^2 k^6\right]^{3/2}}\,, \tag{106}$$

[3] See Mathematica file

where θ is the polar angle in momentum space.

The Berry curvature is well defined in each point except the origin where the bands are degenerate.

The local BC of the spin-split bands of each Kramers pair cancel each other at the same crystal momentum. However, there is a region of crystal momenta populated by a single spin band. In this region – the annulus between the two Fermi lines of the system – alternating positive and negative regions of non-vanishing BC are present (see Fig. 3).