Magnetic Impurity Coupled to Helical Edge States

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Bachelor’s Thesis in Physics

Submitted to the Faculty of Mathematics, Computer Science and Natural Sciences,

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August 2013
Ich versichere, dass ich die Arbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt sowie Zitate kenntlich gemacht habe.

Aachen, den 13.08.2013
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1 Introduction

1.1 Introduction

The discovery of a new state of matter has attracted great attention in the last years: the topological insulator. Topological insulators are band insulators in their bulk, but support conducting states at their surfaces. They were predicted for the first time in 2005 to occur in graphene [6] and in 2006 to occur in CdTe/HgTe/CdTe heterostructures [3]. They could be measured in experiment in 2007 [7]. The surface states hosted by these insulators are stable and protected by time-reversal symmetry. It is interesting to understand these systems, as they can for example possibly be used in quantum computation.

This work is about the edge states in such a CdTe/HgTe/CdTe quantum well. For a given energy, we will find a pair of states, propagating in opposite directions with a kind of pseudo spin also oriented oppositely. Effective Hamiltonians for these edge states are derived with quasi-degenerate perturbation theory. An effective edge Hamiltonian is given in Ref. [5], without further justification as

\[ H_E = v_F \sigma_z k_x + \alpha_R \delta(x)(J_x \sigma_x S^x + J_y \sigma_y S^y + J_z \sigma_z S^z). \]

The first term is proportional to the Fermi velocity \(v_F\) which describes the group velocity of the electrons. The second term stands for a Rashba interaction induced by an electric field and the last term describes a Kondo interaction. The aim of this work is to find a microscopic derivation of this edge Hamiltonian, especially of the Kondo term, which couples a magnetic impurity to the edge states. We also show that the Hamiltonian \(H_E\) is missing important terms induced by an additional BIA (Bulk Inversion Antisymmetry) term. Additionally, we determine the coupling constants numerically which enables us to compare with the experiment and to compare the importance of different terms.
1.2 Formalities

Here one finds the conventions we use throughout the whole work. The Planck constant $\hbar$ and the speed of light $c$ are set to one. If a symbol represents a vector, it will be bold, i.e.: $\mathbf{x} = (x_1, x_2, x_3)^T$. We use $\frac{\partial}{\partial x_i} = \partial_i$ for derivative operators. $\sigma_i$ is used for the Pauli matrices, defined as following:

$$\sigma = \begin{pmatrix} \sigma_x & \sigma_y \\ \sigma_y & \sigma_z \end{pmatrix} \quad \text{with} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.2.1)$$

1.3 Bloch States and Band structure in Type III-IV Semiconductors

1.3.1 Bloch States and $k \cdot p$ theory

The Bloch theorem states that any solution of Schrödinger equation in a crystal can be written as

$$\psi_{nk} = e^{ik \cdot r} u_{nk}(r), \quad (1.3.1)$$

where $u_{nk}(r + \mathbf{R}) = u_{nk}(r)$ is the lattice periodic part with $\mathbf{R}$ a vector of the Bravais lattice and index $n$ refers to a given band. If we leave out the spin-orbit interaction for simplicity of this introduction, the Hamiltonian of the crystal reads

$$H_C = \frac{\mathbf{p}^2}{2m_0} + V(r), \quad (1.3.2)$$

where $V(r)$ is the effective lattice periodic potential. Inserting the Bloch wave into (1.3.2) leads to the following equation for $u_{nk}(r)$

$$\left( \frac{\mathbf{p}^2}{2m_0} + \frac{h^2 k^2}{2m_0} + \frac{\mathbf{p} \cdot \mathbf{k}}{m_0} \right) u_{nk}(r) = \varepsilon_{nk} u_{nk}(r). \quad (1.3.3)$$

The ansatz of $k \cdot p$ theory is to solve the problem for the Bloch vector $k = k_0 = 0$ and regard the terms proportional to $k$ as a small perturbation. This approach is of course only valid for small values of $k$. The functions $u_{nk_0}(r)$ are a full orthonormal set of eigenfunctions and the exact solution of the problem can then be expanded as $u_{nk}(r) = \sum_n c_{nk} u_{nk_0}(r)$. In the envelope function approximation the solutions can be written as the sum over the product of the slowly varying envelope function and the fast varying basis function $u_{nk_0}(r)$:

$$\Psi(r) = \sum_n f(r)_n u_{nk_0}(r), \quad (1.3.4)$$

where the sum over $n$ can exclude remote bands, that are well separated in energy. For the calculation of matrix elements we can later use that $f(r)$ varies significantly slower than
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$u_{nk_0}(r)$ over an atomic unit cell. Using that, we can approximate (as in [1])

$$\int_{\text{Crystal}} d^3r \psi(r)^*\psi(r) = \int_{\text{Crystal}} d^3r \sum_{n} \sum_{n'} f(r)^*_{n} u^*_{nk_0}(r) f(r)_{n'} u_{nk_0}(r)$$

$$\approx \sum_{n} \sum_{n'} \int_{\text{Cell}} d^3r' u^*_{nk_0}(r) u_{nk_0}(r),$$

where the sum over $i$ denotes the sum over all unit cells. This is possible, as $f(r)$ is assumed to be almost constant over a unit cell. With the $u_{nk}$ orthonormal over a unit cell and with $\int_{\text{Cell}} d^3r u^*_{nk_0}(r) u_{nk_0}(r) = V_0 \delta_{nn'}$, we obtain

$$\int_{\text{Crystal}} d^3r \psi(r)^*\psi(r) \approx \sum_{n} \sum_{i} V_0 f(r)^*_{n} f(r)_{n}$$

$$\approx \sum_{n} \int_{\text{Crystal}} d^3r f(r)^*_{n} f(r)_{n'},$$

where we transformed the sum back into an integral. That means, in the envelope function approximation, we are able to concentrate on the envelope functions.

1.3.2 Band structure

The band structure of a solid describes the energy depending on the wave- or Bloch vector of a particle. To get a better feeling of what the band structure is, we first approximate the electrons in a solid as free electrons which can be described with plane waves $\psi \propto e^{i k \cdot r}$, where $k$ is the wave vector. The energy dispersion of free electrons is given by $E = \frac{k^2 k^2}{2m}$, which is a quadratic dispersion. Because of the crystal symmetry, we can reduce our $k$-values to the first Brillouin zone (which is in one dimension: $k < \frac{\pi}{a}$ where $a$ is the period of the potential/crystal). Now we have many possible energies for a chosen $k$-value. Every of these energies gets an index $n$ so that we have $E(k)_n$, where $E(k)_n$ is the $n$th energy band. When we now add a small perturbation to the free electrons in the solid, the Brillouin zone will be lifted in perturbation theory. This leads to band gaps. The different bands can have different important symmetries. The bands will then often be referred by it’s symmetry and called $\Gamma_i$-Band. The $\Gamma_i$-bands in this work are named as conventional and correspond to the specific point group of the band.

1.3.3 Type III-IV Semiconductors

We consider a quantum well consisting of three layers, having a sandwich of a HgTe layer between two Hg$_{1-x}$Cd$_x$Te layers. To describe such a type III-IV semiconductor we can use a reduced eight-band Kane model with the $s$-type $\Gamma_6$ and a $p$-type band (as long as we do not have a spin orbit interaction). Thereby, $s$- and $p$-type band means, that they are quite similar to the different $s$- and $p$- states in atoms. The $s$-type band has a double degeneracy because of the electron spin, while the $p$-type band is six times degenerate. This is a two fold degeneracy
The figure shows the band structure of HgTe and CdTe, the image is taken from [3]. The $\Gamma_6$-band is the conduction band and $\Gamma_8$-band is the valence band of CdTe. We see that HgTe has an inverted band structure, where the $\Gamma_8$ and $\Gamma_6$-band exchange roles. The $\Gamma_7$-band is a spilt-off and will be ignored in all calculations in this work.

because of the spin multiplied by a three times degeneracy because of the band (a kind of orbit quantum number $|m_l = \{-1, 0, 1\}$ ). Using the $J = S + L$ basis, we obtain four quartet states with $J = \frac{3}{2}$ and two doublet states with $J = \frac{1}{2}$. The spin-orbit interaction then causes the $p$-type band to split into the $\Gamma_7$ and the $\Gamma_8$ band, where the first describes the dispersion of the $J = \frac{1}{2}$ states and the second gives the dispersion of the $J = \frac{3}{2}$ states. The $\Gamma_7$-splitoff has negligible effects on the band structure [3], therefore we ignore it and concentrate on the two $s$-type $\Gamma_6$ and four $p$-type $\Gamma_8$ states. That leads to a six band model including the following basis states: $|\Gamma_6, \frac{1}{2}\rangle, |\Gamma_6, -\frac{1}{2}\rangle$ with $J = \frac{1}{2}$ and $|\Gamma_8, \frac{3}{2}\rangle, |\Gamma_8, \frac{1}{2}\rangle, |\Gamma_8, -\frac{1}{2}\rangle, |\Gamma_8, -\frac{3}{2}\rangle$ with $J = \frac{3}{2}$. Figure 1.3.1 shows the energy dispersion of these bands. Considering a quantum well, the six bands then combine to three subbands of the quantum well: $E1, H1, L1$ ([3]). The $L1$ band is separated from the others making it possible to concentrate on the $E1$ and $H1$ bands.

## 1.4 CdTe/HgTe/CdTe Quantum Wells

Stable edge states and the state of a topological insulator has been predicted and already observed in CdTe/HgTe/CdTe quantum wells. Therefore we concentrate on this material. For reasons of simplicity we refer the CdTe/HgTe/CdTe quantum well sandwiches with
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Figure 1.4.1: Left: A sketch of a HgTe/CdTe heterostructure. Right: Example of a 2DEG band structure with n-AlGaAs, i-GaAs and SI-GaAs taken from [2]. For a HgTe/CdTe heterostructure, the band structure will be slightly different but the concept stays the same. The n-AlGaAs and SI-GaAs part then denotes the CdTe region, while the yellow i-GaAs region in the middle stands for the HgTe regions.

HgTe/CdTe quantum wells. It consists of a two layers Hg$_x$Cd$_{1-x}$Te with a very thin layer (about 7nm) of HgTe in between. Such a quantum well induces a 2DEG (two-dimensional electron gas), because of the materials band structure. While in CdTe the $\Gamma_6$ band is the conduction band and higher in energy than the $\Gamma_8$ band, HgTe has an inverted band structure where the $\Gamma_8$ band lays above the $\Gamma_6$. That creates approximately a particle in the box problem (see Figure 1.4.1). When the Fermi energy lays in the potential “box” that is created with the band structure, only low modes or just the ground state can be excited, keeping the system caught in two dimensions. As the “box” is not perfect, the electrons will feel an effective electric field, as a built-in feature of the quantum well. That is an important example for the Rashba interaction, discussed in section 3.4.1.

1.5 What are Surface and Edge States

Before we do extended calculations with surface and edge states, we are going to talk about these states. What makes them “edge” or “surface” states? As the Bloch theorem predicates, states in the bulk of a solid distribute like a modulated plane wave. As shown in subsection 1.3.1, with the Bloch theorem it is possible to derive the envelope function approximation. When it comes to an interface, the solutions for these envelope functions will be states that decay away from the surface. We have more or less a problem, that lives in a two-dimensional space. When we now restrict one coordinate of the surface plane to a finite regime, there can also be states decaying away from that borderline. Now we have a state that for example decays exponentially away in $z$-direction and in $y$-direction from a surface at $z = 0$, $y = 0$. 

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1.6 Basis States and Effective Hamiltonian

Figure 1.5.1: Example probability density of the edge state $\Psi(\xi(1-x)1(1-x))$ which will be determined in the following chapter. The decay lengths at $k_x = 0$ are given by $\lambda_1 = 0.076[\lambda_1]$ and $\lambda_2 = 0.002[\lambda_1]$. We used the Hamiltonian parameters $A = 3.645\text{eV}, B = -68.8\text{eV}Å, D = -51.2\text{eV}Å, M = 0.008\text{eV}$ and $C = -0.006$ as taken from [8].

In other words, it is a state distributing mostly at the one-dimensional $x$-axis. Figure 1.5.1 shows a probability density of such an edge state in the bulk gap. It distributes mainly at the edge $y = 0$ and has almost no probability to be measured in the bulk of the solid.

1.6 Basis States and Effective Hamiltonian

Before we calculate edge states, we take a closer look at our subband states:

$$|E_1, \uparrow\rangle = a(z)|j = \frac{1}{2}, m_j = \frac{1}{2}\rangle + b(z)|j = \frac{3}{2}, m_j = \frac{1}{2}\rangle,$$

$$|E_1, \downarrow\rangle = \bar{a}(z)|j = \frac{1}{2}, m_j = -\frac{1}{2}\rangle + \bar{b}(z)|j = \frac{3}{2}, m_j = -\frac{1}{2}\rangle,$$

$$|H_1, \uparrow\rangle = c(z)|j = \frac{3}{2}, m_j = \frac{3}{2}\rangle,$$

$$|H_1, \downarrow\rangle = \bar{c}(z)|j = \frac{3}{2}, m_j = -\frac{3}{2}\rangle.$$

Ref. [4] gives us a table with the parities of the envelope functions and states, that $\bar{a}(z) = a^*(z)$, $\bar{b}(z) = -b^*(z)$, $\bar{c}(z) = c^*(z)$ and $\tau|E_1, \uparrow\rangle = |E_1, \downarrow\rangle$, $\tau|H_1, \uparrow\rangle = |H_1, \downarrow\rangle$, where $\tau$ is the time-reversal operator. In this table find that $a,a^*,c,c^*$ are even functions and $b,b^*$ are odd functions of $z$. The basis states $\{|j = \frac{1}{2}, m_j = \frac{1}{2}\rangle\}$ are orthonormal.

We can use $\mathbf{k} \cdot \mathbf{p}$ perturbation theory to derive an effective in-plane Hamiltonian to describe the surface subbands $E_1$ and $H_1$. We start with a six band Hamiltonian $H_6(\mathbf{k})$ (the explicit form is not important here, see ([3])) written in the six component basis we introduced above.

