

Kondo-model for quantum-dots with spin-orbit coupling

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Abstract

Cotunneling through a spin-orbit coupled quantum dot

Starting from the Anderson model for a quantum dot, with Rashba type spin-orbit (SO) interactions, coupled to two metallic electrodes, we derive an effective low-energy Hamiltonian describing the dynamical spin-fluctuations, i.e. the cotunneling processes, which remain in the Coulomb blockade regime. This projection to the low-energy states of the Hilbert space is performed by means of two consecutive unitary transformations. First we eliminate the spin-orbit coupling to second order in the SO-coupling, which results in an Anderson model with different spin-quantization axis on the dot and in the metallic electrodes. Subsequently, we eliminate all but second order charge-fluctuations, leaving the quantum dot with a single electron, i.e. a single spin-1/2, which can be flipped by the cotunneling conduction electrons traversing the dot. Due to the spin-dependent tunneling amplitude deriving from the SO-coupling, we end up with an effective Kondo-model having a very low spin rotational symmetry in a finite magnetic field. We show that this can give rise to a nonlinear conductance which is asymmetric under reversal of the applied bias-voltage.

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Chapter 1

Introduction

1.1 Experimental motivation

Consider a device structure where a scattering region (quantum dot) is connected to the outside world by coupling to two metal leads labeled by index $\alpha = L, R$ for left and right. The leads have voltages V_L and V_R and are assumed to be described by non-interacting electrons. By applying a bias-voltage across the device, it is possible to control the amount of current running through. This device is described by an Anderson-type model[4] where the quantum dot plays the role of a magnetic impurity with which the conduction electrons can interact.

The low-temperature transport through such quantum dots is mainly restricted to the so-called charge-degeneracy points at which the number of electrons on the dot becomes uncertain. Away from these points, transport is strongly suppressed by a Coulomb blockade, reflecting the fact that the capacitive charging energy of the dot is too large for electrons to freely tunnel onto and off the dot.

Meanwhile, virtual quantum processes in which an electron visits the dot only in a sufficiently short time, are allowed by the uncertainty principle and these give rise to a small cotunneling conductance. In the case where the dot holds an effective magnetic moment, repeated cotunneling involving spin-flip processes will accumulate logarithmic singularities and instigate a manner of correlated transport across the dot. Lowering the temperature, this so-called Kondo effect lifts the Coulomb blockade completely and results in perfect transmission through the correlated junction.

Experiments by T. Jespersen et al. in 2006 [12] have demonstrated the presence of Kondo-effect in quantum dot devices based on InAs quantum wires. This material has substantial spin-orbit coupling, with a g-factor close to 8-10.

Also traditional GaAs quantum dots have strong SO-coupling and still exhibit Kondo effect[8][26]. One might wonder why Kondo-effect is observed in such materials where spin is no longer a good quantum number.

If an external magnetic field is applied, the Kondo peak is Zeeman split into

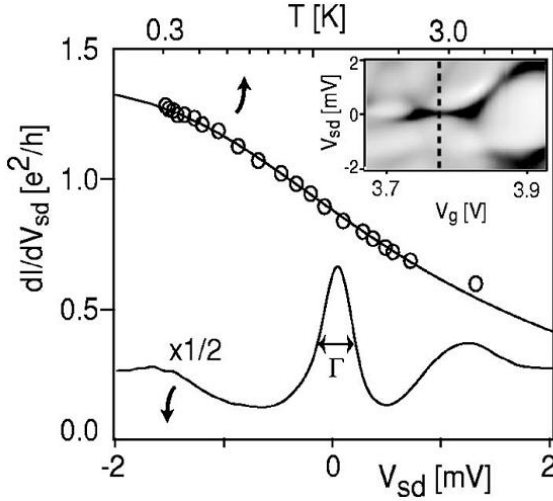


Figure 1.1: Kondo conductance peak at zero bias-voltage in an InAs quantum dot, building up when lowering temperature [12].

two peaks. Experiments have showed an asymmetry in these peaks [5][12]. This asymmetry can not be explained by the Kondo model for a quantum dot where SO interactions are not present.

1.2 Spin Orbit interaction

The spin-orbit coupling is a relativistic effect which follows directly from the Dirac equation. Consider an electron moving with velocity \mathbf{v} in an electric field \mathbf{E} . In its rest frame, the electron will experience a magnetic field¹

$$\mathbf{B}_{\text{RF}} = \gamma (\mathbf{v} \times \mathbf{E}) / c^2$$

where γ is the Lorentz factor $\gamma = (1 - v^2/c^2)^{-1/2}$. In the following we shall restrict ourselves to the case where this can be set to one. The magnetic moment of the electron couples to the magnetic field, leading to an energy that we would expect to be $-(e\hbar/2mc)\sigma \cdot \mathbf{B}_{\text{RF}}$. It has been showed by L.H. Thomas that a more careful treatment which would take into account the energy associated with the precession of the electron spin would result in a reduction in this energy of a factor of two[21]. While Thomas showed this within the framework of classical electrodynamics, the same result is achieved in the nonrelativistic solutions to the

¹This follows directly from the transformation properties of electric and magnetic field in special relativity. Performing a Lorentz transformation and assuming the magnetic field in the laboratory frame to be zero yields the magnetic field $\mathbf{B}_{\text{RF}} \neq 0$ in the rest frame of the electron.

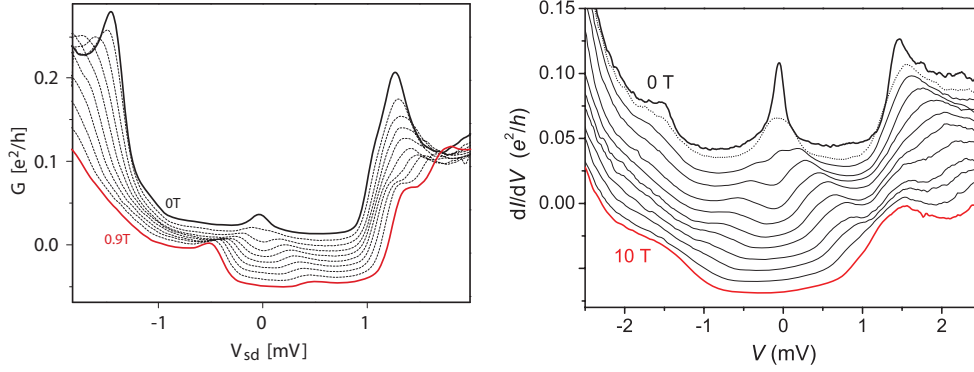


Figure 1.2: (Color online) Left: Differential conductance, dI/dV , as a function of bias voltage, V , for an InAs-wire based quantum dot at $T = 0.3\text{K}$. The data were taken at magnetic fields perpendicular to the wire. $B_{\perp} = 0$ (thick), 0.1 (dotted), ..., 0.9 T (red), and the curves were offset by $0.008e^2/h$ for clarity. The data were taken for an odd occupied Coulomb diamond at gate voltage $V_g = -2.35\text{V}$. [12] Right: dI/dV as a function of V for a carbon nanotube quantum dot at $T = 0.08\text{K}$. $B_{\perp} = 0$ (thick), 0.1 (dotted), 1 (thin), 2, 3, ..., 9, 10 T (red), and the curves were offset by $0.008e^2/h$ for clarity. The data were taken for an odd occupied Coulomb diamond at gate voltage $V_g = -4.96\text{V}$. [23] (Note that at finite magnetic fields features are broadened due to noise induced by the magnet power supply).