The quantum well is grown in the $e_z$-direction [001], therefore we use the envelope function ansatz $\psi(k_x, k_y, z) = e^{i(k_x x + k_y y)} Z(z)$. We first need to solve the Schrödinger equation for every of the three different layers (at $k_x = 0$ and $k_y = 0$), as the material parameters change
discontinuously at the boundaries. The three solutions are then coupled by the boundary
conditions of the wave functions continuity and the continuity of the probability current
across the interfaces. We take a closer look at the ansatz for the wave function of the E1
subband made in [3], as we later need to know especially the details of the E1 band:

$$\Psi_I = \begin{pmatrix} e^{\alpha z} C_1 \\ 0 \\ 0 \\ e^{\alpha z} C_4 \end{pmatrix}, \quad \Psi_{II} = \begin{pmatrix} (e^{\delta z} + e^{-\delta z}) V_1 \\ 0 \\ 0 \\ (e^{\delta z} - e^{-\delta z}) V_4 \end{pmatrix}, \quad \Psi_{III} = \begin{pmatrix} e^{-\alpha z} C_1 \\ 0 \\ 0 \\ -e^{-\alpha z} C_4 \end{pmatrix}. \quad (1.6.5)$$

It is written in the basis $|j = \frac{1}{2}, m_j = \frac{1}{2}|, |j = \frac{1}{2}, m_j = -\frac{1}{2}|, |j = \frac{3}{2}, m_j = \frac{3}{2}|, |j = \frac{3}{2}, m_j = -\frac{3}{2}|$. The $\Psi$’s represent the state in the different regions of the quantum well. We need to match the wave functions and their first derivatives at the
boundary at $z = \pm \frac{d}{2}$, where $d$ is the width of the quantum well. That gives us $V_1 = C_1 \frac{1}{1+e^{\alpha d}}$
and $V_4 = C_4 \frac{1-e^{-\alpha d}}{1+e^{-\alpha d}}$. Taking another equation given by [3], we find the relation between $C_1$ and $C_4$ to be $(E_c(z) - A(z) \alpha^2 - E) C_1 = i \sqrt{3} P \alpha C_4$. The values $E_c(z)$ and $A(z)$
are real material parameters modeled as step functions of $z$. They change in the different materials
of the quantum well. $C_1$ need to be determined so, that the wave function is normalized:

$$\frac{|C_1|^2 e^{-\alpha d}}{\alpha} + \frac{|V_1|^2 + |V_4|^2}{\delta} (e^{\delta d} - e^{-\delta d}) + |V_1|^2 - |V_4|^2 2d = 1 \quad (1.6.6)$$

As it can be multiplied with a complex phase, we choose $C_1$ to be real. That means $C_4$ is
purely imaginary. With the equations taken from [3]

$$\frac{E_c^{(Cd)} - A^{(Cd)} \alpha^2(E) - E}{\sqrt{\frac{3}{2} P \alpha(E)}} = \frac{\sqrt{\frac{3}{2} P \alpha(E)}}{E_c^{(Cd)} + (\gamma_1^{(Cd)} + 2 \gamma_2^{(Cd)}) \alpha^2(E) - E}, \quad (1.6.7)$$

$$\frac{E_c^{(Hg)} - A^{(Hg)} \delta^2(E) - E}{\sqrt{\frac{3}{2} P \delta(E)}} = \frac{\sqrt{\frac{3}{2} P \delta(E)}}{E_c^{(Hg)} + (\gamma_1^{(Hg)} + 2 \gamma_2^{(Hg)}) \delta^2(E) - E}, \quad (1.6.8)$$

we are able to find $\alpha(E)$ and $\delta(E)$ as a function of the energy. The parameters $\gamma_1, \gamma_2$ are the
effective Luttinger parameters of the valence band. $E_c$ and $E_v$ are the conduction and valence
band edges, $P = -\frac{h}{m_0} \langle s|p_s|X \rangle$ is the Kane matrix element between the $s$ and $p$ bands
with $m_0$ the electron mass. The parameter $A = \frac{h^2}{2m_0} (\frac{2 \sum_j \Gamma_j (|S|p_s|u_j\rangle|^2)}{E_c(z) - E_j(z)} + 1) = \frac{h^2}{2m_0} (2F + 1)$ taken
from [4], describes an effective mass approximation. The notation $X^{(Cd)}$ means the value of the
parameter in the CdTe material, while $X^{(Hg)}$ refers to the value in the HgTe material.

With another formula given by [3], the energy can be numerically determined:

$$\frac{E_c^{(Cd)} - A^{(Cd)} \alpha^2(E) - E}{\alpha(E)} = -\tanh \left( \frac{\delta(E)d}{2} \right) \left( \frac{E_c^{(Hg)} - A^{(Hg)} \delta^2(E) - E}{\delta(E)} \right) \quad (1.6.9)$$

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1.6 Basis States and Effective Hamiltonian

With all the parameters given, we are able to calculate the envelope functions for (1.6.1)

\[ a(z) = \begin{cases} 
  e^{\alpha z}C_1 & \text{for } z \leq \frac{d}{2} \\
  (e^{\delta z} + e^{-\delta z})V_1 & \text{for } |z| < \frac{d}{2}, \\
  e^{-\alpha z}C_1 & \text{for } z \geq \frac{d}{2}, 
\end{cases} \quad (1.6.10) \]

and therefore also \( a^\ast (z), b^\ast (z) \). With similar steps, we can derive the \( E_1 \) and \( H_1 \) states. Taking the new basis for the subband states \( |E_1, \uparrow \rangle, |H_1, \uparrow \rangle, |E_1, \downarrow \rangle, |H_1, \downarrow \rangle \) (where \( |E_1, \uparrow \rangle = |E_1, \frac{1}{2} \rangle, |H_1, \uparrow \rangle = |H_1, \frac{3}{2} \rangle, \ldots \)), we can determine the effective \( 4 \times 4 \) Hamiltonian in first order with quasi degenerate perturbation theory ([12]):

\[ H_{ij}^{\text{eff}}(k_x, k_y) = \int_{-\infty}^{\infty} dz \langle \psi_j | \hat{H}_{0}(k_x, k_y, -i\partial_z) | \psi_i \rangle, \quad (1.6.12) \]

where \( \psi_i \) are the four basis subband states introduced above. This integral has to be split up into the three regions and then be calculated with respect to the different material parameters in the different regions. Taking the results from [3], we have

\[ H(k_x, k_y) = \begin{pmatrix} 
  \epsilon_k + \mathcal{M}(k) & Ak_- & 0 & 0 \\
  Ak_+ & \epsilon_k - \mathcal{M}(k) & 0 & 0 \\
  0 & 0 & \epsilon_k + \mathcal{M}(k) & -Ak_- \\
  0 & 0 & -Ak_+ & \epsilon_k - \mathcal{M}(k) 
\end{pmatrix}, \quad (1.6.13) \]

with \( \epsilon_k = C - D(k_x^2 + k_y^2), \mathcal{M} = M - B(k_x^2 + k_y^2), k_\pm = k_x \pm ik_y \). \( A, B, C, D, M \) are constants that depend on the special HgTe quantum well width. This Hamiltonian is an effective surface Hamiltonian, which describes states that mainly distribute at the interface between the HgTe and CdTe regions. This Hamiltonian induces stable helical edge states, if the width \( d \) of the quantum well exceeds a critical thickness \( d_c = 6.3\text{nm} \). That is where the energy of the \( E_1 \) and \( H_1 \) band are the same. Behind this point, the energies of both bands separate again, leading into an inverted regime, where the \( H_1 \) band is higher than the \( E_1 \) band.
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2.1 Toy Model: Dirac Hamiltonian

To get a better understanding of the problem in general, we are going to analyze a simpler two dimensional Dirac-Hamiltonian model. It is a simplification of the effective surface model (1.6.13):

$$H_D = p \cdot \sigma + \sigma_z m,$$  \hspace{1cm} (2.1.1)

with

$$p = \begin{pmatrix} -i \partial_x \\ -i \partial_y \end{pmatrix} \quad \text{and} \quad \sigma = \begin{pmatrix} \sigma_x \\ \sigma_y \end{pmatrix}.$$  \hspace{1cm} (2.1.2)

In matrix form, with the basis $|E_1, \uparrow\rangle$, $|H_1, \uparrow\rangle$, $|E_1, \downarrow\rangle$, $|H_1, \downarrow\rangle$, we get the following representation of the effective 2d-Hamiltonian:

$$H_{\text{eff}} = \begin{pmatrix} H_D(p) & 0 \\ 0 & H_D(-p) \end{pmatrix} = \begin{pmatrix} m & p_x - ip_y & 0 & 0 \\ p_x + ip_y & -m & 0 & 0 \\ 0 & 0 & m & -p_x - ip_y \\ 0 & 0 & -p_x + ip_y & -m \end{pmatrix}.$$  \hspace{1cm} (2.1.3)

We find

$$H_{\text{eff}}^2 = \begin{pmatrix} p_x^2 + m^2 & 0 & 0 & 0 \\ 0 & p_x^2 + m^2 & 0 & 0 \\ 0 & 0 & p_y^2 + m^2 & 0 \\ 0 & 0 & 0 & p_x^2 + m^2 \end{pmatrix}$$  \hspace{1cm} (2.1.4)

which makes it easy to determine the energies

$$E = \pm \sqrt{p_x^2 + m^2} = \pm \sqrt{p_x^2 + p_y^2 + m^2}.$$  \hspace{1cm} (2.1.5)

If we assume a product of plane waves as a solution, we get a band gap of $2m$ at the $\Gamma$–Point $p^2 = 0$, as can be seen in figure 2.1.1.

Now, we consider an one dimensional interface parallel to the $y$-axis at $x = 0$. This will give us effective edge states, describing electrons that only move along an edge (approximately one dimension) of the quantum well. We define $m$ as following:

$$m(x) = \begin{cases} -m_1 & \text{if } x \leq 0 \\ m_2 & \text{if } x > 0 \end{cases} \quad \text{with } m_1, m_2 > 0.$$  \hspace{1cm} (2.1.6)
2.1 Toy Model: Dirac Hamiltonian

Figure 2.1.1: The figure shows the energy dispersion for free bulk solutions \( E = \pm \sqrt{p_x^2 + p_y^2 + m^2} \) with a simple band gap (here \( p_y = 0 \) and \( m = 8 \) meV). We can see, that the gap is given by \( 2m \).

To simulate an inverted band structure. We later send \( m_2 \to \infty \), to create a vacuum for \( x > 0 \). That way, we will find edge states additionally to the free bulk solutions. As the effective Hamiltonian is block-diagonal, we first concentrate on the \( 2 \times 2 \) Hamiltonian \( H_D \). This leads to the following eigenvalue problem:

\[
\begin{pmatrix}
  m(x) & -i \partial_x - \partial_y \\
  -i \partial_x + \partial_y & -m(x)
\end{pmatrix}
\begin{pmatrix}
  \psi_1 \\
  \psi_2
\end{pmatrix}
= E
\begin{pmatrix}
  \psi_1 \\
  \psi_2
\end{pmatrix}.
\]  

(2.1.7)

As \( k_y \) is still a good quantum number and we are searching edge states, this problem can be easily decoupled with the ansatz \( \psi_{1/2} \propto e^{\lambda_D x} e^{ik_y y} \). The first line gives us

\[
\frac{(m(x) - E)}{(i\lambda_D + ik_y)} \psi_1 = \psi_2.
\]  

(2.1.8)

Inserting (2.1.8) in the second line of (2.1.7), we find

\[
(m(x))^2 - E^2 + k_y^2 = \lambda_D^2.
\]  

(2.1.9)

Here we choose \( E^2 = k_y^2 \), which leads to \( E = \pm k_y \) and \( \lambda_D^2 = m(x)^2 \). Considering a solution that can be normalized (with \( m(x) \) as defined above), we find

\[
\psi_2 = A(m(x)) \cdot e^{-m(x)x+ik_y y},
\]  

(2.1.10)

where \( A \) is a normalization constant. The \( x \)-dependency of \( m(x) \) refers to the definition above, thus \( m(x) \) is a constant in both regions. We treat the regions separately and match the wave functions at the end, so that the ansatz of a constant \( \lambda_D \) is valid. Using (2.1.8) and (2.1.12)
2 Edge States

we obtain the two solutions

\[ \psi_{11} = -i (m(x) - k_y) \psi_2 = -i \psi_2 \text{ with } E = k_y, \quad (2.1.11) \]

\[ \psi_{12} = -i (m(x) - k_y) \psi_2 \text{ with } E = -k_y, \]

which give us the states

\[ \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}_1 = A_1(m(x)) e^{-m(x)x + i k_y y} \begin{pmatrix} -i \\ 1 \end{pmatrix}, \]

\[ \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}_2 = A_2(m(x)) e^{-m(x)x + i k_y y} \begin{pmatrix} -i \frac{(m(x) - k_y)}{(m(x) + k_y)} \\ 1 \end{pmatrix}. \quad (2.1.12) \]

Using the boundary condition of continuity at \( x = 0 \), we find

\[ A_1(m_1) = A_1(m_2) = A_1 \quad (2.1.13) \]

and

\[ A_2(m_1) \frac{m_1 - k_y}{m_1 + k_y} = A_2(m_2) \frac{m_2 - k_y}{m_2 + k_y} = A_2. \quad (2.1.14) \]

The latter means, that there is no solution in this block for \( E = k_y \), because the boundary condition maps \( (\psi_1, \psi_2)^T_1 \) to \( (\psi_1, \psi_2)^T_2 \) (after normalization), which has the dispersion relation \( E = k_y \). That means (2.1.12) is our desired solution with \( E = k_y \). We find the normalization constant with the integral:

\[ \int_{-\infty}^{+\infty} dx \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}_1^* \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}_1 = \int_{-\infty}^{+\infty} dx 2 |A_1|^2 e^{-2m x} = 1, \quad (2.1.15) \]

which leads to the result \( A_1 = \sqrt{\frac{m_1 m_2}{m_1 + m_2}} \). When we now send \( m_2 \to \infty \) (to create a vacuum for \( x > 0 \)), our solution still exists with \( (\psi_1, \psi_2)^T = (0, 0)^T \) for \( x > 0 \).

If we repeat the whole procedure with the lower block of \( H_{\text{eff}} \) we obtain a second solution of the surface state type. All in all that gives us the following two edge states:

\[ \Psi_{\downarrow 1} = \Theta(-x) \sqrt{\frac{m_1 m_2}{m_1 + m_2}} e^{-m x + i k_y y} \begin{pmatrix} -i \\ 1 \\ 0 \\ 0 \end{pmatrix} \text{ with } E = k_y, \quad (2.1.16) \]

\[ \Psi_{\downarrow 1} = \Theta(-x) \sqrt{\frac{m_1 m_2}{m_1 + m_2}} e^{-m x + i k_y y} \begin{pmatrix} 0 \\ 0 \\ i \\ 1 \end{pmatrix} \text{ with } E = -k_y, \quad (2.1.17) \]
where $\Theta(x)$ is the Heaviside step function. Looking at the two dispersion relations, we see that we have a pair of electrons moving in opposite directions. Here we already see what characterizes these edge states. We can interpret them as a pairs of “spin” up and “spin” down like states with different movement directions. One state is the time reversed state of the other, making $\Psi_{1\uparrow} = \tau \Psi_{1\downarrow}$, where $\tau$ is the time reversal operator which has the representation $\tau = -i\sigma_y K$. Choosing an energy $E = \epsilon$ we see:

$\begin{align*}
\mathcal{T} \Psi_\uparrow(E = \epsilon) &= \mathcal{T} \sqrt{\frac{m_1 m_2}{m_1 + m_2}} e^{-m x + i \epsilon y} (-i \vert E1, \uparrow \rangle + \vert H1, \uparrow \rangle) \\
&= \sqrt{\frac{m_1 m_2}{m_1 + m_2}} e^{-m x - i \epsilon y} (i \vert E1, \downarrow \rangle + \vert H1, \downarrow \rangle) \\
&= \Psi_\downarrow(E = \epsilon).
\end{align*}$

This is the expected result, as the Hamiltonian is time-reversal invariant, so the states need to be the time reversed of each other because of Kramers degeneracy theorem. $\Psi_\uparrow$ and $\Psi_\downarrow$ are Kramers partners and are called helical edge states.