Dirac equation. The energy is

$$H_{\text{SO}} = -\frac{e\hbar}{4m^2c^2}\sigma \cdot [\mathbf{E} \times \mathbf{p}]$$

where $\mathbf{v} = \mathbf{p}/m$ is the electron velocity. An electric field \mathbf{E} can be described as a gradient of a potential and the time derivative of a vector potential using the Maxwell equation $\mathbf{E} = -\nabla V - \partial\mathbf{A}/\partial t$, where the magnetic field generating the electric field is $\mathbf{B} = \nabla \times \mathbf{A}$. Assuming the field to be constant in time gives $\mathbf{E} = -\nabla V$. Writing out H_{SO} in terms of σ and \mathbf{E} gives the Rashba terms

$$\begin{aligned} H_{\text{SO}} &= -\frac{e\hbar}{4m^2c^2} [-E_y(\sigma_z p_x - \sigma_x p_z) - E_z(\sigma_x p_y - \sigma_y p_x) - E_x(\sigma_y p_z - \sigma_z p_y)] \\ &= \frac{\hbar}{m} \frac{eE_z}{4mc^2} (\sigma_x p_y - \sigma_y p_x) + \frac{\hbar}{m} \frac{eE_y}{4mc^2} (\sigma_z p_x - \sigma_x p_z) + \frac{\hbar}{m} \frac{eE_x}{4mc^2} (\sigma_y p_z - \sigma_z p_y) \\ &= \frac{\hbar}{m} \alpha_z (\sigma_x p_y - \sigma_y p_x) + \frac{\hbar}{m} \alpha_y (\sigma_z p_x - \sigma_x p_z) + \frac{\hbar}{m} \alpha_x (\sigma_y p_z - \sigma_z p_y) \\ &= H_{R_z} + H_{R_y} + H_{R_x} \end{aligned}$$

where the Rashba spin-orbit interaction constant is defined by

$$\alpha_i = \frac{eE_i}{4mc^2} \quad (1.1)$$

This is a coupling constant defining the strength of the coupling between the spin and momentum. It has the unit of 1/length and the inverse

$$\lambda_{SO}^i = 1/\alpha_i$$

is the Rashba spin-orbit length.

For a particle confined in the x -direction ($p_x = p$, $p_y = p_z = 0$) the Hamiltonian describing the particle with Rashba and Zeeman interaction is given by

$$\begin{aligned} H &= H_0 + H_{SO} + H_{Zeeman} \\ &= \frac{p_x^2}{2m} - \frac{\hbar\alpha_z}{m}\sigma_y p_x + \frac{\hbar\alpha_y}{m}\sigma_z p_x - \frac{1}{2}g\mu_B\sigma \cdot \mathbf{B} \end{aligned}$$

The last term is the Zeeman energy which depends on the external magnetic field \mathbf{B} not to confuse with the magnetic field responsible for the spin-orbit interaction. As shown in the next chapter, an external magnetic field (and hence a Zeeman interaction) is necessary in order to have energy bands with non-fixed spin quantization axes (meaning that the spin polarization of the electron is wavevector dependent).

In addition to the Rashba effect, owing to the lack of inversion symmetry in bulk materials, there exists the so-called bulk inversion asymmetry (BIA) or Dresselhaus spin-orbit interaction:

$$H_{Dr} = \frac{\hbar}{m}\beta_z(\sigma_x p_x - \sigma_y p_y)$$

In a photocurrent measurement on n-type InAs quantum wells[7], Ganichev et al have deduced the ratio of the relevant Rashba and Dresselhaus coefficients to

$$\alpha/\beta = 2.15$$

1.2.1 Origin of the electric field

What has not been addressed here is the origin of the electric field that is experienced by the electron through \mathbf{B}_{RF} . Consider a surface of a $n \leq 3$ -dimensional crystal. From the point of view of an electron, the surface is established and maintained due to a confining potential V perpendicular to the surface. No matter what kind of complicated structure of atoms the crystal has, an 'electronic' surface must be due to a potential perpendicular to this. Electrons moving in the corresponding electric field $\mathbf{E}_\perp = \mathbf{e}_\perp dV/dr_\perp$ will have their degeneracy lifted by a Rashba spin-orbit coupling with an interaction constant α_\perp proportional to E_\perp .

3D crystal measures of the surface state on Au(111) has been done in a high-resolution photoemission experiment by LaShell et al.[14] showing a splitting of the parabolic dispersion into two branches. The authors have ruled out other

possible explanations and have argued that the splitting should be interpreted as the effect of a spin-orbit interaction. At the Fermi momentum the splitting is observed to be $\Delta E_{\text{LaShell}} \sim -0.1\text{eV}$.

Assuming the surface electrons in Au(111) to be quasi-2D free electron (confined by a potential V_{\perp}) and including a Rashba spin-orbit coupling, L. Petersen and P. Hedegård[20] have estimated the splitting using calculations on jellium By Lang[13]. For a solid, the work function Φ is the minimum energy needed to remove an electron from a solid to a point immediately outside the solid surface (or energy needed to move an electron from the Fermi energy into vacuum). The work function corresponds to a gradient potential $\nabla V \approx \Phi/\lambda_F$ where λ_F is the Fermi wavelength. Petersen and Hedegård have calculated the splitting caused by this gradient potential to be $\Delta E \sim 10^{-6}\text{eV}$ - five orders of magnitude smaller than the splitting experimentally observed by LaShell. They conclude that in Au(111) the potential corresponding to the work function cannot explain the magnitude of the SO-coupling. Hence the electric field must come from somewhere else: the atom cores. Starting from the Intra-atomic SO-coupling

$$H_{\text{SOC}} = \alpha \mathbf{L} \cdot \mathbf{S} = \frac{\alpha}{2} (L^+ \sigma^- + L^- \sigma^+ + L^z \sigma^z)$$

Petersen and Hedegård formulate a tight-band model for the surface states that includes the SO-interaction. The Hamiltonian for p_z bands with only virtual transitions to p_x, p_y bands is to second order in α, γ and \mathbf{k} is

$$H_{\text{eff}} = \begin{pmatrix} -6\delta + (\frac{3}{2}\delta + 9\gamma^2/w) k^2 & -i(k_x - ik_y) \alpha_R \\ +i(k_x + ik_y) \alpha_R & -6\delta + (\frac{3}{2}\delta + 9\gamma^2/w) k^2 \end{pmatrix}$$

with $\alpha_R := 6\alpha\gamma/w$. Here w and γ are coefficients in the overlap matrix elements in the tight-binding Hamiltonian while α is the intra-atomic SO-coupling constant. The effective Hamiltonian is exactly the Matix form of a Hamiltonian consisting of a free electron part and a Rashba-term. The SO coupling constant α_R is of order of the atomic splitting, and hence the model is able to explain the energy splitting observed by LaShell.

Chapter 2

Eigenstates and eigenvalues of the Rashba Hamiltonian

In this chapter we examine how the quantum dot eigenenergies are modified in the presence of a Rashba spin-orbit interaction. Expressing the appropriate Hamiltonian in matrix representation and diagonalizing the matrix yields the eigenenergies and eigenstates of the dot.

Consider a free particle. The eigenstates are given by the solutions to the Schrödinger equation. In real space representation the wave functions are

$$\varphi_{\mathbf{k}\sigma}(\mathbf{r}) = \langle \mathbf{r} | \mathbf{k}\sigma \rangle = \varphi_{\mathbf{k}}(\mathbf{r}) \chi_{\sigma} = A e^{i\mathbf{k}\cdot\mathbf{r}} \chi_{\sigma}$$

with corresponding eigenenergies $\hbar^2 k^2 / 2m$. Here χ_{σ} are the two-component spinors defined as the following eigenstates of the z component of the spin operator: $\hat{S}_z \chi_{\uparrow/\downarrow} = +/ - (\hbar/2) \chi_{\uparrow/\downarrow}$. To each eigenenergy corresponds four linearly independent wave functions, that is

$$\hbar^2 k^2 / 2m = E(\mathbf{k}, \uparrow) = E(\mathbf{k}, \downarrow) = E(-\mathbf{k}, \uparrow) = E(-\mathbf{k}, \downarrow)$$

and hence the eigenenergies are four-fold degenerate: two-fold degenerate in momentum and two-fold degenerate in spin.

2.1 Spin-orbit coupling and symmetries

For more complicated systems, solving the Schrödinger equation can be quite a task. It is then fruitful to consider symmetries in the physical problem as they can lead to restrictions on the energy dispersion relation.

2.1.1 Time reversal symmetry

Time reversal symmetry (T-symmetry) is the symmetry of physical laws under the time transformation $T : t \rightarrow -t$. The T-symmetry of a system is very dependent

of 1) what is considered a part of the system and what is considered external and 2) at which level the system is described (microscopic or macroscopic). See [21] p. 281.