### 2.2 Quadratic Dirac Hamiltonian

In this section we are going to analyze the more complex surface model, introduced in (1.6)

$$
\mathcal{H}(k_x, k_y) = \begin{pmatrix}
\epsilon_k + \mathcal{M}(k) & A k_- & 0 & 0 \\
A k_+ & \epsilon_k - \mathcal{M}(k) & 0 & 0 \\
0 & 0 & \epsilon_k + \mathcal{M}(k) & -A k_+ \\
0 & 0 & -A k_- & \epsilon_k - \mathcal{M}(k)
\end{pmatrix},
$$

with $\epsilon_k = C - D(k_x^2 + k_y^2)$, $\mathcal{M} = M - B(k_x^2 + k_y^2)$, $k_\pm = k_x \pm i k_y$. The ordered basis of the matrix is again $\vert E1, \uparrow \rangle$, $\vert H1, \uparrow \rangle$, $\vert E1, \downarrow \rangle$, $\vert H1, \downarrow \rangle$. As in the Dirac toy model, the Hamiltonian is block diagonal. Therefore we concentrate on solving the eigenvalue problem of the upper block. For bulk solutions, we can choose the ansatz $\Psi(x, y) \propto e^{ik_x x} e^{ik_y y}$, which makes $k_x$ and $k_y$ good quantum numbers. Now it is easy to diagonalize the Hamiltonian, obtaining two energy branches $\epsilon_k = \pm \sqrt{(M - B(k_x^2 + k_y^2)^2 + A^2(k_x^2 + k_y^2)}$. This shows, that the energy gap for small values of $k_y$ and $k_x$ is of the order of $M$, as can be seen in figure 2.2.1.

For the edge solutions, we consider an interface parallel to the $x$-axis at $y = 0$ and periodic boundary conditions for $x$. The solution will be a superposition of product states like $\Psi = Y(y) X(x)$ where $X(x) = e^{ik_x x}$ and $Y(y) \propto e^{iy}$, where $\lambda$ has to be real and $\lambda > 0$. For $y > 0$ we assume vacuum without any states, thus $Y(y \geq 0) = 0$, which corresponds to the hard wall approximation. $k_x$ is still a good quantum number, while $k_y$ has to be resubstituted by $-i\partial_y$. As $C$ is just a doping parameter (tunable by top and/or bottom gates [8]) proportional to the identity, we choose $E = E - C$, where $E$ is the energy. For simplicity reasons, we refer $E$ with $E$, keeping in mind, that it is possible to dope $E$ with the parameter $C$. That gives us the following pair of equations:
have functions that can be normalized, we just need looking at the result for \( g \). For \( k_y = 0 \) the gap is given by \( M \), while increasing \( k_y \) enlarges the gap. We used the parameters \( A = 3.645 \text{eV}, B = -68.8 \text{eVÅ}, D = -51.2 \text{eVÅ}, M = 0.008 \text{eV} \) and \( C = -0.006 \) as taken from [8].

\[
\begin{align*}
[M - (D + B)(k_x^2 - \partial_y^2)] \psi_1 + A(k_x - \partial_y) \psi_2 &= E\psi_1, \quad (2.2.2) \\
[-M - (D - B)(k_x^2 - \partial_y^2)] \psi_2 + A(k_x + \partial_y) \psi_1 &= E\psi_2. \quad (2.2.3)
\end{align*}
\]

Using the test function \( \psi_{1/2} \propto e^{\lambda y} \) and defining \((B + D) = B_+, (B - D) = B_- \), we obtain

\[
\begin{align*}
[M - B_+(k_x^2 - \lambda^2)] \psi_1 + A(k_x - \lambda) \psi_2 &= E\psi_1, \quad (2.2.4) \\
[-M + B_-(k_x^2 - \lambda^2)] \psi_2 + A(k_x + \lambda) \psi_1 &= E\psi_2. \quad (2.2.5)
\end{align*}
\]

We can express \( \psi_2 = \psi_1 \frac{[M-B_+(k_x^2-\lambda^2)-E]}{A(\lambda-k_x)} \) and use (2.2.5) to find an equation of the form \( \lambda^4 - \frac{p}{2} \lambda^2 + q = 0 \) with \( p = \frac{A^2-2(MB+ED)}{2(B^2-D^2)} + k_x^2 \) and \( q = \frac{A^2-2(MB+ED)k_x^2-E^2+M^2}{(B^2-D^2)} + k_x^2 \). That gives us

\[
\lambda_{1/2}^2 = k_x^2 + F \pm \sqrt{F^2 - \frac{M^2-E^2}{B^2-D^2}}, \quad (2.2.6)
\]

where \( F = \frac{A^2-2(MB+ED)}{2(B^2-D^2)} \). At \( k = 0 \) we can find real \( \lambda \)s for \( B^2 > D^2 \) and \( \frac{A^2}{B_+B_-} > \frac{4M}{B} \) in the energy gap \(|E| < M\) (in respect to the energy dispersion we will find). The condition \( B^2 > D^2 \) keeps \( \frac{M^2-E^2}{B^2-D^2} \) positive, so that \( F \geq \sqrt{F^2 - \frac{M^2-E^2}{B^2-D^2}} \), while the condition \( \frac{A^2}{B_+B_-} > \frac{4M}{B} \) ensures that \( F^2 - \frac{M^2-E^2}{B^2-D^2} \geq 0 \).

Looking at the result for \( \lambda \), we see that we have four solutions: \( \pm \lambda_1 \) and \( \pm \lambda_2 \). As we need to have functions that can be normalized, we just need \( +\lambda_{1/2} \), using the ansatz:

\[
\begin{align*}
\psi_1(y) &= Z e^{\lambda_1 y} + T \cdot e^{\lambda_2 y} \quad (2.2.7) \\
\psi_2(y) &= \tilde{Z} e^{\lambda_1 y} + \tilde{T} \cdot e^{\lambda_2 y} \quad (2.2.8)
\end{align*}
\]
As already mentioned, we use the hard wall approximation, which means the wave function equals zero for the whole region above the interface at $y \geq 0$ (vacuum). In this approximation, we may just use the boundary condition of the wave functions continuity, but not the continuity of the first derivative. With the boundary condition $\psi_{1/2}(0) = 0$, we get:

$$Z = -T.$$ (2.2.9)

Using equation (2.2.2) to derive:

$$\left( M - B_+ k_x^2 \right) \psi_1 + A k_x \psi_2 + B_+ \cdot Z \left( \lambda_1^2 e^{\lambda_1 y} - \lambda_2^2 e^{\lambda_2 y} \right)$$

$$+ A Z \left( \lambda_1 e^{\lambda_1 y} - \lambda_2 e^{\lambda_2 y} \right) = E \psi_1,$$ (2.2.10)

we can order the components in front of each exponential function to find two equations $G(\lambda_1) e^{\lambda_1 y} = 0$ and $G(\lambda_2) e^{\lambda_2 y} = 0$ (with $Z = \eta Z$):

$$B_+ \left( \lambda_1^2 - k_x^2 \right) + A \eta (k_x - \lambda_1) - (E - M) = 0,$$ (2.2.11)

$$-B_+ \left( \lambda_2^2 - k_x^2 \right) - A \eta (k_x - \lambda_2) + (E - M) = 0.$$ (2.2.12)

If we add (2.2.11) and (2.2.12) we can determine $\eta = \frac{B_+ (\lambda_1 + \lambda_2)}{A}$. Subtracting both equations leads to a self consistent equation for the energy:

$$E_+ = M - B_+ \lambda_1 \lambda_2 + B_+ (\lambda_1 + \lambda_2) k_x - B_+ k_x^2.$$ (2.2.13)

To solve this equation, we expand $E$ in orders of $k_x$: $E = \sum E_i k_x^i$; the terms $\lambda_1 \lambda_2$ up to the first order and $(\lambda_1 + \lambda_2)$ to the zeroth order in $k_x$. That gives us

$$E_0 + E_1 k_x = M - B_+ \left( \sqrt{\frac{M^2 - E_0^2}{B_+ B_-}} - \sqrt{\frac{M^2 - E_0^2}{B_+ B_-}} \frac{E_0 E_1}{B_+ B_-} k_x \right) + B_+ A \sqrt{\frac{B_+}{B_-}} k_x.$$ (2.2.14)

Comparing coefficients leads us to $E_+ = -\frac{DM}{B} + A \sqrt{\frac{B_+ B_-}{B^2}} k_x + O(k_x^2)$. There is another solution $E_0 = M$, but this solution is in conflict with the second line of the eigenvalue problem (2.2.3). This second line leads to $E = -M$ and $E = E_+$, which makes $E_+$ the final energy dispersion for the upper block of the Hamiltonian. Repeating all the steps with the lower block of the Hamiltonian (2.2.1) gives us $\eta = \eta = \frac{B_+ (\lambda_1 + \lambda_2)}{A}$ and

$$E_- = M - B_+ \lambda_1 \lambda_2 - B_+ (\lambda_1 + \lambda_2) k_x - B_+ k_x^2$$ (2.2.15)

leading to an energy-$k_x$ dispersion of $E_- = -\frac{DM}{B} - A \sqrt{\frac{B_+ B_-}{B^2}} k_x + O(k_x^2)$). Extended calculations with Mathematica show, that all coefficients $E_i$ for quadratic and higher-order terms in $k_x$ vanish, what makes our solution exact for this model. Recalling that we can dope $E_\pm$ with the parameter $C = \frac{DM}{B}$ makes it possible to gain a linear dispersion relation without offset:

$$E_\pm = \pm A \sqrt{\frac{B_+ B_-}{B^2}} k_x = \pm v_F k_x.$$ (2.2.16)
2 Edge States

Figure 2.2.2: This plot shows the linear dispersion of helical edge states (blue) $E_{\pm} = \pm v_F k_x$ and the dispersion of the bulk states $E_{\text{Bulk}} = \epsilon_k \pm \sqrt{(M - B(k_x^2 + k_y^2)^2 + A^2(k_x^2 + k_y^2)^2)}$, plotted for different $k_y$ (black). We see that the edge states do not cross in the middle of the gap, but next to the positive bulk energies. This position in the gap is determined by the ratio $D_B$, for $D = B$ the crossing point would touch the lowest point of the positive energy branch. We used the parameters $A = 3.645\text{eV}, B = -68.8\text{eVÅ}, D = -51.2\text{eVÅ}, M = 0.008\text{eV}$ and $C = -0.006$ as taken from [8].

$\nu_F$ is the Fermi velocity (see figure 2.2.2). It describes the group velocity of the moving wave. All in all we have the states:

$$\Psi_\uparrow = \Theta(-y) Z e^{ik_x x} (e^{\lambda_1 y} - e^{\lambda_2 y}) \begin{pmatrix} 1 \\ \eta \\ 0 \\ 0 \end{pmatrix} \quad \text{with dispersion } E = E_+,$$

(2.2.17)

$$\Psi_\downarrow = \Theta(-y) Z e^{ik_x x} (e^{\lambda_1 y} - e^{\lambda_2 y}) \begin{pmatrix} 0 \\ 0 \\ 1 \\ \eta \end{pmatrix} \quad \text{with dispersion } E = E_-,$$

(2.2.18)

where $Z = \sqrt{\frac{2\lambda_1 \lambda_2 (\lambda_1 + \lambda_2)}{(1 + \eta^2)(\lambda_1 - \lambda_2)^2}}$ is a normalization constant. The up state is the time reversed state of the down state ($\mathcal{T} \Psi_\uparrow = -i\sigma_y K \Psi_\downarrow = \Psi_\downarrow$), making them Kramers partners. With $\nu_F = \frac{\partial E}{\partial k}$, we see that the electrons move in opposite $x-$directions. They distribute mainly at the edge $y = 0$ (see figure 1.5.1).
3 Edge Hamiltonians in Degenerate Perturbation Theory

3.1 Perturbation Method

In the chapter before, we discussed the edge states we found in our model for HgTe-quantum wells. We now introduce a set of Hamiltonians, that leads to a weak coupling of the edge states with the bulk states. We will derive effective Hamiltonians in the subspace of the edge states, using the quasi-degenerate perturbation theory called Löwdin partitioning or Schrieffer-Wolff transformation [12]. We can write our Hamilton operator as a sum

\[ H = H^0 + H', \]

(3.1.1)

where \( H^0 \) is diagonal with eigenvalues \( E_n \) and eigenfunctions \( |n\). \( H' \) is treated as perturbation and should therefore only lead to a weak coupling between the subspace of states A, which are the ones we are interested in and states B, which refer to the rest. In our case it should have a weak coupling between the bulk and the edge states compared with the energy gap. The aim of the Schrieffer-Wolff transformation is to find a unitary transformation \( e^{-SHe^S} \) with \( S \) anti-Hermitian, which maps \( H' \) block-diagonal, so that all matrix elements between states from set A and states from set B vanish. The exact derivation can be found in [12].

In first order, we find an effective Hamiltonian

\[ (H_{\text{eff}}^{(1)})_{ij} = \langle m_j | H' | m_i \rangle, \]

(3.1.2)

where the \( |m_j\rangle \)s are the eigenstates of \( H^0 \) in the subspace A. The second order term reads

\[ (H_{\text{eff}}^{(2)})_{ij} = \frac{1}{2} \sum_l (m_i | H' | k_l \rangle \langle k_l | H' | m_j \rangle \left[ \frac{1}{E_i - E_l} + \frac{1}{E_j - E_l} \right], \]

(3.1.3)

with the \( |k_l\rangle \)s as the eigenkets of \( H^0 \) in subspace B. As we use the envelope function approximation, \( \langle m_j | H' | m_i \rangle \) denotes to \( \sum_{ab} \int dz dy f(z, y)_{m_i}^{a} f(z, y)_{m_j}^{b} |a|H'|b\rangle \), where \(|a\rangle, |b\rangle\) are elements of the six basic bands as explained in subsection 1.3.3. The \( x \)-dependency is left untouched, to obtain an effective model in the \( x \)-space.

3.2 Edge States in Perturbation Theory

Now we are going to solve the quadratic Dirac Hamiltonian (2.2.1) in \( k \cdot p \) perturbation theory up to first order in \( k \). This is a simple method to determine the energy dispersion for
the helical edge states. First, we solve the problem of for \( k_x = 0 \) and see the terms \( \propto k_x \) as a small perturbation. We use the same ansatz and find \( \lambda(k_x) \) as in (2.2.6) with \( k_x = 0 \), making the \( \lambda \) \( k_x \)-independent. Equation (2.2.13) here becomes

\[
E_+(k_x = 0) = M - B_+ \lambda_1 \lambda_2. \tag{3.2.1}
\]

It can be easily solved for \( E \), finding \( E_1 = M \) and \( E_2 = -\frac{DM}{B} \). The solution \( E_1 = M \) is not compatible with \( E_+(k_x = 0) = -M - B_- \lambda_1 \lambda_2 \) which can be derived from the second line of the eigenvalue problem. It has the solutions \( E_1 = -M \) and \( E_2 = -\frac{DM}{B} \). Therefore \( E = -\frac{DM}{B} \) is the right energy for \( k_x = 0 \). As for the exact solution, our eigenvector is still \( \upsilon = (1, 1)^T \), where \( \upsilon = \frac{B_+ (\lambda_1 + \lambda_2)}{A} \). That gives us the exact same states as in (2.2.17) and (2.2.18), just with \( 1/2 \) at \( k_x = 0 \).

We now calculate the effective Hamiltonian \( (H_{eff})_{ij} = \langle \Psi_j | H_{k_x} | \Psi_i \rangle \), where \( i, j \in \{\uparrow, \downarrow\} \). \( H_{k_x} \) is the Hamiltonian proportional to all terms linear in \( k_x \). The matrix elements are calculated as following:

\[
\langle \Psi_{\uparrow} | H_A | \Psi_{\uparrow} \rangle = \frac{1}{1 + \eta^2} \begin{pmatrix} 1 & \frac{1}{\eta} \\ 0 & \frac{1}{\eta} \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & A k_x & 0 & 0 \\ 0 & 0 & -A k_x & 0 \\ 0 & 0 & 0 & -A k_x \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{\eta} \\ 0 \\ 0 \end{pmatrix} = \frac{2A k_x \eta}{1 + \eta^2} \tag{3.2.2}
\]

In the same way, we find the other matrix elements to be:

\[
\langle \Psi_{\downarrow} | H_{k_x} | \Psi_{\downarrow} \rangle = \frac{-2A k_x \eta}{1 + \eta^2}, \tag{3.2.3}
\]

\[
\langle \Psi_{\uparrow} | H_{k_x} | \Psi_{\downarrow} \rangle = \langle \Psi_{\downarrow} | H_{k_x} | \Psi_{\uparrow} \rangle = 0. \tag{3.2.4}
\]

Calculating \( \eta \) for \( k_x = 0 \) gives us \( \eta = \sqrt{\frac{B_+}{B_-}} \). If we put that into (3.2.2) and (3.2.3), we obtain

\[
H_{Aeff} = \begin{pmatrix} A k_x \sqrt{\frac{B_+ B_-}{B_-}} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -A k_x \sqrt{\frac{B_+ B_-}{B_-}} & 0 \end{pmatrix} = \begin{pmatrix} v_F k_x & 0 & 0 \\ 0 & 0 & -v_F k_x \end{pmatrix}. \tag{3.2.6}
\]

This matrix is diagonal, giving us the perturbed energies directly. If we compare it with (2.2.16), we see that both are identical. With this method, we are able to find the first order energy dispersion for our problem way easier, than with the exact method.
3.3 Additional Hamiltonians

We now introduce the following terms (\(H_D\) and \(H_R\) are given by [8]) as perturbation of the original Hamiltonian (2.2.1):

\[
H_{\text{per}} = H_D + H_R + H_V
\]

\[
= h(\cos(2\theta)\sigma_y + \sin(2\theta)\sigma_x)s_y + R_0 \left( \frac{s_z + 1}{2} (k_x\sigma_y - k_y\sigma_x) \right) \quad (3.3.1)
\]

\[
+ V_0 \delta(x) S \cdot J_s \quad , \quad (3.3.3)
\]

\[
\text{where } \sigma \text{ acts in the pseudo spin space of the edge states while } s \text{ acts in the } (E_1, H_1)\text{-space.}
\]

The coupling constants \(h, R_0\) and \(V_0\) need to be small in comparison to the energy gap, so that the edge states couple just weakly with the bulk states. The Dresselhaus Term is a bulk inversion asymmetry term, which is not invariant under rotation in the \(xy\)-plan. Therefore, \(\theta\) describes the angle between the \(x\)-axis and the [100] crystal direction. The Rashba term corresponds to an electric potential and the impurity term describes a magnetic impurity interacting with the electrons. In the following, the single terms are discussed more precisely.

3.4 First Order Calculations

3.4.1 Rashba Term

The Rashba term is switched on with an electric field in the \(z\)-direction of the quantum well. It is important, even if there is no artificial external field in the experiment, because the quantum well can have an effective electric field as a build-in feature. That makes a discussion of the Rashba term very important. The leading-order Rashba term is

\[
H_R = R_0 \left( \frac{s_z + 1}{2} (k_x\sigma_y - k_y\sigma_x) \right), \quad (3.4.1)
\]

which is a good approximation of the Rashba effect in the small \(k_x\) limit we are researching. In the ordered basis of \(E_1\) and \(H_1\) bands, \(H_R\) reads:

\[
\left(\begin{array}{cccc}
0 & 0 & -(k_y + ik_x)R_0 & 0 \\
0 & 0 & 0 & 0 \\
-(k_y - ik_x)R_0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{array}\right) \quad (3.4.2)
\]

One can easily see, that the diagonals are given by

\[
\langle \Psi_\uparrow | H_R | \Psi_\uparrow \rangle = \frac{1}{1 + \eta^2} \left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
\end{array}\right) \left(\begin{array}{cccc}
0 & 0 & -(k_y + ik_x)R_0 & 0 \\
0 & 0 & 0 & 0 \\
-(k_y - ik_x)R_0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{array}\right) \left(\begin{array}{c}
1 \\
\eta \\
0 \\
0 \\
\end{array}\right) = 0 \quad (3.4.3)
\]
and in the same way, \( \langle \Psi_\uparrow | H_A | \Psi_\downarrow \rangle = 0 \). For the off-diagonal elements we get
\[
\langle \Psi_\uparrow | H_R | \Psi_\downarrow \rangle = \frac{R_o}{1 + \eta^2} \int dy \left[ (-i)k_x Z^2 (e^{\lambda_1 y} - e^{\lambda_2 y})^2 ight. \\
+ i Z^2 (e^{\lambda_1 y} - e^{\lambda_2 y}) \partial_y (e^{\lambda_1 y} - e^{\lambda_2 y}) \left. \right] \\
= -i R_o k_x \frac{1}{1 + \eta^2} 
\]
(3.4.4)
(3.4.5)
(3.4.6)

The term proportional to \( k_y \) does not contribute, as we can see from
\[
\int dy \left[ \mu(y) \partial_y \mu(y) \right]_{\text{P.I.}} = (\mu(y)^2)_{-\infty}^\infty - \int dy [\mu(y) \partial_y \mu(y)] = 0, \text{ for vanishing } \mu(y)\big|_{-\infty}^0.
\]
With the same argument, we obtain \( \langle \Psi_\downarrow | H_A | \Psi_\uparrow \rangle = -i R_o k_x \frac{1}{1 + \eta^2} \). That gives us the form
\[
H_R = \begin{pmatrix}
0 & -i \alpha_R k_x \\
-i \alpha_R k_x & 0
\end{pmatrix} = \alpha_R k_x \sigma_y,
\]
(3.4.7)

where \( \alpha_R = \frac{R_o}{1 + \eta^2} \) is the coupling constant for the Rashba interaction.

### 3.4.2 Dresselhaus Term

The Dresselhaus term has, in contrast to the Rashba term, no \( k \)-dependence. Additionally, it is not rotationally invariant, therefore it introduces the angle \( \theta \). It refers to the angle between the crystal [100] direction and the \( x \)-direction in the chosen coordinate system. As a consequence of that, physics will in general depend on \( \theta \) thus we keep it as a parameter. The Hamiltonian reads
\[
H_D = \hbar (\cos(2\theta) \sigma_y + \sin(2\theta) \sigma_x) s_y.
\]
(3.4.8)

Before we just calculate the effective Hamiltonian, we can already make a statement of what we will expect: The effective Dresselhaus Hamiltonian in first order perturbation theory has to be zero or proportional to the identity. Kramers theorem of degeneracy tells us, that we need to have at least a twice degenerate system, if the Hamiltonian is time-reversal invariant. Now, we do have just time-reversal invariant terms and our unperturbated energies \( E_{\pm} = \frac{-BM}{\hbar} + C \) at \( k = 0 \) are twice degenerate, as we expect. If we found an effective Hamiltonian with off-diagonal elements, that would separate the energies. As example, the matrix
\[
P = \begin{pmatrix}
L & W \\
N & L
\end{pmatrix}
\]
(3.4.9)

has the eigenvalues \( \lambda_{1/2} = L \pm \sqrt{NW} \). If \( L \) is a constant and \( NW \) does not have a degree of freedom like \( k_x \) (\( \theta \) is a fixed parameter for our system) which could map \( \lambda_1 \) on \( \lambda_2 \), the degeneracy would be broken. That can not happen, as long as we do not break time-reversal invariance, so the off diagonal elements of the effective Dresselhaus Hamiltonian need to be zero. In the next step, we need to calculate the diagonal elements and we are also going to
3.4 First Order Calculations

calculate the off-diagonal elements, to proof our claim:

\[ \langle \Psi_\uparrow \vert H_D \vert \Psi_\downarrow \rangle = Z^2 \begin{pmatrix} 1 \\ \eta \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & -he^{i2\theta} \\ 0 & 0 & he^{i2\theta} & 0 \\ 0 & he^{-i2\theta} & 0 & 0 \\ -he^{i2\theta} & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ \eta \\ 0 \\ 0 \end{pmatrix} = Z^2 (\eta \eta - h\eta) e^{i2\theta} = 0 \] (3.4.10)

\[ \langle \Psi_\uparrow \vert H_D \vert \Psi_\uparrow \rangle = Z^2 \begin{pmatrix} 1 \\ \eta \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & -he^{i2\theta} \\ 0 & 0 & he^{-i2\theta} & 0 \\ 0 & he^{-i2\theta} & 0 & 0 \\ -he^{i2\theta} & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ \eta \\ 0 \\ 0 \end{pmatrix} = 0. \] (3.4.11)

The other matrix elements are also obtained to be zero, confirming our prediction that the Dresselhaus term has no influence on our system in first order perturbation theory.

3.4.3 Magnetic Impurity

We now introduce a term in our Hamiltonian, that describes a magnetic impurity located at \( x = 0 \) which couples to the edge states of the system

\[ H_M = V_0 \delta(x) S \cdot J_s, \] (3.4.12)

where \( J_s \) is the spin operator of the edge states, while \( S \) is the operator that acts on the impurity spin. It is important, that the strength of the potential is smaller than \( M \), which is the constant that mainly defines the gap between the bulk states. Only in this regime, the perturbation calculations are valid. \( H_M \) has no \( y \)-dependancy, which is equivalent to an impurity smeared out in \( y \)-direction. It is also possible to introduce an impurity that is exactly localized at \( y = y_0 \). It has the form \( H_{My_0} = V_0 \delta(x) \delta(y - y_0) S \cdot J_s \). One has to pay attention to not choose \( y_0 \geq 0 \), because the states are defined to equal zero for \( y \geq 0 \), so that an impurity would have no effect there. If we use \( H_{My_0} \), it does not change any calculation here dramatically beside a global factor \( Q(y_0) \) (see figure 3.4.1). We use \( S \cdot J_s = S^z J_s^z + \frac{1}{2} (S^+ J_s^- + S^- J_s^+) \) with \( J_s^+ = J_s^x + iJ_s^y \) and \( J_s^- = J_s^x - iJ_s^y \) to bring the Hamiltonian to the form

\[ H_M = V_0 \delta(x) [S^z J_s^z + \frac{1}{2} (S^+ J_s^- + S^- J_s^+)]. \] (3.4.13)

The edge states we found in section (3.2) are \( |\Psi_\uparrow \rangle = \psi(y, x) \langle 1 \vert E1, \uparrow \rangle + \eta \vert H1, \uparrow \rangle \rangle \) and \( |\Psi_\downarrow \rangle = \psi(y, x) \langle 1 \vert E1, \downarrow \rangle + \eta \vert H1, \downarrow \rangle \rangle \) (see equations (2.2.17) and (2.2.18)). That gives us an effective \( 2 \times 2 \) matrix. Because of the parities given in section 1.6, we do not have any coupling between
3 Edge Hamiltonians in Degenerate Perturbation Theory

Figure 3.4.1: The figure shows a plot of the global factor \( Q(y_0) = (e^{\lambda_1 y_0} - e^{\lambda_2 y_0})^2 \frac{2\lambda_1 \lambda_2 (\lambda_1 + \lambda_2)}{(\lambda_1 - \lambda_2)^2} < 1 \). This factor modulates the effective Hamiltonian \( H_M \rightarrow Q(y_0)H_M \) when considering an impurity exactly localized at \( y_0 \). The modulation is proportional to the probability density of the wave functions \( y \)-part. With this factor inserted, the calculations are exactly the same as for a blurred impurity.

\[ a(z), \tilde{a}(z), c(z), \tilde{c}(z) \text{ and } b(z), \tilde{b}(z) \text{ terms.} \]

The matrix elements are calculated as following:

\[
\langle \Psi | H_M | \Psi \rangle = \frac{1}{1+\eta^2} \left( \langle H1, \uparrow | \eta^* \rangle + \langle E1, \uparrow | \rangle H_M (| E1, \uparrow \rangle + \eta | H1, \uparrow \rangle) \right) \tag{3.4.14}
\]

\[
= \frac{1}{1+\eta^2} \langle E1, \uparrow | (H_M)| E1, \uparrow \rangle + \eta^2 \frac{1}{1+\eta^2} \langle H1, \uparrow | (H_M)| H1, \uparrow \rangle
\]

\[
= (1) = \frac{1}{2} S^z V_0 \delta(x) \quad \text{and} \quad (2) = \frac{3}{2} S^z V_0 \delta(x)
\]

\[
+ \eta \frac{1}{1+\eta^2} \langle E1, \uparrow | (H_M)| H1, \uparrow \rangle + \eta \frac{1}{1+\eta^2} \langle H1, \uparrow | (H_M)| E1, \uparrow \rangle
\]

\[
= (3) = 0 \quad \text{and} \quad (4) = 0
\]

\[
= \frac{(1\frac{1}{2} + \frac{3}{2} \eta^2) V_0 S^z \delta(x)}{1+\eta^2}.
\]

The integral of the position space is left out, if it just leads to a factor one, because of the states normalization. The term \((1) = \frac{1}{2} S^z V_0 \delta(x)\) and \((2) = \frac{3}{2} S^z V_0 \delta(x)\) come out that way, because only the \(J^z\) operator with \( J^z | j, m_j \rangle = m_j | j, m_j \rangle \) leaves the states untouched, so that \( (j, m_j | j, m_j) = \delta_{ij} \) equals one. The terms \((3)\) and \((4)\) could have a possible coupling between the \( j = \frac{3}{2} \) terms, but because of the parities of the envelope functions, these terms are also
Therefore we find that