Consider an electron experiencing a Rashba spin-orbit coupling

$$H_{\text{SO}} = -\frac{e\hbar}{4m^2c^2}\sigma \cdot [\mathbf{E} \times \mathbf{p}]$$

due to an external potential $-\nabla V = \mathbf{E}$. Both the spin and the momentum are antisymmetric under time reversal¹. The electric and magnetic field have different transformations under TR: $\mathbf{E} \rightarrow \mathbf{E}$ and $\mathbf{B} \rightarrow -\mathbf{B}$. Hence the Rashba SO-coupling is invariant under TR. Similarly, the Zeeman term $\propto \sigma \cdot \mathbf{B}$ as well as the free energy term $\propto p^2$ is also invariant under TR. So the Hamiltonian describing a spinning electron in an external magnetic field and with a Rashba SO-coupling is invariant under TR.

General restrictions on the eigenenergies can be derived from the assumption of T-symmetry. In quantum mechanics time reversal must be represented as an anti-unitary operator. Anti-unitary means that for arbitrary states φ', φ , T fulfils $\langle \varphi | T^\dagger T | \varphi' \rangle = \langle \varphi' | \varphi \rangle$. Furthermore, it has to have a two-dimensional representation with the property $T^2 = -1$. Following the convention of Sakurai Eq. (4.4.79)[22], a valid representation for a spin 1/2 particles is

$$T = e^{-i(\pi/2)\sigma_y} K$$

where K denotes complex conjugation. Let H be a T-symmetric Hamiltonian with eigenstate and corresponding eigenenergy given by $H\psi = E\psi$. Then $T\psi$ is also an eigenstate with the same eigenenergy, since

$$H(T\psi) = ([H, T] + TH)\psi = [H, T]\psi + E(T\psi) = E(T\psi)$$

These eigenstates are orthogonal since

$$\langle T\psi | \psi \rangle = -\langle T\psi | T(T\psi) \rangle = -\langle T\psi | \psi \rangle$$

¹According to the standard account an active time transformation must be of such character that the spatial velocity \mathbf{v} and current \mathbf{j} flip under active time reversal, while the charge density ρ is invariant. The standard procedure is then to assume that the Maxwell equations and the Lorentz force law $q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) = m\mathbf{a}$ are invariants under TR. This together with the transformation properties of \mathbf{v} , \mathbf{j} and ρ leads to the transformation properties

$$(\mathbf{v}, \mathbf{j}, \mathbf{E}, \mathbf{B}, \rho, \nabla, t) \xrightarrow{T} (-\mathbf{v}, -\mathbf{j}, \mathbf{E}, -\mathbf{B}, \rho, \nabla, -t)$$

However, in Time and Chance[1] (2000) David Albert has argued that the magnetic field is TR invariant and hence the classical EM theory is not TR invariant. This controversial claim has started an ongoing debate among researchers in the philosophy of physics. Notable papers are [15] and [3]. For practical purposes the standard point of view and application gives the right results. The mentioning of the controversy should be considered an information for the reader particularly interested in this topic.

where first step follows from the fact that for half-integer spin $T^2 = 1$ and last step follows from anti-unitarity. This result goes by the name of Kramers' Theorem. So to each eigenvalue E corresponds (at least) two linearly independent eigenstates. All eigenstates have a two-fold degeneracy. Labeling the eigenstates with the index $\lambda \in \{+, -\}$, the eigenstates are ψ_λ with corresponding eigenvalue E .

Consider a crystal. The crystal structure is defined by a periodic lattice. The Bloch Theorem states that each eigenenergy is characterized by a Bloch wave vector \mathbf{k} and Bloch wave state

$$\psi_{\mathbf{k}\lambda}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}\lambda}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \begin{pmatrix} u_{\mathbf{k}\lambda}^\uparrow(\mathbf{r}) \\ u_{\mathbf{k}\lambda}^\downarrow(\mathbf{r}) \end{pmatrix}$$

where u is periodic. Acting on this Bloch wave state with the time reversal operator yields

$$T\psi_{\mathbf{k}\lambda}(\mathbf{r}) = e^{i(-\mathbf{k})\cdot\mathbf{r}} \begin{pmatrix} -u_{\mathbf{k}\lambda}^{\downarrow*}(\mathbf{r}) \\ u_{\mathbf{k}\lambda}^{\uparrow*}(\mathbf{r}) \end{pmatrix} = \psi_{-\mathbf{k}-\lambda}(\mathbf{r})$$

where the last identification can be made since the expression is a Bloch wave state with wave vector $-\mathbf{k}$ and since we know that T maps an eigenstate with index λ into its time reversed eigenstate, having index $-\lambda$. Letting H act on each side and using that a state and its time inverted have same eigenenergy gives

$$E(\mathbf{k}, \lambda) = E(-\mathbf{k}, -\lambda)$$

2.1.2 Spatial inversion symmetry

Parity is represented as a unitary operator P acting on a state function as $P\psi(\mathbf{r}) = \psi(-\mathbf{r})$. If $\psi_{\mathbf{k}\lambda}(\mathbf{r})$ is an eigenstate of P with eigenvalue κ , then $P^2\psi_{\mathbf{k}\lambda}(\mathbf{r}) = \kappa^2\psi_{\mathbf{k}\lambda}(\mathbf{r}) = \psi_{\mathbf{k}\lambda}(\mathbf{r})$. The eigenvalue is thus a phase $\kappa = e^{i\varphi}$. For a crystal that is invariant under P , that is $[H, P] = 0$, then if $\psi_{\mathbf{k}\lambda}$ is an eigenstate of H corresponding to eigenenergy $E_{\mathbf{k}\lambda}$, so is the transformed:

$$H(P\psi_{\mathbf{k}\lambda}) = ([H, P] + PE_{\mathbf{k}\lambda})(\psi_{\mathbf{k}\lambda}) = E_{\mathbf{k}\lambda}(P\psi_{\mathbf{k}\lambda})$$

Explicitly applying P to $\psi_{\mathbf{k}\lambda}(\mathbf{r})$ gives a Bloch state with Bloch vector $-\mathbf{k}$. Since there is double degeneracy in λ (and since this is the only degeneracy), this vector must be in span $\{\psi_{-\mathbf{k}\lambda}(\mathbf{r}), \psi_{-\mathbf{k}-\lambda}(\mathbf{r})\}$ and hence be a linear combination of these:

$$P\psi_{\mathbf{k}\lambda}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}} \begin{pmatrix} u_{\mathbf{k}\lambda}^\uparrow(-\mathbf{r}) \\ u_{\mathbf{k}\lambda}^\downarrow(-\mathbf{r}) \end{pmatrix} = a\psi_{-\mathbf{k}\lambda}(\mathbf{r}) + b\psi_{-\mathbf{k}-\lambda}(\mathbf{r})$$

This leads to $E(\mathbf{k}, \lambda) = E(-\mathbf{k}, \lambda)$ and together with the restriction from T -symmetry, we have that

$$E(\mathbf{k}, \lambda) = E(\mathbf{k}, -\lambda)$$

The conclusion is that for time reversal invariant systems, spin splitting $E(\mathbf{k}, \lambda) \neq E(\mathbf{k}, -\lambda)$ can only occur if the parity is broken, that is if $[H, P] \neq 0$.

Bulk Au have fcc lattice structure and since the fcc lattice has (3D) inversion symmetry, bulk Au cannot have a spin-orbit split band structure. However, the surface of any crystal, there is no inversion symmetry in the direction perpendicular to the surface. This means that we are not able to rule out the possibility of spin splitting.

2.2 Simple Rashba-term and B-field along x

Single-particle Hamiltonian for translational invariant wire along the x-axis, including a Rashba term due to E-field along z-axis and an external magnetic field along the x-axis

$$H = \frac{p_x^2}{2m} - \frac{\hbar\alpha_z}{m}\sigma_y p_x - \frac{1}{2}g\mu_B\sigma_x B_x + V(x)$$

2.3 The splitting of the electron band

For $B = 0$ the effect of the S-O coupling $\sigma_y p_x$ is to split the band $\epsilon(k) = (k^2 + V)$ into two distinct bands

$$\epsilon_1(k) = (k^2 + V) + 2\alpha_z k = (k + \alpha_z)^2 - \alpha_z^2 + V$$

$$\epsilon_2(k) = (k^2 + V) - 2\alpha_z k = (k - \alpha_z)^2 - \alpha_z^2 + V$$

crossing at $(0, V(0))$. The spin expectation values are

$$(\langle\sigma_x\rangle_1, \langle\sigma_y\rangle_1, \langle\sigma_z\rangle_1) = (0, +1/2, 0)$$

$$(\langle\sigma_x\rangle_2, \langle\sigma_y\rangle_2, \langle\sigma_z\rangle_2) = (0, -1/2, 0)$$

and hence the branch $\epsilon_1(k)$ ($\epsilon_2(k)$) is characterized by spin pointing parallel to $+y$ ($-y$). By relabeling the branches $(\epsilon_{s=\uparrow}, \epsilon_{s=\downarrow}) := (\epsilon_1, \epsilon_2)$ the splitting of the energy band into two distinct bands of different spin is emphasized.

As a external magnetic field $\mathbf{B} = (B_x, 0, 0)$ is applied, the Zeeman term will cause a splitting of the energy band. In the absence of spin-orbit interactions the energy bands are given by $\epsilon_a = k^2 + B_x$ and $\epsilon_b = k^2 - B_x$.

In the presence of both a spin-orbit interaction $-\sigma_y p_x$ and a Zeeman term $-\sigma_x B_x$ will result in a mixing of the Rashba-split subbands. The splitting is shown in fig. ???. By forming a local gap at $k = 0$ the energy branches avoid crossing. For large $|k|$ values the spin will be orientated approx. as it was before applying the external B-field. The spin rotates in a small region around the gap at $k = 0$. It is no longer possible to associate a fixed spin direction with each

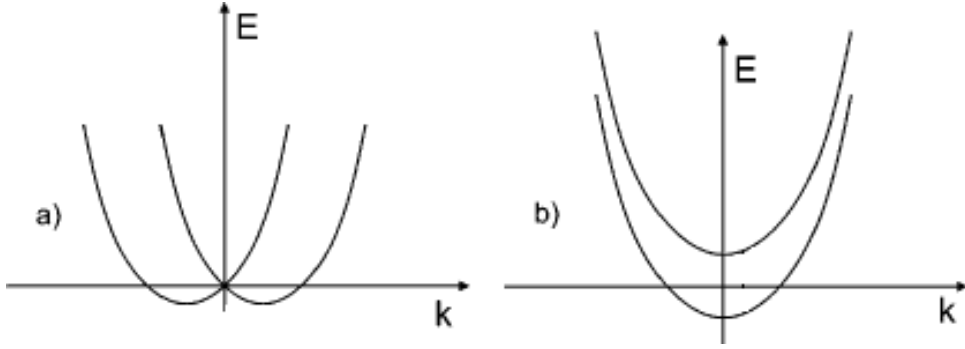
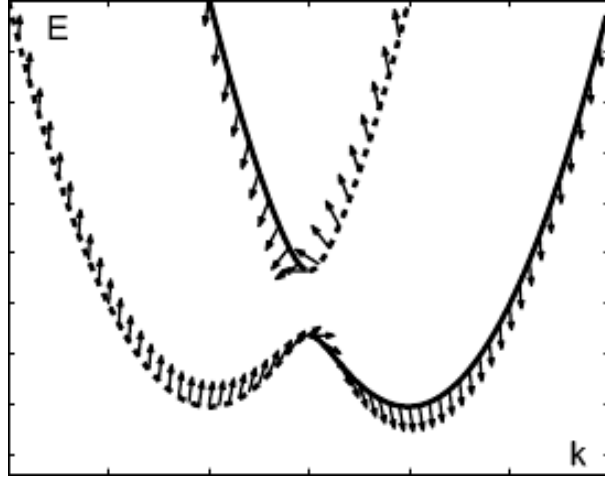


Figure 2.1: Schematic representation of a conduction band structure where the spin-degeneracy is broken a) by a spin-orbit interaction as described by the Rashba Hamiltonian and b) by a Zeeman interaction of the spin with an external magnetic field [17]

Figure 2.2: Schematic representation of a conduction band structure where the spin-degeneracy is broken by both a Rashba SO interaction and a Zeeman interaction. The spin expectation value is plotted on the branches. Note that each branch is no longer associated with a single spin. Fig. from [25]



band. Due to the Rashba SO coupling together with the Zeeman splitting, spin and momentum do not constitute a set of good quantum numbers. Instead we must label the bands with an index $\eta = \pm$ that is not associated with a single spin. We may think of η as a pseudo-spin and denote the \pm values as \uparrow / \downarrow .

The question now arises as to what effect this mixing of the spin degree of freedom with the orbital motion will have on electrons tunneling through the quantum dot. An electron from lead $\alpha = L, R$ in an energy eigenstate $|\alpha \mathbf{k} \sigma\rangle$ given by momentum and spin (the lead label α is only written for bookkeeping purposes) can tunnel into the dot region, where the energy eigenstates are $|\mathbf{k} \eta\rangle$. This process can be described by a tunneling Hamiltonian in an Anderson-type model for the electron transport through the junction.

Chapter 3

Anderson Model with SO interaction

3.1 Second quantization formulation

In the following, both k and p will be used as names for particle de Broglie wavenumber. When dealing with the tunneling Hamiltonian, k will be associated with states on the quantum dot and p with lead states. A scattering region (quantum dot) is coupled to two metal leads ($\alpha = L, R$) as well as a gate electrode used to shift the chemical potential on the dot. The lead electrons are assumed to be free noninteracting electrons while the dot electrons are described by a Hamiltonian containing a Rashba SO interaction, a Zeeman splitting, a charging energy and a confining harmonic oscillator potential. The second-quantized Hamiltonian reads

$$H = H_{LR} + H_D + H_T \quad (3.1)$$

where

$$\begin{aligned} H_{LR} &= H_L + H_R = \sum_{p\sigma} \xi_{Lp} c_{Lp\sigma}^\dagger c_{Lp\sigma} + \sum_{p\sigma} \xi_{Rp} c_{Rp\sigma}^\dagger c_{Rp\sigma} \\ H_D &= H_{D0} + H_{S-O} + H_{\text{Zeeman}} \\ H_T &= \sum_{\alpha p k \sigma} (t_{\alpha p k} c_{\alpha p \sigma}^\dagger d_{k\sigma} + t_{\alpha p k}^* d_{\alpha \sigma}^\dagger c_{\alpha p \sigma}) \end{aligned}$$

3.2 Cotunneling and Kondo effect in the absence of SO interaction

Fig 3.1 shows the potential landscape of a quantum dot along the transport direction. The states in the leads are filled up to the electrochemical potentials μ_L and μ_R which are connected via the externally applied bias-voltage $V =$

$(\mu_L - \mu_{RL})/e$. This energy window is called the bias window. For energies within the bias window, the electron states in one reservoir is filled whereas states in the other are empty. At zero temperature sequential tunneling occurs only if there is an appropriate electrochemical potential level on the dot within the bias window. Electron tunneling through the dot thus depends critically on the alignment of the electrochemical potential on the dot with those of the leads.

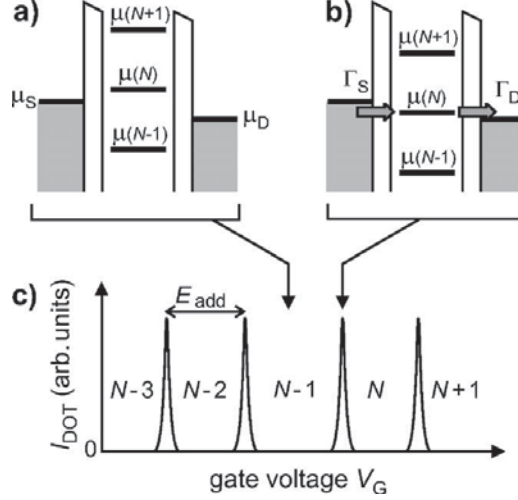


Figure 3.1: Quantum dot in the regime of low bias. (a) Coulomb blockade. Sequential tunneling through the dot is not possible. (b) A charge-degenerate point at which the number of electrons can fluctuate and thus permitting electrons to tunnel through the junction. (c) The oscillatory dependence of current on gate-voltage [11]

The electrochemical potential for the transition between the N -electron ground state and the $(N-1)$ -electron ground state on the dot is

$$\mu(N) = E(N) - E(N-1)$$

All electrochemical potentials have the same linear dependence on the gate voltage V_g . Therefore shifting V_g will move the whole 'ladder' of electrochemical potentials without altering the distance between them.