As shown above, we can choose zero as result. In the second line of \((1) = 3.4\) First Order Calculations

\[
(1) = (E_1, \uparrow \uparrow | (H_M)|E_1, \uparrow) \quad (3.4.15)
\]

\[
= \int_{-\infty}^{\infty} dz \left( \frac{1}{1+\eta^2} (j = \frac{1}{2}, m_j = \frac{1}{2}) \right) \left| a(z) a^*(z) V_0 | S^+ J_s^z + \frac{1}{2} (S^+ J_s^z + S_- J_s^z) \right| |j = \frac{1}{2}, m_j = \frac{1}{2} \rangle
\]

\[
= \frac{1}{2} \eta \delta(\eta) | d(z) | a^*(z) \rangle, \text{ just } S_\uparrow \text{leaves the state untouched with eigenvalue } \frac{1}{2}.
\]

\[
+ \frac{1}{2} \eta \delta(\eta) | d(z) | b^*(z) \rangle, \text{ just } S_\uparrow \text{leaves the state untouched with eigenvalue } \frac{1}{2}.
\]

\[
+ \eta \frac{1}{1+\eta^2} | d(z) | b^*(z) \rangle, \text{ just } S_\uparrow \text{leaves the state untouched with eigenvalue } \frac{1}{2}.
\]

\[
= \frac{1}{2} V_0 \delta(x) S^z.
\]

\[
(3) = (E_1, \uparrow \uparrow | (H_M)|H_1, \uparrow) \quad (3.4.16)
\]

\[
= \int_{-\infty}^{\infty} dz \left( \langle j = \frac{1}{2}, m_j = \frac{1}{2} | c(z) a^*(z) V_0 | S^+ J_s^z + \frac{1}{2} (S^+ J_s^z + S_- J_s^z) \rangle |j = \frac{1}{2}, m_j = \frac{3}{2} \rangle \right)
\]

\[
= 0 \text{ because } j = \frac{3}{2} \text{ does not couple with } j = \frac{1}{2}.
\]

\[
+ \langle j = \frac{3}{2}, m_j = \frac{1}{2} | c(z) b^*(z) V_0 | S^+ J_s^z + \frac{1}{2} (S^+ J_s^z + S_- J_s^z) \rangle |j = \frac{3}{2}, m_j = \frac{3}{2} \rangle \rangle
\]

\[
= 0 \text{ because even and odd parity of } c(z) \text{ and } b^*(z).
\]

\[
= 0.
\]

In the second line of (3), the operator \(J_\uparrow \) would couple the states, but here the parity leads to zero as result. In (1) we used \( \int dz \ a(z) a^*(z) + \int dz \ b(z) b^*(z) = 1 \). We calculate the other three matrix elements in the same way as above, giving us:

\[
\langle \Psi_{\uparrow} | H_M | \Psi_{\uparrow} \rangle = \frac{V_0 \delta(x)}{1 + \eta^2} \left( \frac{1}{2} + \frac{3}{2} \eta^2 \right) S^z = J_z S^z \quad (3.4.17)
\]

\[
\langle \Psi_\downarrow | H_M | \Psi_\downarrow \rangle = -\frac{V_0 \delta(x)}{1 + \eta^2} \left( \frac{1}{2} + \frac{3}{2} \eta^2 \right) S^z = -J_z S^z \quad (3.4.18)
\]

\[
\langle \Psi_{\uparrow} | H_M | \Psi_\downarrow \rangle = \frac{1}{2} \frac{V_0 \delta(x)}{1 + \eta^2} \int dz (a(z)^2 - 2b(z)^2) S^+ = J_x 1 S^+ \quad (3.4.19)
\]

\[
\langle \Psi_\downarrow | H_M | \Psi_{\uparrow} \rangle = \frac{1}{2} \frac{V_0 \delta(x)}{1 + \eta^2} \int dz (a^*(z)^2 - 2b^*(z)^2) S^- = J_{x2} S^- \quad (3.4.20)
\]

As shown above, we can choose \( a(z) \) to be real, which gives us a totally imaginary \( b(z) \). Therefore we find that \( J_{x1} = J_{x2} = J_x = J_y \) (these terms are coupling constants and do not
need to correspond to the expected value of the operator components of $J_S$ and our effective Kondo Hamiltonian reads:

$$H_K = \delta(x)(J_x \sigma_x S^x + J_y \sigma_y S^y + J_z \sigma_z S^z), \quad (3.4.21)$$

with

$$J_x = J_y = \frac{V_0}{2(1 + \eta^2)} \int dz \left( a(z)^2 - 2b(z)^2 \right), \quad (3.4.22)$$

$$J_z = \frac{V_0}{1 + \eta^2} \left( \frac{1}{2} + \frac{3}{2} \eta^2 \right), \quad (3.4.23)$$

The $\sigma$-matrices act on the pseudo-spin space. If we want to calculate $J_z$ and $J_x$, we just need to know the envelope functions $a(z)$ and $b(z)$ and the parameters of the Hamiltonian (2.2.1).

Additionally we give the first order effective Hamiltonian in the surface ($E_1, H_1$)-space

$$H_{MS} = \delta(x) \left( \begin{array}{ccc}
\frac{1}{2} V_0 S^z & 0 & J_z (S_x + iS_y) \\
0 & \frac{3}{2} V_0 S^z & 0 \\
J_z (S_x - iS_y) & 0 & -\frac{1}{2} V_0 S^z \\
0 & 0 & -\frac{3}{2} V_0 S^z
\end{array} \right), \quad (3.4.24)$$

which we use in the second order perturbation calculations.

### 3.5 Second Order Calculations

In second order perturbation theory, we receive terms that can be larger than some first order terms, because we do have different “small” parameters. The second order effective Hamiltonian reads in this case

$$(H^{(2)}_{\text{eff}})_{ij} = \frac{1}{2} \int d^3k \langle m_i | H' | k \rangle \langle k | H' | m_j \rangle \frac{2}{E_i - E_k}, \quad (3.5.1)$$

where the $|k\rangle$‘s are the bulk states and $E_i$ is the degenerate energy of the edge-states at $k = 0$. Approximately we can reduce the $E_k$‘s, which are the bulk state energies, to the two dominant energies of our problem $E_{H1} = -M + C$ and $E_{E1} = M + C$. Therefore $\int d^3k \frac{1}{E_i - E_k} |k\rangle \langle k|$ becomes a projector onto the subspace of every of the both energies. Then the subspaces are given by $\{|E1\uparrow\rangle, |E1\downarrow\rangle\} \in S_{E1}$ and $\{|H1\uparrow\rangle, |H1\downarrow\rangle\} \in S_{H1}$, giving us the projector

$$G = \int d^3k \frac{|k\rangle \langle k|}{E_i - E_k} = \frac{P_{S_{E1}}}{E_i - E_{E1}} + \frac{P_{S_{H1}}}{E_i - E_{H1}}, \quad (3.5.2)$$

It has the matrix representation

$$G = \left( \begin{array}{cccc}
\frac{1}{E_i - E_{E1}} & 0 & 0 & 0 \\
0 & \frac{1}{E_i - E_{H1}} & 0 & 0 \\
0 & 0 & \frac{1}{E_i - E_{E1}} & 0 \\
0 & 0 & 0 & \frac{1}{E_i - E_{H1}}
\end{array} \right). \quad (3.5.3)$$
As $H' = H_A + H_R + H_D + H_M$, we will find an effective Hamiltonian with the form $\sum_{ij} H_i G H_j$, where $i, j \in \{A, R, D, M\}$. That gives us six new possible combinations of Hamilton operator terms and four “diagonal” terms $H_i G H_i$. Ignoring these diagonal terms $H_i G H_i$, there are four relevant combinations $(H_D, H_A)$, $(H_D, H_M)$, $(H_M, H_A)$ and $(H_D, H_R)$. The other two combinations do contribute only weakly. This leads to the following symmetrized Hamiltonians

\[
\begin{align*}
H_{DA} &= \beta k_x (\sigma_x \cos(2\theta) - \sigma_y \sin(2\theta)), \\
H_{DM} &= \tilde{J}_x (\cos(2\theta) \sigma_x - \sin(2\theta) \sigma_y) S^z \delta(x) - \tilde{J}_y \sigma_z (\cos(2\theta) S^x + \sin(2\theta) S^y) \delta(x), \\
H_{AM} &= \gamma k_x S^z \delta(x), \\
H_{DR} &= \mu k_x \sigma_x \sin(2\theta),
\end{align*}
\] 

with $\beta = -\frac{2\hbar k_v}{1 + \eta^2} \left( \frac{1}{C - M} - \frac{\eta^2}{C + M} \right)$, $\tilde{J}_x = \frac{2\hbar v_0}{1 + \eta^2} \left[ \frac{1}{2(C+M)} - \frac{3}{2(C-M)} \right]$, $\tilde{J}_y = \frac{\hbar}{(M+C)(1+\eta^2)}$, $\gamma = \frac{24(\frac{3}{2}M+C+\frac{1}{2}(C-M))}{C-M^2(1+\eta^2)}$, and $\mu = \frac{2\hbar R_0}{(M+C)(1+\eta^2)}$ (see Appendix A for calculations in Mathematica). It is important to see, that the $H_{DM}$ does not depend on $k_x$. That means in the limit $k_x \to 0$ it does not vanish and will therefore, together with the impurity Hamiltonian, become the most important term. In this regime, the physics will be dominated by the impurity.

### 3.6 Total Edge Hamiltonian

We are now able to give a total effective edge Hamiltonian in the pseudo spin up and down basis in first order perturbation theory:

\[
H_E = \nu_F \sigma_z k_x + \alpha_R \sigma_y k_x + \delta(x) (J_x \sigma_x S^x + J_y \sigma_y S^y + J_z \sigma_z S^z) + \beta k_x (\sigma_x \cos(2\theta) - \sigma_y \sin(2\theta)) + \gamma k_x S^z \delta(x) + \mu k_x \sigma_x \sin(2\theta) + \delta(x) (\tilde{J}_x (\cos(2\theta) \sigma_x - \sin(2\theta) \sigma_y) S^z - \tilde{J}_y \sigma_z (\cos(2\theta) S^x + \sin(2\theta) S^y))
\]

The first line has exactly the form as the one used in [5]. We are going to review the important steps in the microscopic derivation, which led to the result above:

There should be an additional constant term proportional to the identity $E_{\text{add}} = -\frac{DM}{B} + C$. As the energy can be doped, we can choose $C = \frac{DM}{B}$ and erase this constant offset. For the form of the Rashba term, it is important that $|\Psi_1\rangle$ and $|\Psi_2\rangle$ have the same envelope functions in their $y$-dependency, making the contribution of all terms proportional to $k_y$ equal zero (see (3.4.4)).

There are different important steps, to obtain the form of the Kondo interaction above. From the microscopic derivation, we see that this very symmetric Kondo Hamiltonian is a feature of the envelope functions parities and coefficients. Just because of the even and odd parities of $c(z)$ and $b(z)$, we do not get a term $\propto S^z \sigma_z$ and $\propto S^y \sigma_z$ (see (3.4.16)). We also need to take into account that we can choose the envelope function $a(z)$ to be real, which makes $b(z)$ imaginary. Without that condition, if $a(z)$ or $b(z)$ are complex, which induces $a(z)^2 \neq a^*(z)^2$, $b(z)^2 \neq b^*(z)^2$, $J_{x1}(3.4.20)$ and $J_{x2}(3.4.19)$ will be different. Therefore, the terms proportional to $S^x$ and $S^y$ will be more complicated.
3 Edge Hamiltonians in Degenerate Perturbation Theory

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$P$</th>
<th>$E_c$</th>
<th>$E_v$</th>
<th>$\gamma_1$</th>
<th>$\gamma_2$</th>
<th>$F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value (HgTe)</td>
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<td>-0.303</td>
<td>0</td>
<td>4.1</td>
<td>0.5</td>
<td>0</td>
</tr>
<tr>
<td>Value (CdTe)</td>
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<td>1.036</td>
<td>-0.570</td>
<td>1.47</td>
<td>-0.28</td>
<td>2</td>
</tr>
<tr>
<td>Value (Hg$<em>{0.32}$Cd$</em>{0.68}$Te)</td>
<td>8.43</td>
<td>0.579</td>
<td>-0.388</td>
<td>2.31</td>
<td>-0.03</td>
<td>1.36</td>
</tr>
</tbody>
</table>

(a) Material parameters of HgTe and CdTe at $T = 0$ as taken from [10]

<table>
<thead>
<tr>
<th></th>
<th></th>
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<th></th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>Value</td>
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<td>-68.6</td>
<td>-51.2</td>
<td>-0.008</td>
<td>-0.156</td>
<td>0.0016</td>
<td>-0.0060</td>
</tr>
</tbody>
</table>

(b) Typical parameters for a quantum well width of 70Å taken from [8] (beside $C$ which is determined to erase the offset of the Fermi velocity term)

Table 3.1: Material parameters and quantum well geometry for $d = 7$ nm

The second and third line arise from an approximate treatment of second order perturbation, which has the aim to give an estimate for their magnitude. In [5] they are completely ignored. We are researching the limit $k_x \rightarrow 0$, what means that terms proportional to $k_x$ are important. Second order in the Schrieffer-Wolff transformation is not equal to the second order in $k_x$. All following orders of the Schrieffer-Wolff transformation will produce terms proportional to $k_x$. Their strength is suppressed by the energy gap, but in second order Schrieffer-Wolff, they are still comparable with the first order terms. We discuss their strength more precisely in the next section.

3.7 Numerical Calculations

3.7.1 Parameters

Having obtained an effective one dimensional edge model in first order perturbation theory, we are now going to calculate the coupling constants with our microscopic knowledge. We use the computational software Mathematica to do the numerical calculations. The worksheets can be found in Appendix B. We do all calculations for Hg$_{1-x}$Cd$_x$Te quantum wells. As we can add a constant to the energy, we choose the valence band edge $E_v^{(Hg)} = 0$ and use the material parameters from table 3.1. For the quantum well width, we consider $d = 70$Å. The offset between the valence band of HgTe and CdTe is about $E_{v,\text{Off}} = 570$ meV at $T = 0$ [10]. We assume $E_{v,\text{Off}}$ to vary linear in $x$ [11] and $E_v[eV] = E_v - E_c = -0.303(1-x) + 1.606x - 0.132x(1-x)$ [9]. All other parameters are extrapolated linear in $x$. There can be found many different values for parameters, like the Luttinger parameters. Furthermore many of the material values also depend on the temperature. Keeping that in mind, the numerical results here can be seen as an estimate of their magnitude, but probably need more precise calculations to be more exact for a specific problem.
3.7 Numerical Calculations

3.7.1 Figure 3.7.1: Top: Both sides of equation (1.6.9) plotted for a Hg$_{0.32}$Cd$_{0.68}$Te/HgTe quantum well, where “Side1” refers to the formula proportional to tanh($\frac{d}{2}$). “Side1” has no imaginary part. Therefore the solutions can be found only in the small window, where both functions are real. We need to find the lowest energy solution, thus the crossing point of both functions next to zero gives the desired energy. Bottom: The energy of the E1-Band plotted versus the quantum well width at $k_x = k_y = 0$. The result is in fine agreement with [3].