We shall here assume that the temperature is very low compared to the energy-level spacing. In the low-bias regime the bias window is very narrow. Sweeping the gate-voltage will give an almost discrete dependence of current as function of gate-voltage as shown in fig 3.1. At a charge-degenerate point there is a level μ_D in the bias window so the number of electrons on the dot can alternate, thus current can flow. Away from these points, transport is strongly suppressed by a Coulomb blockade, reflecting the fact that the capacitive changing energy of the dot is too large for electrons to freely tunnel onto and off the dot. The sequential tunneling rate is given by Fermi's golden rule to lowest order in the tunneling, H_T .

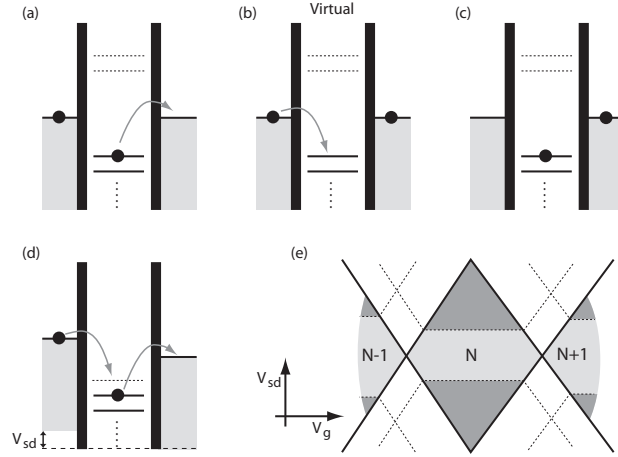


Figure 3.2: (a)-(c) Cotunneling. The intermediate state can occur as long as the system only exist in the virtual state for a time sufficiently short not to violate the Heisenberg uncertainty principle. (d) For larger bias, inelastic cotunneling becomes available. (3) Cotunneling is possible in the dark area of the Coulomb diamond. Fig from ref. Fig. from [12]

For strong couplings to the lead, this is not a correct description as there are higher order contributions to the tunneling. Transitions in which the intermediate state has an energy larger than the initial energy can occur as a virtual process due to the uncertainty principle. This happens in cotunneling which is of second order in the tunneling. The process is illustrated in fig 3.2. An expression for the transition rates is obtained by using the generalized Fermi's golden rule [4, p. 88].

In the case where the quantum dot holds an effective magnetic moment, the dot and the metallic electrodes constitute a system similar to a metal with a single magnetic impurity. The Hamiltonian (3.1) can be brought on a form that includes a spin-spin interaction term expressing scattering on the dot due to virtual scattering in and out of the dot. This causes a correlated transport across the dot. Contrary to the case of metals, this scattering on the dot increases the conductance through the dot. Lowering the temperature this Kondo-effect lifts the Coulomb blockade completely. As an example of a Kondo-peak, see the measurement by Wiel in fig 3.4.

In order to determine how this picture is modified by the presence of a Rashba spin-orbit interaction we have a two step plan: First we shall transform away the SO interaction by means of a unitary transformation. Then we shall follow Schrieffer-Wolff and transform away the charge fluctuations, bringing the Hamiltonian on the form of a spin-spin interaction.

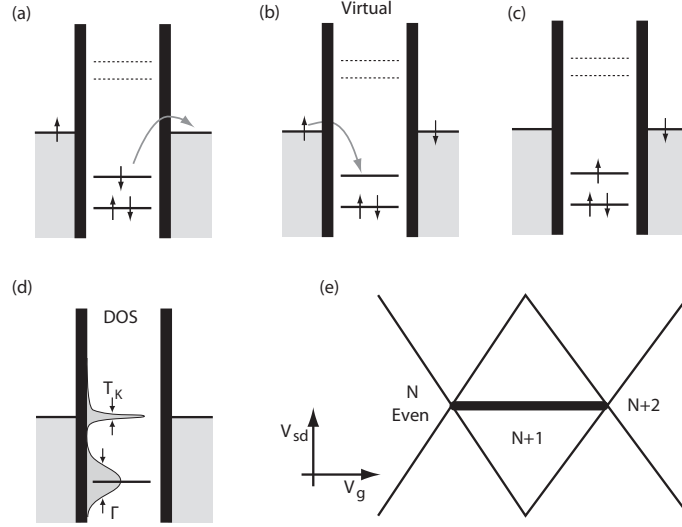


Figure 3.3: The process leading to the Kondo effect in an odd- N quantum dot. Being a quantum particle, the spin-down electron may tunnel out of the dot to briefly occupy a classically forbidden 'virtual state' outside the dot, and then be replaced by an electron from the lead. This can effectively flip the spin of the quantum dot. (d) Many such events combine to produce the Kondo effect, which leads to the appearance of an extra resonance at the Fermi energy. Since transport properties, such as conductance, are determined by electrons with energies close to the Fermi level, the extra resonance can dramatically change the conductance. (e) The enhanced conductance takes place only at low bias (black area). Fig. from [12]

3.3 Transforming away the SO interaction

3.3.1 Simple Rashba-term

We first consider the simplest Hamiltonian covering a Rashba spin-orbit interaction

$$H = \frac{p^2}{2m} + \frac{\hbar\alpha}{m}\sigma_y p + V(x), \quad p = p_x.$$

If there exist a unitary operator U , such that $UHU^\dagger = \frac{p^2}{2m} + V(x)$, then the eigenvalues and eigenfunctions of H can be found by solving the eigenvalue problem for the rotated Hamiltonian. Let ψ' denote an eigenstate of UHU^\dagger with eigenenergy E' . Then $U^\dagger\psi'$ is an eigenstate of H with eigenenergy E' , as can be seen from $(UHU^\dagger)\psi' = E'\psi' \Leftrightarrow H(U^\dagger\psi') = E'(U^{-1}\psi') = E'(U^\dagger\psi')$.

Let $U = e^{iS}$ for an operator S , that we will specify in the following. UHU^\dagger

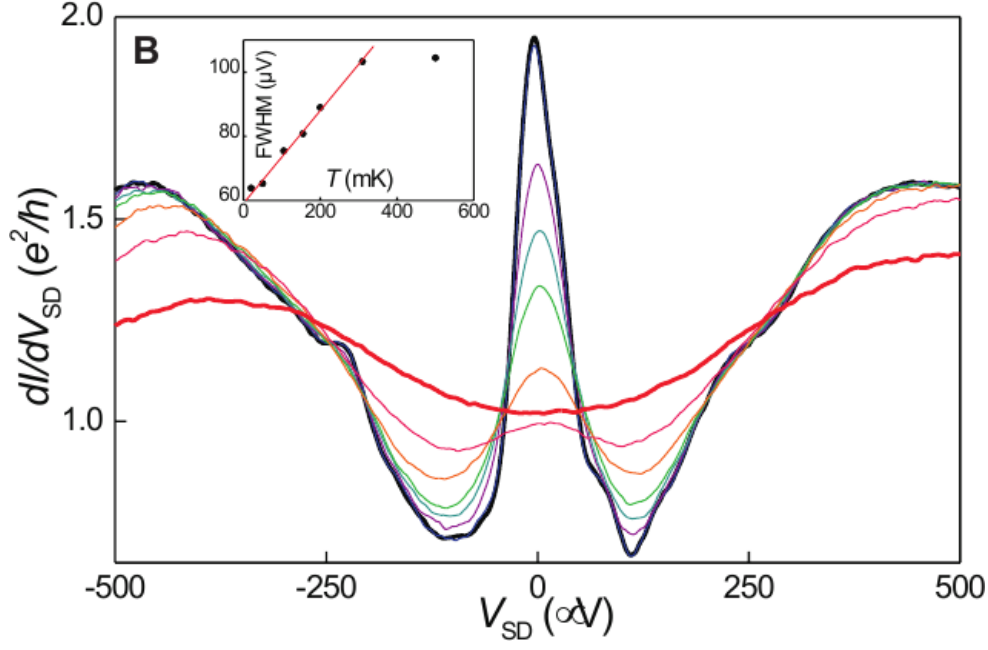


Figure 3.4: Measurements on a semiconductor quantum dot. dI/dV as function of bias V for $T = 15$ mK (thick black trace) up to 900 mK (thick red trace). The left inset shows that the width of the zero-bias peak, measured from the full-width-at-half-maximum (FWHM) increases linearly with T . The red line indicates a slope of 1.7 mV/K, where k_B is the Boltzmann constant. At 15 mK the FWHM = 64 μ V and it starts to saturate around 300 mK. [26]

can be evaluated using the Baker-Campbell-Hausdorff formula

$$e^{\tau A} B e^{-\tau A} = \sum_{m=0}^{\infty} \frac{\tau^m}{m!} B_m \quad (3.2)$$

where

$$B_m = [A, B]_m = [A, [A, B]_{m-1}] \quad , \quad B_0 = B$$

The goal is to find a suitable operator S , such that the Rashba term is cancelled out when performing the unitary transformation. First we examine $U H U^\dagger$ to linear order in S

$$\begin{aligned} U H U^\dagger &= e^{iS} \left(\frac{p^2}{2m} + V(X) + \frac{\hbar\alpha}{m} \sigma_y p \right) e^{-iS} \\ &\approx \frac{p^2}{2m} + V(X) + \frac{\hbar\alpha}{m} \sigma_y p + i \left[S, \frac{p^2}{2m} + V(X) \right] + i \left[S, \frac{\hbar\alpha}{m} \sigma_y p \right] \end{aligned}$$

The Rashba term can be cancelled out with the first commutator if we let $S = \alpha x \sigma_y$ such that $e^{iS} = e^{i\alpha x \sigma_y}$:

$$\begin{aligned} i \left[S, \frac{p^2}{2m} + V(X) \right] &= \frac{\alpha i}{2m} x [\sigma_y, p^2] + \frac{\alpha i}{2m} [x, p^2] \sigma_y \\ &\quad + \alpha i x [\sigma_y, V(x)] + \alpha i [x, V(x)] \sigma_y \\ &= -\frac{\hbar \alpha}{m} \sigma_y p \end{aligned}$$

The second commutator is just a constant

$$i \left[S, \frac{\hbar \alpha}{m} \sigma_y p \right] = \frac{i \alpha^2 \hbar}{m} [x \sigma_y, \sigma_y p] = \frac{i \alpha^2 \hbar}{m} \sigma_y [x, p] \sigma_y = -\frac{\alpha^2 \hbar^2}{m} \sigma_y^2 = -(\hbar^2/m) \alpha^2$$

Here we have used the basic identities

$$\begin{aligned} [p_{x_i}, x_j^2] &= (-2i\hbar) x_i \delta_{ij} \\ [x_i, p_{x_j}^2] &= 2i\hbar p_{x_i} \delta_{ij} \end{aligned}$$

as well as the commutator between Pauli matrices

$$[\sigma_a, \sigma_b] = 2i \sum_c \epsilon_{abc} \sigma_c$$

Note that this term is quadratic in the Rashba spin-orbit interaction constant α . To linear order in α , the Hamiltonian has thereby been diagonalized: $UHU^\dagger = \frac{p^2}{2m} + V(x) + O(\alpha^2)$.

To second order in S , UHU^\dagger is given by

$$\begin{aligned} UHU^\dagger &\approx \frac{p^2}{2m} + V(X) + i \left[S, \frac{\hbar \alpha}{m} \sigma_y p \right] \\ &\quad - \frac{1}{2} \left[S, [S, \frac{p^2}{2m} + V(X)] \right] - \frac{1}{2} \left[S, [S, \frac{\hbar \alpha}{m} \sigma_y p] \right] \\ &= \frac{p^2}{2m} + V(X) + i \left[S, \frac{\hbar \alpha}{m} \sigma_y p \right] - \frac{i}{2} \left[S, \frac{\hbar \alpha}{m} \sigma_y p \right] - 0 \\ &= \frac{p^2}{2m} + V(X) - \frac{1}{2} \frac{\hbar^2 \alpha^2}{m} \end{aligned}$$

Since $H_2 = [S, H]_2 = [S, [S, H]] = -\frac{\alpha^2 \hbar^2}{2m}$ is a constant, it is clear that all higher order contributions are zero: $B_3 = [S, [S, H]_2] = 0$ and $B_{m>3} = [S, [S, H]_{m-1}] = [S, 0] = 0$. We arrive at the exact relation

$$UHU^\dagger = \frac{p^2}{2m} + V(X) - \frac{\hbar^2 \alpha^2}{2m}$$

The transformation is nothing more than a momentum shift $p \rightarrow p + \hbar\alpha\sigma_y$, as can be seen from

$$H = \frac{p^2}{2m} + \frac{\hbar\alpha}{m}\sigma_y p + V(x) = \frac{(p + \hbar\alpha\sigma_y)^2}{2m} - \frac{\hbar^2\alpha^2}{2m} + V(x)$$

This is also clear since $S = \alpha x\sigma_y$ is a generator of momentum translation.

If the confining potential is an harmonic oscillator potential

$$V(x) = \frac{1}{2}m\omega_0^2 x^2$$

then $H' = UHU^\dagger$ is the Hamiltonian for a harmonic oscillator with eigenfunctions ψ'_n and corresponding eigenenergies E'_n given by

$$\begin{aligned}\psi'_n &= H_n(x/a) (n!2^n a\pi^{1/2})^{-1/2} e^{-x^2/2a^2} \\ E'_n &= \left(n + \frac{1}{2}\right) \hbar\omega_0 - \frac{\alpha^2 \hbar^2}{2m}\end{aligned}$$

The oscillator length a is given by

$$a = (\hbar/m\omega_0)^{1/2}$$

and $H_n(x)$ is the Hermite polynomials defined by the recursive relation

$$\begin{aligned}H_{n+1}(y) &= 2yH_n(y) - 2nH_{n-1}(y) \\ H_0(y) &= 1 \\ H_1(y) &= 2y\end{aligned}$$

The ground state of the harmonic oscillator is $\psi'_0 = (a\pi^{1/2})^{-1/2} e^{-x^2/2a^2}$ and $\frac{d}{dx}\psi'_0 = -\frac{x}{a^2}\psi'_0$. Since $UHU^\dagger\psi' = E'\psi' \Leftrightarrow H(U^\dagger\psi') = E'(U^\dagger\psi')$, the eigenfunctions and eigenenergies of H are

$$\psi_n = U^\dagger\psi'_n = \frac{H_n(x/a)}{(n!2^n a\pi^{1/2})^{1/2}} e^{-i\alpha x\sigma_y} e^{-x^2/2a^2}, \quad E_n = \left(n + \frac{1}{2}\right) \hbar\omega_0 - \frac{\alpha^2 \hbar^2}{2m}$$

By finding a unitary transformation between the Hamiltonian concerned and a Hamiltonian with known solutions, the problem is solved. All one has to do is to apply the hermitian conjugate transformation (for a unitary transformation, this is the inverse transformation) to the set of known solutions. This is often much easier than to solve the problem from scratch. Using the Baker-Campbell-Hausdorff expansion to write out the transformed Hamiltonian in terms of the operator S makes it a bit easier to find an S that does the job.

Using a unitary operator on the form e^{iS} and using the Baker-Campbell-Hausdorff formula to calculate the transformed Hamiltonian is a neat way of making perturbation theory. The BCH-formula is a series expansion in the original Hamiltonian. Since the Rashba spin-orbit coupling α enters linearly in both S and H , the element B_m in (3.2) will contain terms up to order $O(\alpha^{m+1})$.

3.3.2 Rashba-term and an external magnetic field

In this section we shall use the techniques of above to find eigenstates of the two-dimensional Hamiltonian

$$\begin{aligned} H_D &= H_d + H_{Ra} + H_Z \\ &= \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega_0^2(x^2 + y^2) + \frac{\hbar\alpha}{m}(\sigma_x p_y - \sigma_y p_x) - \frac{1}{2}g\mu_B \boldsymbol{\sigma} \cdot \mathbf{B} \end{aligned}$$

following Golovach[9]. The Hamiltonian describes a particle in a 2-D harmonic oscillator potential, subject to a Rashba spin-orbit interaction and a magnetic field. The eigenstates are then used to calculate the tunneling coefficients in the tunneling Hamiltonian that describe tunneling between the leads and the dot.