3.7.2 Envelope Functions

First we need to calculate the envelope functions $a(z), b(z)$. We use (1.6.7) and (1.6.8) to determine the decay lengths $\alpha(E)$ and $\delta(E)$ and find four solutions for both variables. We can sort out two of them, as we are searching for positive results which ensure that the states can be normalized. Inserting the decay lengths which give the lowest $E$ solutions into equation (1.6.9), gives us a self consistent equation for the energy, which we can solve numerically. We see in figure 3.7.1, that there is just a small window where both sides of the equation are real. We can only have solutions in this window, as one side is always real. Numerically solved, we find the lowest energy solution to be $E = -31$ meV for HgTe/CdTe quantum wells and $E = -33$ meV for Hg$_{0.32}$Cd$_{0.68}$Te/HgTe quantum wells. Figure 3.7.1 shows the energy of the E1-band depending on the quantum well width $d$, which is in fine agreement with [3]. Substituting the energy back into the equations for $\alpha(E)$ and $\delta(E)$, we obtain the decay lengths of the envelope functions. Normalizing the states gives us their coefficients. As result, we have the full envelope functions
Figure 3.7.2: The plot shows the probability density in $z$-direction $|a(z)|^2 + |b(z)|^2$ for a Hg$_{0.32}$Cd$_{0.68}$Te/HgTe quantum well with a thickness of $d = 70\text{Å}$. We see that the state mainly distributes at the edges $d = \pm 35\text{Å}$. Although, the probability to be measured in the bulk does not vanish.

$$a(z) = \begin{cases} e^{\alpha z} C_1 & \text{for } z \leq \frac{d}{2} \\ (e^{\delta z} + e^{-\delta z}) V_1 & \text{for } |z| < \frac{d}{2} \\ e^{-\alpha z} C_1 & \text{for } z \geq \frac{d}{2} \end{cases}$$  \hspace{1cm} (3.7.1)

$$b(z) = \begin{cases} e^{\alpha z} C_4 & \text{for } z \leq \frac{d}{2} \\ (e^{\delta z} - e^{-\delta z}) V_4 & \text{for } |z| < \frac{d}{2} \\ -e^{-\alpha z} C_4 & \text{for } z \geq \frac{d}{2} \end{cases}$$  \hspace{1cm} (3.7.2)

with $\alpha = 0.097\text{Å}^{-1}$, $\delta = 0.011\text{Å}^{-1}$, $C_1 = 2.82$, $C_4 = -3.73i$, $V_1 = 0.04$ and $V_4 = 0.16i$ for HgTe/CdTe wells and $\alpha = 0.062\text{Å}^{-1}$, $\delta = 0.011\text{Å}^{-1}$, $C_1 = 0.79$, $C_4 = -1.04i$, $V_1 = 0.04$ and $V_4 = 0.16i$ for Hg$_{0.32}$Cd$_{0.68}$Te/HgTe wells. Figure 3.7.2 shows how the Hg$_{0.32}$Cd$_{0.68}$Te/HgTe solution is distributed.

### 3.7.3 Coupling Constants Main Term and Rashba Term

The coupling constant of the main term is the Fermi velocity, thus the moving velocity (group velocity) of the electrons:

$$v_F = A \sqrt{\frac{B_+ B_-}{B^2}} = 2.426eV\text{Å},$$  \hspace{1cm} (3.7.3)

which corresponds to a speed in SI-Units $v_{F\text{SI}} = 368570 \frac{m}{s}$.

The Rashba constant $\alpha_R$ mainly consists of the original coupling constant for the two dimensional Hamiltonian $R_0$ and can therefore be calculated to

$$\alpha_R = \frac{R_0}{1 + \eta^2} = 0.130R_0$$  \hspace{1cm} (3.7.4)
With $\frac{R_0}{\nu} = -15.6\text{nm}^2$ and typical electrical fields $E = 3\text{mV/nm}$, we have $R_0 = -468\text{meVÅ}$. The Rashba coupling is very weak compared to the main term proportional to $v_F$. The coupling constant of the second order terms calculates to
\[ \beta = -1.47eV \text{ and } \mu = 0.018eVÅ. \] (3.7.5)

The $\beta$-term can match up to the $v_F$-term and the $\mu$-term can be compared with the Rashba interaction. Thus the Hamiltonian $H_{AD} + H_{DR}$ is important and cannot easily be ignored.

### 3.7.4 Coupling Constants Kondo Hamiltonian

If we want to find the coupling strength between the edge states and a magnetic impurity, we need to calculate the coupling constants $J_z$ and $J_x = J_y$. The first one can be easily computed inserting all parameters in the formula (3.4.23):
\[ J_z = \frac{V_0}{1 + \eta^2} \left( \frac{1}{2} + \frac{3}{2} \eta^2 \right) S_z = 0.685V_0. \] (3.7.6)

For the calculation of $J_x$, we need to integrate the envelope functions
\[ J_x = \frac{1}{2} \frac{V_0}{1 + \eta^2} \left( \int dz (a(z)^2 - 2b(z)^2) \right) \] (3.7.7)
\[ = \frac{1}{2} \frac{V_0}{1 + \eta^2} \left[ \frac{C_1^2 + 2C_4^2}{\alpha} e^{-\alpha d} + \frac{V_1^2 + 2V_4^2}{\delta} (e^{\delta d} - e^{-\delta d}) + 2(V_1^2 - V_4^2) \right] \]
\[ = \begin{cases} 
-0.0238V_0 & \text{for CdTe/HgTe} \\
-0.0300V_0 & \text{for Hg}_{0.32}\text{Cd}_{0.68}\text{Te/HgTe} 
\end{cases} \]

This calculation shows, that for a typically HgTe/CdTe quantum well (here $d = 7\text{nm}$), the coupling constant $J_z$ is way stronger than $J_x$ and has an opposite sign. This Kondo term alone mainly affects out-of-plane spins. The ratio $\frac{J_z}{J_x}$ lays between 30 and 20 and can just slightly be tuned by the stoichiometry of the quantum well as can be seen in (3.7.7). We compare the results with example values for $J_x$ and $J_z$ as used in [5] where $\frac{J_z}{a_0} = 50\text{meV}$ and $\frac{J_x}{a_0} = 5\text{meV}$ with the Bohr radius $a_0$. The ratio between both needs to be tuned by about an factor of 2, to fulfill our results. Furthermore $V_0$ needs to be about $39\text{meVÅ}$. As the bulk states for the H1-band are only separated by an energy gap of $|E_{\text{gap}}| = \frac{MB^3D}{B^2}$, which is for our quantum well geometry about $2\text{meV}$ (see figure 2.2.2), $V_0$ is above the relevant gap parameter. Thus the perturbation model for the edge states is not valid in this regime.

The constants for the second order impurity term contribute
\[ \tilde{J}_z = 0.834V_0, \quad \tilde{J}_x = 0.001V_0 \text{ and } \gamma = 1724.55V_0\text{Å}. \] (3.7.8)

The term for $\tilde{J}_z$ is very small and can probably be ignored in edge calculations, but the term proportional to $\tilde{J}_z$ is in strong competition with the $J_z$ term. It will influence how the impurity spin couples to the edge states. The coupling constant $\gamma$ seems to be large but the Hamiltonian $H_{AV}$ is proportional to $k_x$ and for $|V_0| < |E_{\text{gap}}|$, it is comparably with the other terms proportional to $k_z$. Thus the Hamiltonian in [5] is missing important parts, which will likely change the physics.
4 Conclusion

In this bachelor’s work, we studied the helical edge states present in a topological insulator which can be realized with HgTe/CdTe-quantum wells. First, we calculated edge states in $k\cdot p$-theory and the envelope function approximation. Then we introduced different perturbation Hamiltonians which denote a Rashba interaction, a not rotationally invariant Dresselhaus term and a magnetic impurity. From these, we derived an effective edge Hamiltonian for the low energy limit, with the focus on the interaction of the edge states with the magnetic impurity. We compared this effective Hamiltonian with the one used in [5], and found that important terms are missing in the latter. These missing terms are a result of second order perturbation theory, which can produce relevant terms because we do have more than one small parameter. It mainly is the Dresselhaus term, not able to lift the Kramers degeneracy in first order, which combines with the other terms in second order perturbation theory and produces these additionally relevant terms. As we want to be able to compare the results with the experiment, we calculated all coupling constants numerically and found, that the Kondo coupling with the out-of-plane impurity spin is stronger than the in-plan coupling for typical quantum wells with a width of $d = 70\text{Å}$. Our results for the energy of the E1-band depending on the quantum well thickness are in fine agreement with [3], which supports the correctness of our numerical computations. Still, all material parameters depend on temperature, stoichiometry of the used well materials and more, which makes it is difficult to determine the right parameters that should be used in the computations for a specific problem. Therefore, the results here are values that give informations about the coupling constants magnitude, but are probably far from being exact. A next step could be a more precise calculation of the relevant coupling constants and parameters.
Acknowledgements

I want to thank my supervisor Prof. Dr. Fabian Hassler for making this interesting work possible. I am grateful for the time he took to answer my questions and supporting me in the important steps of my work. I also want to thank Jascha Ulrich for giving me good advises and helping me with my questions.
Bibliography


Appendix A: Second Order Calculations

HdV0 = \[
\begin{pmatrix}
    a & 0 & j & p & 0 \\
    0 & b & 0 & 0 & 0 \\
    j & m & 0 & -a & 0 \\
    0 & 0 & 0 & -b & 0
\end{pmatrix}
\times
\begin{pmatrix}
    1/\, -e_1 & 0 & 0 & 0 \\
    0 & 1/\, -e_2 & 0 & 0 \\
    0 & 0 & 1/\, -e_1 & 0 \\
    0 & 0 & 0 & 1/\, -e_2
\end{pmatrix}
\times
\begin{pmatrix}
    a & 0 & j & p & 0 \\
    0 & b & 0 & 0 & 0 \\
    j & m & 0 & -a & 0 \\
    0 & 0 & 0 & -b & 0
\end{pmatrix}
\]

\[
\begin{pmatrix}
    0 & 0 & 0 & -h & p \\
    0 & 0 & h & p & 0 \\
    0 & h & m & 0 & 0 \\
    -h & m & 0 & 0 & 0
\end{pmatrix}
\times
\begin{pmatrix}
    1/\, -e_1 & 0 & 0 & 0 \\
    0 & 1/\, -e_2 & 0 & 0 \\
    0 & 0 & 1/\, -e_1 & 0 \\
    0 & 0 & 0 & 1/\, -e_2
\end{pmatrix}
\times
\begin{pmatrix}
    a & 0 & j & p & 0 \\
    0 & b & 0 & 0 & 0 \\
    j & m & 0 & -a & 0 \\
    0 & 0 & 0 & -b & 0
\end{pmatrix}
\]

\[
\begin{pmatrix}
    0 & a & h & m & j & p & 0 \\
    0 & b & h & j & m & p & 0 \\
    0 & a & h & m & j & p & 0 \\
    0 & b & h & j & m & p & 0
\end{pmatrix}
\]

\[
\begin{pmatrix}
    1, \eta, 0, 0 \} \cdot \text{HdV0.} \{1, \eta, 0, 0 \} \\
    \{1, \eta, 0, 0 \} \cdot \text{HdV0.} \{0, 0, 1, \eta \} \\
    \{0, 0, 1, \eta \} \cdot \text{HdV0.} \{0, 0, 1, \eta \} \\
    \{0, 1, \eta \} \cdot \text{HdV0.} \{1, \eta, 0, 0 \}
\end{pmatrix}
\]

\[
\begin{pmatrix}
    \text{hp jm} \, \eta \\
    \text{hm jp} \, \eta \\
    \text{hm jm} \, \eta \\
    \text{hm hj} \, \eta
\end{pmatrix}
\]

\[
\begin{pmatrix}
    a & h & p & 0 \\
    0 & b & h & p \\
    a & h & m & j \\
    0 & b & h & m
\end{pmatrix}
\]

\[
\begin{pmatrix}
    \text{hp jm} \, \eta \\
    \text{hm jp} \, \eta \\
    \text{hm jm} \, \eta \\
    \text{hm hj} \, \eta
\end{pmatrix}
\]
\[ V_0 \left( \begin{array}{c} 1 - e_1 \\ 1 - e_2 \\ 1 - e_2 \\ 1 - e_2 \\ 1 - e_2 \\ 1 - e_2 \end{array} \right) = 0 \]
\[
\begin{align*}
\text{Out}[18] &= \begin{pmatrix}
0 & 1/e_1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1/e_2 & 0 \\
0 & 0 & 0 & 1/e_2 & 0 \\
0 & 0 & 0 & 1/e_2 & 0
\end{pmatrix} + \\
& \begin{pmatrix}
a & 0 & j_0 & 0 \\
0 & b & 0 & 0 \\
0 & j_0 & -a & 0 \\
0 & 0 & 0 & -b
\end{pmatrix}
\begin{pmatrix}
1/e_1 & 0 & 0 & 0 \\
0 & 0 & 1/e_2 & 0 \\
0 & 0 & 1/e_2 & 0 \\
0 & 0 & 1/e_2 & 0
\end{pmatrix}
\begin{pmatrix}
a & 0 & j_0 & 0 \\
0 & b & 0 & 0 \\
0 & j_0 & -a & 0 \\
0 & 0 & 0 & -b
\end{pmatrix}.
\end{align*}
\]

\[
\begin{align*}
\text{Out}[19] &= \left\{\begin{array}{c}
\frac{2a^2}{e_1} - \frac{2jmj_p}{e_1}, 0, 0, 0 \\
0, -\frac{2b^2}{e_2}, 0, 0, 0
\end{array}\right\}, \\
\left\{\begin{array}{c}
0, 0, -\frac{2a^2}{e_1} - \frac{2jmj_p}{e_1}, 0, 0, 0
\end{array}\right\}
\]

\[
\text{Out}[20] = \begin{pmatrix}
0 & 0 & -R_0 * I * k m_0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix} + \\
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
1/e_1 & 0 & 0 & 0 \\
0 & 1/e_2 & 0 \\
0 & 1/e_2 & 0 \\
0 & 1/e_2 & 0
\end{pmatrix}
\begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\]

\[
\begin{align*}
\text{Out}[21] &= \text{Simplify}[ (1/(1 + \eta^2)) \{1, \eta, 0, 0\} . \text{HRHD}. \{1, \eta, 0, 0\}] \\
&= \text{Simplify}[ (1/(1 + \eta^2)) \{1, \eta, 0, 0\} . \text{HRHD}. \{0, 0, 1, \eta\}] \\
&= \text{Simplify}[ (1/(1 + \eta^2)) \{0, 0, 1, \eta\} . \text{HRHD}. \{0, 0, 1, \eta\}] \\
&= \text{Simplify}[ (1/(1 + \eta^2)) \{0, 0, 1, \eta\} . \text{HRHD}. \{1, \eta, 0, 0\}]
\end{align*}
\]

\[
\begin{align*}
\text{Out}[22] &= \frac{i (h m k m - h p k p) R_0 \eta}{e_1 (1 + \eta^2)}
\end{align*}
\]

\[
\begin{align*}
\text{Out}[23] &= \frac{i (h m k m - h p k p) R_0 \eta}{e_1 (1 + \eta^2)}
\end{align*}
\]

\[
\text{Out}[24] = 0
\]
Out[25]=

\[
\begin{pmatrix}
a & 0 & j p & 0 \\
0 & b & 0 & 0 \\
j m & 0 & - a & 0 \\
0 & 0 & 0 & - b
\end{pmatrix}
\begin{pmatrix}
1 - e l & 0 & 0 & 0 \\
0 & 1 - e 2 & 0 & 0 \\
0 & 0 & 1 - e l & 0 \\
0 & 0 & 0 & 1 - e 2
\end{pmatrix}
\begin{pmatrix}
0 & 0 & - A * k x & 0 \\
A * k x & 0 & 0 & 0 \\
0 & 0 & 0 & - A * k x \\
0 & 0 & 0 & 0
\end{pmatrix}
\]

\[
\begin{pmatrix}
0 & A * k x & 0 & 0 \\
A * k x & 0 & 0 & 0 \\
0 & 0 & 0 & - A * k x \\
0 & 0 & - A * k x & 0
\end{pmatrix}
\begin{pmatrix}
1 - e l & 0 & 0 & 0 \\
0 & 1 - e 2 & 0 & 0 \\
0 & 0 & 1 - e l & 0 \\
0 & 0 & 0 & 1 - e 2
\end{pmatrix}
\begin{pmatrix}
a & 0 & j p & 0 \\
0 & b & 0 & 0 \\
j m & 0 & - a & 0 \\
0 & 0 & 0 & - b
\end{pmatrix}
\]