We want a unitary operator $U = e^S$, such that $U H U^\dagger = H_d + H_Z$. That is, such that the Rashba spin-orbit interaction is transformed out. As in the previous section, the strategy is to find an operator S , such that the part $[S, H_d + H_Z]$ of the first commutator in the Baker-Campbell-Hausdorff expansion cancels out the spin-orbit term. On order to identify S , we first rewrite $-H_{Ra}$ as:

$$\begin{aligned} -\frac{\hbar\alpha}{m}(\sigma_x p_y - \sigma_y p_x) &= -\frac{\hbar\alpha}{m} \left(\frac{1}{2i\hbar} [y, p_y^2] \sigma_x + \frac{1}{2i\hbar} [-x, p_x^2] \sigma_y \right) \\ &= i\alpha \left(\left[y, \frac{p_x^2 + p_y^2}{2m} \right] \sigma_x + \left[-x, \frac{p_x^2 + p_y^2}{2m} \right] \sigma_y \right) \\ &= i \sum_i [\xi_i, H_d + H_Z] \sigma_i \\ &= \underbrace{\left[i \sum_i \xi_i \sigma_i, H_d + H_Z \right]}_{[S_1, H_d + H_Z]} - i \sum_i \xi_i [\sigma_i, H_d + H_Z] \end{aligned}$$

where we have defined $\boldsymbol{\xi} = (\alpha y, -\alpha x, 0) = \left(\frac{y}{\lambda_{SO}}, \frac{-x}{\lambda_{SO}}, 0 \right)$ with $\lambda_{SO} = 1/\alpha$ being the spin-orbit length. In order to bring $-H_{Ra}$ on the right commutator form, we got an additional term, that is not immediately on the right form. It can however

be brought into the commutator form

$$\begin{aligned}
-i \sum_i \xi_i [\sigma_i, H_d + H_Z] &= -g\mu_B B \alpha (y n_y \sigma_z - y n_z \sigma_y - x n_z \sigma_x + x n_x \sigma_z) \\
&= -g\mu_B B \alpha \left((-n_z) [p_y, V(x, y)] \sigma_y + (-n_z) [p_x, V(x, y)] \sigma_x \right. \\
&\quad \left. + n_y [p_y, V(x, y)] \sigma_z + n_x [p_x, V(x, y)] \sigma_z \right) \frac{i}{2\hbar} \frac{1}{\frac{1}{2} m \omega_0^2} \\
&= -g\mu_B B \alpha \left([-n_z \partial_y, H_d + H_Z] \sigma_y + [-n_z \partial_x, H_d + H_Z] \sigma_x \right. \\
&\quad \left. [n_y \partial_y + n_x \partial_x, H_d + H_Z] \sigma_z \right) \frac{i}{2\hbar} \frac{1}{\frac{1}{2} m \omega_0^2} (-i\hbar) \\
&= -\frac{g\mu_B B \alpha}{m \omega_0^2} \left[-n_z \partial_x \sigma_x - n_z \partial_y \sigma_y \right. \\
&\quad \left. + (n_y \partial_y + n_x \partial_x) \sigma_z, H_d + H_Z \right] + O(B^2) \\
&= \left[-\frac{g\mu_B B}{m \omega_0^2} [\mathbf{n} \times \boldsymbol{\zeta}] \cdot \boldsymbol{\sigma}, H_d + H_Z \right] + O(B^2)
\end{aligned}$$

where $\boldsymbol{\zeta} = (-\alpha \partial_y, \alpha \partial_x, 0) = \left(-\frac{1}{\lambda_{SO}} \partial_y, \frac{1}{\lambda_{SO}} \partial_x, 0 \right)$ and $\mathbf{n} = \mathbf{B}/B$. We thus have

$$[S, H_d + H_Z] = -H_{Ra} + O(B^2)$$

with

$$S = S_1 + S_2 = i\boldsymbol{\xi} \cdot \boldsymbol{\sigma} - \frac{g\mu_B B}{\hbar \omega_0} a^2 [\mathbf{n} \times \boldsymbol{\zeta}] \cdot \boldsymbol{\sigma}$$

and to linear order in B , the rotated Hamiltonian is given by

$$\tilde{H}_D = U H_D U^\dagger \approx H_d + H_Z + \frac{1}{2} [S, H_{Ra}] \quad (3.3)$$

Note that $\frac{1}{2} [S, H_{Ra}]$ has terms up to quadratic order in the coupling since S is linear in α . Restricting ourselves to one dimension, the quadratic contribution to the rotated Hamiltonian is

$$\frac{1}{2} [S, H_{Ra}] = \frac{\alpha^2 \hbar^2}{m} + \frac{1}{m} \left(\frac{a}{\lambda_{SO}} \right)^2 \frac{g\mu_B \mathbf{B}}{\hbar \omega_0} \cdot (\sigma_x, 0, \sigma_z) p_x^2$$

The second term is an anisotropic correction to the g-factor which is negligible if the dot is much smaller than the Rashba spin orbit length

$$a \ll \lambda_{SO}$$

and if the Zeeman splitting is much smaller than the level splitting

$$g\mu_B B \ll \hbar \omega_0$$

. In the following we shall assume this to be the case and thus

$$\tilde{H}_D = H_d + H_Z$$

Acting with U on the harmonic oscillator eigenfunctions gives eigenfunctions of H . In the following, we shall consider a quantum dot where transitions to excited states can only happen as virtual processes allowed by the uncertainty principle. Our hope is that this is sufficient to describe the characteristics of the spin-orbit effect on the tunneling through a quantum dot.

The ground state wave functions of the two-dimensional harmonic oscillator are

$$\varphi_{00}(x, y)|\sigma\rangle = \varphi_0(x)\varphi_0(y)|\sigma\rangle = (a\pi^{1/2})^{-1} e^{-(x^2+y^2)/2a^2}|\sigma\rangle$$

for spins $\sigma = \uparrow, \downarrow$. We choose the quantization axis along the z-axis. That is, $|\sigma\rangle$ is an eigenstate of S_z and S^2 . The spin-orbit interaction gives rise to a new branch index $\eta = \pm 1$, that we will here symbolize as a pseudo-spin $\eta \in \{+1, -1\} = \{\uparrow, \downarrow\}$. Multiplying with the identity operator and using

$$\begin{aligned} (\sigma_x, \sigma_y, \sigma_z)|\uparrow\rangle &= (|\downarrow\rangle, i|\downarrow\rangle, |\uparrow\rangle) \\ (\sigma_x, \sigma_y, \sigma_z)|\downarrow\rangle &= (|\uparrow\rangle, -i|\uparrow\rangle, -|\downarrow\rangle) \end{aligned}$$

the ground states of H are given by

$$\begin{aligned} |0\uparrow\rangle &= (1 - S)|00\rangle|\uparrow\rangle \\ &= |00\rangle|\uparrow\rangle - i\alpha(y\sigma_x - x\sigma_y)|\uparrow\rangle|00\rangle \\ &\quad + g\mu_B B \frac{\alpha}{m\omega_0^2} [(-n_z\partial_x)\sigma_x + (-n_z\partial_y)\sigma_y + (n_x\partial_x + n_y\partial_y)\sigma_z]|\uparrow\rangle|00\rangle \\ &= \left(1 + g\mu_B B \frac{\alpha}{m\omega_0^2} (n_x\partial_x + n_y\partial_y)\right)|00\rangle|\uparrow\rangle \\ &\quad + \left(i^2\alpha x - i\alpha y - g\mu_B B \frac{\alpha}{m\omega_0^2} n_z(\partial_x + i\partial_y)\right)|00\rangle|\downarrow\rangle \end{aligned}$$

and

$$\begin{aligned} |0\downarrow\rangle &= \left(-i^2\alpha x - i\alpha y - g\mu_B B \frac{\alpha}{m\omega_0^2} n_z(\partial_x - i\partial_y)\right)|00\rangle|\uparrow\rangle \\ &\quad + \left(1 - g\mu_B B \frac{\alpha}{m\omega_0^2} (n_x\partial_x + n_y\partial_y)\right)|00\rangle|\downarrow\rangle \end{aligned}$$

Comparing the spin-up part of ψ_{\uparrow} to the spin-down part of ψ_{\downarrow} , there is a lack of symmetry regarding signs. This is due to σ_z having different eigenvalues associated with $|\uparrow\rangle$ and $|\downarrow\rangle$. Similarly, the difference between the spin-down part of

ψ_{\uparrow} and the spin-up part of ψ_{\downarrow} is due to different eigenvalues of σ_y .