Out[25]=

\[
\left\{\left\{0, - \frac{a A k x}{e l} - \frac{b k x}{e 2}, 0, \frac{A j p k x}{e l} \right\}, \left\{\frac{a A k x}{e l} - \frac{b k x}{e 2}, 0, - \frac{A j p k x}{e l} \right\}, \left\{0, - \frac{A j m k x}{e l}, 0, \frac{a A k x}{e l} - \frac{b k x}{e 2} \right\} \right\}
\]

Out[26]=

\[2 A (b e l + a e 2) k x \eta
\]

\[e l e 2 (1 + \eta^2)
\]

Out[28]=

\[2 A (b e l + a e 2) k x \eta
\]

\[e l e 2 (1 + \eta^2)
\]

Out[29]=

\[0
\]

Out[30]=

\[
\begin{pmatrix}
a & 0 & j p & 0 \\
0 & b & 0 & 0 \\
j m & 0 & - a & 0 \\
0 & 0 & 0 & - b
\end{pmatrix}
\begin{pmatrix}
1 - e l & 0 & 0 & 0 \\
0 & 1 - e 2 & 0 & 0 \\
0 & 0 & 1 - e l & 0 \\
0 & 0 & 0 & 1 - e 2
\end{pmatrix}
\begin{pmatrix}
0 & 0 & 0 & - R 0 * I * k m 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\]

\[
\begin{pmatrix}
0 & 0 & - R 0 * I * k m 0 \\
0 & 0 & 0 & 0 \\
I * R 0 * k p 0 & 0 & 0 & 0 \\
I * R 0 * k p 0 & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
1 - e l & 0 & 0 & 0 \\
0 & 1 - e 2 & 0 & 0 \\
0 & 0 & 1 - e l & 0 \\
0 & 0 & 0 & 1 - e 2
\end{pmatrix}
\begin{pmatrix}
a & 0 & j p & 0 \\
0 & b & 0 & 0 \\
j m & 0 & - a & 0 \\
0 & 0 & 0 & - b
\end{pmatrix}
\]

Out[30]=

\[
\left\{\frac{i j m k m R 0}{e l}, \frac{- i j p k p R 0}{e l}, 0, 0, 0 \right\}, \left\{0, 0, 0, 0 \right\}, \left\{0, 0, 0, 0 \right\}
\]

Out[31]=

\[
\frac{i j m k m R 0}{e l} - \frac{i j p k p R 0}{e l}, 0, 0, 0, 0, 0, 0, 0
\]
\[ b_1 = -68.6 \]
\[ d = -51.2; \]
\[ m = -0.008; \]
\[ h = 0.0016; \]
\[ c = d \times m / b_1; \]
\[ e_1 = m + c \]
\[ e_2 = -m + c \]
\[ a = 0.5 \times V_0 \times S_z \]
\[ b = 3 / 2 \times V_0 \times S_z \]
\[ R_0 = 0.468 \]
\[ j_m = -0.03 \times V_0 \times T_p \]
\[ j_p = -0.03 \times V_0 \times T_m \]
\[ \eta = -2.587 \]
\[ A = 3.645 \]
\[ h = 0.0016 \]
\[ h_p = h \times E^{2 \times I \times \theta} \]
\[ h_m = h \times E^{(-2 \times I \times \theta)} \]
In[64]:= Simplify[(1/(1+\eta^2))\{1, \eta, 0, 0\}.\text{V0V0.}\{1, \eta, 0, 0\}]
Simplify[(1/(1+\eta^2))\{1, \eta, 0, 0\}.\text{V0V0.}\{0, 0, 1, \eta\}]
Simplify[(1/(1+\eta^2))\{0, 0, 1, \eta\}.\text{V0V0.}\{1, \eta, 0, 0\}]
Simplify[(1/(1+\eta^2))\{0, 0, 1, \eta\}.\text{V0V0.}\{1, \eta, 0, 0\}]

Out[64] = 0. - 1924.73 Sz^2 V0^2 + 0.0167486 Tm Tp V0^2

Out[59] = 0.
Out[58] = 0. - 1924.73 Sz^2 V0^2 + 0.0167486 Tm Tp V0^2
Out[57] = 0.

In[53]:= Simplify[(1/(1+\eta^2))\{1, \eta, 0, 0\}.\text{HdHA.}\{1, \eta, 0, 0\}]
Simplify[(1/(1+\eta^2))\{1, \eta, 0, 0\}.\text{HdHA.}\{0, 0, 1, \eta\}]
Simplify[(1/(1+\eta^2))\{0, 0, 1, \eta\}.\text{HdHA.}\{1, \eta, 0, 0\}]
Simplify[(1/(1+\eta^2))\{0, 0, 1, \eta\}.\text{HdHA.}\{1, \eta, 0, 0\}]

Out[53] = 0.
Out[54] = -1.47359 e^{21\eta} \text{Kx}
Out[55] = 0.
Out[56] = -1.47359 e^{-21\eta} \text{Kx}

In[57] := 0.065 * 11.335
Out[57] = 0.736775

In[58] := V0 * 0.68
Out[58] = 0.68 V0

In[59] := Simplify[(1/(1+\eta^2))\{1, \eta, 0, 0\}.\text{HRHD.}\{1, \eta, 0, 0\}]
Simplify[(1/(1+\eta^2))\{1, \eta, 0, 0\}.\text{HRHD.}\{0, 0, 1, \eta\}]
Simplify[(1/(1+\eta^2))\{0, 0, 1, \eta\}.\text{HRHD.}\{1, \eta, 0, 0\}]
Simplify[(1/(1+\eta^2))\{0, 0, 1, \eta\}.\text{HRHD.}\{1, \eta, 0, 0\}]

Out[59] = (0. + 0.0180247 i) e^{-21\eta} \text{Km} - (0. + 0.0180247 i) e^{21\eta} \text{Kp}
Out[60] = 0. + 0. i
Out[61] = (0. - 0.0180247 i) e^{-21\eta} \text{Km} + (0. + 0.0180247 i) e^{21\eta} \text{Kp}
Out[62] = 0. + 0. i

In[63] =
In[64] =
\[\text{Out[65]} = \text{Simplify}[(1/(1 + \eta^2)) \cdot \{1, \eta, 0, 0\} \cdot \text{HdV0.}\{1, \eta, 0, 0\}]\]
\[\text{Simplify}[1/(1 + \eta^2) \cdot \{1, \eta, 0, 0\} \cdot \text{HdV0.}\{0, 0, 1, \eta\}]\]
\[\text{Simplify}[1/(1 + \eta^2) \cdot \{0, 0, 1, \eta\} \cdot \text{HdV0.}\{1, \eta, 0, 0\}]\]
\[\text{Out[65]} = 0.00115543 e^{-2i\theta} \text{Tm V0} + 0.00115543 e^{2i\theta} \text{Tp V0}\]
\[\text{Out[66]} = 0.834034 e^{2i\theta} \text{Sz V0}\]
\[\text{Out[67]} = -0.00115543 e^{-2i\theta} \text{Tm V0} - 0.00115543 e^{2i\theta} \text{Tp V0}\]
\[\text{Out[68]} = 0.834034 e^{-2i\theta} \text{Sz V0}\]
\[\text{Out[69]} = \text{Simplify}[(1/(1 + \eta^2)) \cdot \{1, \eta, 0, 0\} \cdot \text{HAV0.}\{1, \eta, 0, 0\}]\]
\[\text{Simplify}[1/(1 + \eta^2) \cdot \{1, \eta, 0, 0\} \cdot \text{HAV0.}\{0, 0, 1, \eta\}]\]
\[\text{Simplify}[1/(1 + \eta^2) \cdot \{0, 0, 1, \eta\} \cdot \text{HAV0.}\{0, 0, 1, \eta\}]\]
\[\text{Simplify}[1/(1 + \eta^2) \cdot \{0, 0, 1, \eta\} \cdot \text{HAV0.}\{1, \eta, 0, 0\}]\]
\[\text{Out[69]} = 0. \cdot 1724.55 \text{kx Sz V0}\]
\[\text{Out[70]} = 0.\]
\[\text{Out[71]} = 0. \cdot 1724.55 \text{kx Sz V0}\]
\[\text{Out[72]} = 0.\]
\[\text{Out[73]} =\]
\[\text{Out[74]} = \text{Simplify}[(1/(1 + \eta^2)) \cdot \{1, \eta, 0, 0\} \cdot \text{HRV0.}\{1, \eta, 0, 0\}]\]
\[\text{Simplify}[1/(1 + \eta^2) \cdot \{1, \eta, 0, 0\} \cdot \text{HRV0.}\{0, 0, 1, \eta\}]\]
\[\text{Simplify}[1/(1 + \eta^2) \cdot \{0, 0, 1, \eta\} \cdot \text{HRV0.}\{0, 0, 1, \eta\}]\]
\[\text{Simplify}[1/(1 + \eta^2) \cdot \{0, 0, 1, \eta\} \cdot \text{HRV0.}\{1, \eta, 0, 0\}]\]
\[\text{Out[74]} = 0. \cdot (-0. + 0.130639 i) \text{ kp Tm V0} + (0. + 0.130639 i) \text{ km Tp V0}\]
\[\text{Out[75]} = 0.\]
\[\text{Out[76]} = 0. \cdot (-0. + 0.130639 i) \text{ kp Tm V0} + (0. + 0.130639 i) \text{ km Tp V0}\]
\[\text{Out[77]} = 0.\]
Appendix B: Numerical Constant Calculations

(*Calculation of Constants*)
\begin{verbatim}
In[3]:= b = -68.6;
d = -51.2;
m = -0.008;
h = 0.0016;
c = d * m / b;
A = 3.645;
R0 = -15.6 * 3 * 10^-3;
pCD = 0.68
pHG = 1 - pCD
EcCD = -0.57 * pCD + (-0.303 (1 - pCD) + 1.606 * pCD - 0.132 * pCD (1 - pCD))
EcHG = -0.303;
EvCD = -0.57 * pCD
EvHG = 0;
PCD = 8.43;
PHG = 8.43;
gamma1CDa = 1.47;
gamma2CDa = -0.28;
gamma1HGa = 4.1;
gamma2HGa = 0.5;

\text{\textbf{gamma1CD}} = pCD * gamma1CDa + pHG * gamma1HGa
\text{\textbf{gamma2CD}} = pCD * gamma2CDa + pHG * gamma2HGa
\text{\textbf{gamma1HG}} = 4.1;
\text{\textbf{gamma2HG}} = 0.5;
En = -d * m / b + c;
AHG = 3.810;
ACDe = 5 * AHG
ACD = pHG * AHG + pCD * ACDe
E0proA = 3.81;
ky = 0;
\end{verbatim}

Out[10]= 0.68
Out[11]= 0.32
Out[12]= 0.578797
Out[13]= -0.3876
Out[22]= 2.3116
Out[23]= -0.0304
Out[28]= 19.05
Out[29]= 14.1732
In[32]= Clear[Ener]

43
In[33]:= equa = (EcCD - ACD * alpha^2 - Ener) / ((PCD / I) * alpha * (2/3)^(1/2)) ==
(2/3)^(1/2) * (PCD / I) * alpha / 
(EvCD + E0proA * (gamma1CD + 2 gamma2CD) * alpha^2 - Ener)

Out[33] = 
1
(0. + 0.145284 i) (0.578797 - 14.1732 alpha^2 - Ener) ==
alpha
(0. + 6.88307 i) alpha
- 0.3876 + 8.57555 alpha^2 - Ener

In[34]:= equa2 = (EchG - AHG * delta^2 - Ener) / ((PHG / I) * delta * (2/3)^(1/2)) ==
(2)^(1/2) * (PHG / I) * delta / 
(EvHG + E0proA * (gamma1HG + 2 gamma2HG) * delta^2 - Ener)

Out[34] = 
(0. + 0.145284 i) (-0.301 - 3.81 delta^2 - Ener)
(delta == (0. + 11.9218 i) delta)

Out[34] = 19.431 delta^2 - Ener

In[35]:= alphav = NSolve[equa, alpha]
deltav = NSolve[equa2, delta]

Solve::ratnz :
Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result. >>

Out[35] = {
{alpha -> -3.47802 \times 10^{-22} \sqrt{(1.96678 \times 10^{42} + 1.90362 \times 10^{41} Ener - 
1. \sqrt{(3.74208 \times 10^{84} + 6.41298 \times 10^{83} Ener + 5.98501 \times 10^{83} Ener^2))},
{alpha -> -3.47802 \times 10^{-22} \sqrt{(1.96678 \times 10^{42} + 1.90362 \times 10^{41} Ener - 
1. \sqrt{(3.74208 \times 10^{84} + 6.41298 \times 10^{83} Ener + 5.98501 \times 10^{83} Ener^2))},
{alpha -> -3.47802 \times 10^{-22} \sqrt{(1.96678 \times 10^{42} + 1.90362 \times 10^{41} Ener + 
\sqrt{(3.74208 \times 10^{84} + 6.41298 \times 10^{83} Ener + 5.98501 \times 10^{83} Ener^2))},
{alpha -> -3.47802 \times 10^{-22} \sqrt{(1.96678 \times 10^{42} + 1.90362 \times 10^{41} Ener + 
\sqrt{(3.74208 \times 10^{84} + 6.41298 \times 10^{83} Ener + 5.98501 \times 10^{83} Ener^2))}}

Solve::ratnz :
Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result. >>

Out[36] = {
deleta -> -8.90724 \times 10^{-16} \sqrt{(6.48417 \times 10^{29} - 1.32976 \times 10^{29} Ener - 
1. \sqrt{(4.20444 \times 10^{59} - 1.65945 \times 10^{59} Ener + 3.91415 \times 10^{58} Ener^2))},
{deleta -> -8.90724 \times 10^{-16} \sqrt{(6.48417 \times 10^{29} - 1.32976 \times 10^{29} Ener - 
1. \sqrt{(4.20444 \times 10^{59} - 1.65945 \times 10^{59} Ener + 3.91415 \times 10^{58} Ener^2))},
{deleta -> -8.90724 \times 10^{-16} \sqrt{(6.48417 \times 10^{29} - 1.32976 \times 10^{29} Ener + 
\sqrt{(4.20444 \times 10^{59} - 1.65945 \times 10^{59} Ener + 3.91415 \times 10^{58} Ener^2))},
{deleta -> -8.90724 \times 10^{-16} \sqrt{(6.48417 \times 10^{29} - 1.32976 \times 10^{29} Ener + 
\sqrt{(4.20444 \times 10^{59} - 1.65945 \times 10^{59} Ener + 3.91415 \times 10^{58} Ener^2))}}

Out[37] = alphav = alpha /. alphav[[2]];
deltav = delta /. deltatv[[2]];

Out[39] = Clear[Ener]

Out[40] = Clear[Ener]

Clear[Erg]
Clear[EnEquation]
EnergyL = Table[0, {i, 1, 4000}];
For \( i = 1, i < 4001, i++ \), EnEquation = \((E_{CCD} - ACD \cdot \alpha V^2 - Ener) / \alpha V = -\text{Tanh}[deltaV \cdot (40 + (i / 100)) / 2] ((E_{CHG} - AHG \cdot \delta V^2 - Ener) / \delta V)\); 
Erg = FindRoot[EnEquation, {{Ener, -0.04, -3, 3}}, MaxIterations -> 10000]; 
Eni = Ener /. Erg; 
EnergyL[[i]] = Eni; 
Clear[Ener]; 
Clear[Erg]; 
Clear[EnEquation];

FindRoot::lstol: The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances. \(\triangleright\)

FindRoot::lstol: The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances. \(\triangleright\)

FindRoot::lstol: The line search decreased the step size to within tolerance specified by AccuracyGoal and PrecisionGoal but was unable to find a sufficient decrease in the merit function. You may need more than MachinePrecision digits of working precision to meet these tolerances. \(\triangleright\)

General::stop: Further output of FindRoot::lstol will be suppressed during this calculation. \(\triangleright\)

EnergyL;

E1BandPlot = ListLinePlot[EnergyL, DataRange -> {40, 80}, AxesLabel -> {"d[Å]", "Energy[eV]"}]

Ener = EnergyL[[3000]]

-0.0327018
EnergyEquation = Plot[
{Re[(-Tanh[deltaV * 70 / 2]) ((EcHG - AHG * deltaV^2 - Ener) / deltaV)],
Re[(EcCD - ACD * alphaV^2 - Ener) / alphaV],
Im[(EcCD - ACD * alphaV^2 - Ener) / alphaV]},
{Ener, -2, 2}, PlotStyle -> {Black, Red, Blue},
PlotLegends -> {"Re[Side1]", "Re[Side2]", "Im[Side2]"},
Frame -> True, FrameLabel -> {"Energy[eV]", ""}],

Out[50]=

In[51]:=

In[52]:=

In[53]:=

In[54]:= (EcCD - ACD * alphaV^2 - Ener) / alphaV
   - Tanh[deltaV * 70 / 2] ((EcHG - AHG * deltaV^2 - Ener) / deltaV)

Out[54]= 9.05358

Out[55]= 9.05358

In[56]:=

alphaV
   deltaV

Out[56]= 0.0616016

Out[57]= 0.0107371

In[58]:=

In[59]:=

b1 = b + d;
   b2 = b - d;

In[60]:= F = (A^2 - 2 * (m * b + En * d)) / (2 * (b1 * b2));
In[83]:  \[
\text{lambda1} = \sqrt{\text{P} + \sqrt{\text{P}^2 - (m^2 - En^2) / (b1 \cdot b2)}};
\]
\[
\text{lambda2} = \sqrt{\text{P} - \sqrt{\text{P}^2 - (m^2 - En^2) / (b1 \cdot b2)}};
\]
\[
\text{lambda}
\]
Out[85]:  0.076432

In[86]:  \[
\text{eta} = (d + b) \cdot (\text{lambda1} + \text{lambda2}) / A
\]
Out[86]:  -2.58744

In[87]:  \[
\text{Enkp} = \text{En} + \sqrt{b1 \cdot b2 / b^2} \cdot A \cdot kx
\]
\[
\text{Enkm} = \text{En} - \sqrt{b1 \cdot b2 / b^2} \cdot A \cdot kx
\]
Out[87]:  0. + 2.42592 kx
Out[88]:  0. - 2.42592 kx

In[89]:  \[
\text{ky} = 0.001
\]
Out[89]:  0.001

In[70]:  \[
\text{Enerp} = c - d \cdot (kx^2 \cdot ky^2) + \sqrt{(m - b \cdot (ky^2 + kx^2))^2 + A^2 \cdot (ky^2 + kx^2)}
\]
\[
\text{Enerpm} = c - d \cdot (kx^2 \cdot ky^2) - \sqrt{(m - b \cdot (ky^2 + kx^2))^2 + A^2 \cdot (ky^2 + kx^2)}
\]
Out[70]:  -0.00597085 + 51.2 \cdot (1. \times 10^{-6} + kx^2) + \\
\sqrt{(13.286 (1. \times 10^{-6} + kx^2) + (-0.008 + 68.6 (1. \times 10^{-6} + kx^2))^2)}
Out[71]:  -0.00597085 + 51.2 \cdot (1. \times 10^{-6} + kx^2) - \\
\sqrt{(13.286 (1. \times 10^{-6} + kx^2) + (-0.008 + 68.6 (1. \times 10^{-6} + kx^2))^2)}

In[72]:  \[
\text{C4} = \text{C1} \cdot (\text{EcCD} - \text{ACD} \cdot \text{alphaV}^2 - \text{Ener}) / ((2 / 3) \cdot (1 / 2) \cdot \text{PCD} \cdot \text{alphaV} \cdot I)
\]
Out[72]:  (0. - 1.31534 i) \text{C1}

In[73]:  \[
\text{V1} = \text{C1} \cdot \text{E} \cdot (-\text{alphaV} \cdot 0.5 \cdot \text{wi}) / (\text{E} \cdot (-\text{deltaV} \cdot 0.5 \cdot \text{wi}) + \text{E} \cdot (\text{deltaV} \cdot 0.5 \cdot \text{wi}))
\]
\[
\frac{\text{C1} \cdot e^{-0.0308008 \cdot \text{wi}}}{e^{-0.00536853 \cdot \text{wi}} + e^{0.00536853 \cdot \text{wi}}}
\]
Out[73]:  

In[74]:  \[
\text{V4} = \text{C4} \cdot \text{E} \cdot (-\text{alphaV} \cdot 0.5 \cdot \text{wi}) / (\text{E} \cdot (-\text{deltaV} \cdot 0.5 \cdot \text{wi}) - \text{E} \cdot (\text{deltaV} \cdot 0.5 \cdot \text{wi}))
\]
\[
\frac{(0. + 1.31534 i) \text{C1} \cdot e^{0.0308008 \cdot \text{wi}}}{e^{-0.00536853 \cdot \text{wi}} - e^{0.00536853 \cdot \text{wi}}}
\]
Out[74]:  

In[75]:  \[
(*) \text{V4 imaginary, infront V4^2 - instead of + *)}
\]
\[
\text{normEqua} = 1 = \text{C1}^2 \cdot \text{E} \cdot (-\text{alphaV} \cdot \text{wi}) / \text{alphaV} + ((\text{V1}^2 \cdot \text{V4}^2) / \text{deltaV}) \cdot \text{E} \cdot (\text{wi} \cdot \text{deltaV}) - \text{E} \cdot (-\text{wi} \cdot \text{deltaV})) + (\text{V1}^2 \cdot \text{V4}^2) \cdot 2 \cdot \text{wi}
\]
Out[76]:  1 = 16.2333 \text{C1}^2 \cdot e^{-0.0616016 \cdot \text{wi}} + 93.1354 \cdot \left(-e^{-0.0107371 \cdot \text{wi}} + e^{0.0107371 \cdot \text{wi}}\right) \\
\left(\frac{1.73012 + 0. i}{}\right) \text{C1}^2 \cdot e^{-0.0616016 \cdot \text{wi}} \\
\cdot \left(\text{e}^{-0.00536853 \cdot \text{wi}} - e^{0.00536853 \cdot \text{wi}}\right)^2 \right) + \\
\left(1.73012 + 0. i\right) \text{C1}^2 \cdot e^{-0.0616016 \cdot \text{wi}} \\
\cdot \left(\text{e}^{-0.00536853 \cdot \text{wi}} - e^{0.00536853 \cdot \text{wi}}\right)^2 \right) \text{wi
In[77] := \[Out\[77\]] = Csol = Solve[normEqua, \{C1\}]

\[Out\[77\]] := \{\{C1 \to \frac{1}{\sqrt{\left(16.2333 \cdot e^{-0.0616016 \cdot wi} - \left(\frac{(161.135 + 0 \cdot i) \cdot e^{-0.0723387 \cdot wi}}{\left(e^{-0.00536853 \cdot wi} - 1 \cdot e^{0.00536853 \cdot wi}\right)^2} - \frac{(161.135 + 0 \cdot i) \cdot e^{-0.0508645 \cdot wi}}{\left(e^{-0.00536853 \cdot wi} - 1 \cdot e^{0.00536853 \cdot wi}\right)^2}\right) + \frac{93.1354 \cdot e^{-0.0723387 \cdot wi}}{\left(e^{-0.00536853 \cdot wi} + e^{0.00536853 \cdot wi}\right)^2} + \frac{93.1354 \cdot e^{-0.0508645 \cdot wi}}{\left(e^{-0.00536853 \cdot wi} + e^{0.00536853 \cdot wi}\right)^2}\right) + \frac{2 \cdot e^{-0.0616016 \cdot wi \cdot L}}{\left(e^{-0.00536853 \cdot wi} + e^{0.00536853 \cdot wi}\right)^2}\right)\}\}

\[Out\[77\]] := \{\{C1 \to \frac{1}{\sqrt{\left(16.2333 \cdot e^{-0.0616016 \cdot wi} - \left(\frac{(161.135 + 0 \cdot i) \cdot e^{-0.0723387 \cdot wi}}{\left(e^{-0.00536853 \cdot wi} - 1 \cdot e^{0.00536853 \cdot wi}\right)^2} - \frac{(161.135 + 0 \cdot i) \cdot e^{-0.0508645 \cdot wi}}{\left(e^{-0.00536853 \cdot wi} - 1 \cdot e^{0.00536853 \cdot wi}\right)^2}\right) + \frac{93.1354 \cdot e^{-0.0723387 \cdot wi}}{\left(e^{-0.00536853 \cdot wi} + e^{0.00536853 \cdot wi}\right)^2} + \frac{93.1354 \cdot e^{-0.0508645 \cdot wi}}{\left(e^{-0.00536853 \cdot wi} + e^{0.00536853 \cdot wi}\right)^2}\right) + \frac{2 \cdot e^{-0.0616016 \cdot wi \cdot L}}{\left(e^{-0.00536853 \cdot wi} + e^{0.00536853 \cdot wi}\right)^2}\right)\}\}

In[78] := C1 = C1 / Csol[[2]];
In[79] := C1 * E^(- (wi * 0.5) * alphaV);
In[80] := V1 *(E^(- (wi * 0.5) * deltaV) + E^(- (wi * 0.5) * deltaV));
In[81] := -V4 *(E^(- (wi * 0.5) * deltaV) - E^(- (wi * 0.5) * deltaV));
In[82] := C4 * E^(- (wi * 0.5) * alphaV);
In[83] := JxproV0 = 0.5 * (1 + eta^2) * ((C1^2 + 2 * C4^2) / alphaV) * E^(- (alphaV * wi)) + ((V1^2 + 2 * V4^2) / deltaV) * (E^(- (wi * deltaV)) - E^(- (wi * deltaV))) + 2 * (V1^2 - 2 * V4^2) * wi);
In[84] := JzproV0 = (0.5 / (1 + eta^2)) * (1/2 + (3/2) * eta^2);
Out[84] := 0.685021
In[85] :=
In[86]:= Plot[JxproV0, {wi, 63.5, 70}]

Out[86]=

In[87]:= wi = 70
Out[87]= 70

In[88]:= 63.52
Out[88]= 63.52

In[89]:= JxproV0
Out[89]= -0.0299753 + 0. i

In[90]:= C1
Out[90]= 0.789151 + 0. i

In[91]:= C4
Out[91]= 0. -1.038 i

In[92]:= V1
Out[92]= 0.042638 + 0. i

In[93]:= V4
Out[93]= 0. + 0.156199 i

Out[94]=

In[95]:= Plot[Piecewise[{{(C1 \[Exponent] \[Alpha] V \[Exponent] y) \[Exponent] 2, y < -35},
{(C1 \[Exponent] \[Alpha] V \[Exponent] y) \[Exponent] 2, y > 35}}], {y, -50, 50}, PlotRange -> {0, 0.01}]

Out[95]=
EdgeStatesz = 
Plot[
Piecewise[
{{(C1 * E^((alphaV * y)))^2, y < -35},
{(V1 * (E^(-deltaV * y) + E^((deltaV * y))))^2 -
(V4 * (E^(-deltaV * y) - E^((deltaV * y))))^2, -35 < y < 35},
{{(C1 * E^(-alphaV * y)))^2 - (-C4 * E^(-alphaV * y)))^2, y > 35}]},
{y, -50, 50},
PlotRange -> {0, 0.03}, AxesLabel -> {"z[A]", "Probability Density"}]

\[\text{Out[96]}\] =

\[\text{In[97]}\] = deltaV * 35
\[\text{Out[97]}\] = 0.375797

\[\text{In[98]}\] = Func = (E^((lambda1 * y0) - E((lambda2 * y0)))^2 * 
(2 * (lambda1 * lambda2 * (lambda1 + lambda2))) / (lambda1 - lambda2)^2)
\[\text{Out[98]}\] = 0.00501912 \((-e^{0.00129261 y0} + e^{0.0676432 y0})^2\)

\[\text{In[99]}\] = Y0Factor = Plot[Func, {y0, -400, 0}, 
Frame -> True, FrameLabel -> {"x[A]", "Modulation Factor"}]

\[\text{Out[99]}\] =

\[\text{In[100]}\] = (*Export["Bachelorarbeit/images/Y0Factor.pdf",Y0Factor] 
*) Export["Bachelorarbeit/images/EdgeStatesz.pdf",EdgeStatesz] (* 
Export["Bachelorarbeit/images/E1BandPlot.pdf",E1BandPlot]*)
\[\text{Out[100]}\] = Bachelorarbeit/images/EdgeStatesz.pdf

\[\text{In[101]}\] =
\[\text{In[102]}\] =