We now restrict our attention to one dimension. We denote by C_i the ratio between the Zeeman splitting and the level spacing

$$C_i = g\mu_B B \frac{n_i}{m\omega_0^2 a^2} = \frac{g\mu_B B_i}{\hbar\omega_0} \ll 1 \quad (3.4)$$

which we assume to be much smaller than one. The energy eigenstates are

$$\begin{aligned} |0 \uparrow\rangle &= \left(1 + g\mu_B B \frac{\alpha}{m\omega_0^2} n_x \partial_x\right) |0\rangle |\uparrow\rangle + \left(i^2 \alpha x - g\mu_B B \frac{\alpha}{m\omega_0^2} n_z \frac{\partial}{\partial x}\right) |0\rangle |\downarrow\rangle \\ &= (1 - C_x \alpha x) |0\rangle |\uparrow\rangle + (i^2 \alpha x + C_z \alpha x) |0\rangle |\downarrow\rangle \end{aligned}$$

$$\begin{aligned} |0 \downarrow\rangle &= \left(-i^2 \alpha x - g\mu_B B \frac{\alpha}{m\omega_0^2} n_z \partial_x\right) |0\rangle |\uparrow\rangle + \left(1 - g\mu_B B \frac{\alpha}{m\omega_0^2} n_x \partial_x\right) |0\rangle |\downarrow\rangle \\ &= (-i^2 \alpha x + C_z \alpha x) |0\rangle |\uparrow\rangle + (1 + C_x \alpha x) |0\rangle |\downarrow\rangle \end{aligned}$$

A general dot state $|n \uparrow\rangle$ ($|n \downarrow\rangle$) is likewise given by applying the inverse transformation $(1 - S)$ to the oscillator eigenstate $|n\rangle |\uparrow\rangle$ ($|n\rangle |\downarrow\rangle$):

$$|n, \eta = \pm 1\rangle = \sum_{n'\sigma'=\uparrow,\downarrow} |n'\sigma'\rangle \langle n'\sigma'| (1 - S) |n\rangle |\sigma = \pm 1\rangle$$

Here the notation gets a bit tricky. It is important to stress that $|n, \eta = \pm 1\rangle = |n, \eta = \uparrow / \downarrow\rangle$ is a dot state determined by n and pseudo-spin, whereas $|\sigma = \pm 1\rangle = |\sigma = \uparrow / \downarrow\rangle$ is a normal spin state. In order to keep track of where which spin σ came from and to be able to write a general expression, we use an alternative notation, namely

$$\sigma_\eta = \begin{cases} \uparrow & \text{for } \eta = \uparrow \\ \downarrow & \text{for } \eta = \downarrow \end{cases}$$

3.4 Tunneling coefficients

A conduction electron in the lead $\alpha \in \{L, R\}$ is initially in the state $|\alpha k \sigma\rangle$ determined by its momentum and spin. The alpha in the ket is only written for bookkeeping purposes. The Hybridization Hamiltonian that describes tunneling of electrons between the leads and the dot is

$$H_T = \sum_{\substack{\alpha=L,R \text{ } k \\ \sigma=\uparrow,\downarrow \text{ } \eta=\uparrow,\downarrow}} t_{\alpha k n}^{\sigma \eta} c_{\alpha k \sigma}^\dagger d_{n \eta} + t_{\alpha k n}^{\sigma \eta *} d_{n \eta}^\dagger c_{\alpha k \sigma}$$

where the tunneling coefficients are given by the overlap

$$\begin{aligned} t_{\alpha kn}^{\sigma\eta} &= \langle \alpha k \sigma | H_T | n \eta \rangle \\ &= \sum_{n' \sigma'} \langle \alpha k \sigma | H_T | n' \sigma' \rangle \langle n' \sigma' | n \eta \rangle \\ &= \sum_{n' \sigma'} t_{\alpha kn'}^{\sigma \sigma'} m_{n' n}^{\sigma' \eta} \end{aligned}$$

In this expression $t_{\alpha kn'}^{\sigma \sigma'} := \langle \alpha k \sigma | H_T | n' \sigma' \rangle$ is the tunneling coefficient between a metallic lead and a dot with oscillator eigenstates where no SO-interaction is present. This problem is well known, so in this thesis the tunneling coefficient $t_{\alpha kn'}^{\sigma \sigma'}$ is taken as model parameter. In order to find the coefficients $m_{n' n}^{\sigma' \eta} = \langle n' \sigma' | n \eta \rangle$ we first find the kets to multiply:

$$\begin{aligned} |n \eta\rangle &= (1 - S) |n\rangle |\sigma_\eta\rangle \\ &= |n\rangle |\sigma_\eta\rangle + i\alpha x \sigma_y |\sigma_\eta\rangle |n\rangle + g\mu_B \frac{\alpha}{m\omega_0^2} [-n_z \partial_x \sigma_x + n_x \partial_x \sigma_z] |\sigma_\eta\rangle |n\rangle \\ &= \left(1 + C_x a^2 \alpha |\sigma_\eta| \partial_x\right) |n\rangle |\sigma_\eta\rangle + \left(i^2 \alpha x |\sigma_\eta| - C_z a^2 \alpha \partial_x\right) |n\rangle |\overline{\sigma_\eta}\rangle \end{aligned}$$

By $|\sigma_\eta|$ we just mean $+1$ for $\eta = \uparrow$ and -1 for $\eta = \downarrow$. The coefficients are given by

$$\begin{aligned} m_{n' n}^{\sigma' \eta} &= \delta_{n' n} \delta_{\sigma' \sigma_\eta} + |\sigma_\eta| C_x a^2 \alpha \delta_{\sigma' \sigma_\eta} \langle n' | \partial_x | n \rangle \\ &\quad - \alpha |\sigma_\eta| \delta_{\sigma' \overline{\sigma_\eta}} \langle n' | x | n \rangle - C_z a^2 \alpha \delta_{\sigma' \overline{\sigma_\eta}} \langle n' | \partial_x | n \rangle \end{aligned}$$

The inner products concerning x are [16]

$$\langle n' | x | n \rangle = \frac{a}{\sqrt{2}} \left[\sqrt{n'} \delta_{n, n'-1} + \sqrt{n'+1} \delta_{n, n'+1} \right]$$

The differential operator acting on a harmonic oscillator state $|n\rangle$ is

$$\partial_x |n\rangle = -\frac{x}{a^2} |n\rangle + \theta_1(n) \frac{\sqrt{2}\sqrt{n}}{a} |n-1\rangle$$

where $\theta_1(n)$ is the Heaviside step function with $\theta_1(0) = 0$ and $\theta_1(n > 0) = 1$. Sandwiching the operator between harmonic oscillator states gives the inner product:

$$\begin{aligned} \langle n' | \partial_x | n \rangle &= -a^{-2} \langle n' | x | n \rangle + \theta_1(n) 2^{1/2} a^{-1} \sqrt{n} \langle n' | n-1 \rangle \\ &= -a^{-1} 2^{-1/2} \left[\sqrt{n'} \delta_{n, n'-1} + \sqrt{n'+1} \delta_{n, n'+1} \right] + \theta_1(n) 2^{1/2} a^{-1} \sqrt{n} \delta_{n' n-1} \end{aligned}$$

and hence the m-coefficients are

$$\begin{aligned}
m_{n'n}^{\sigma'\eta} &= \delta_{n'n} \delta_{\sigma'\sigma_\eta} - \alpha |\sigma_\eta| \delta_{\sigma'\overline{\sigma_\eta}} a 2^{-1/2} \left[\sqrt{n'} \delta_{n,n'-1} + \sqrt{n'+1} \delta_{n,n'+1} \right] \\
&\quad + |\sigma_\eta| C_x a^2 \alpha \delta_{\sigma'\sigma_\eta} \left(-a^{-1} 2^{-1/2} \left[\sqrt{n'} \delta_{n,n'-1} + \sqrt{n'+1} \delta_{n,n'+1} \right] \right. \\
&\quad \left. + \theta_1(n) 2^{1/2} a^{-1} \sqrt{n} \delta_{n'n-1} \right) \\
&\quad - C_z a^2 \alpha \delta_{\sigma'\overline{\sigma_\eta}} \left(-a^{-1} 2^{-1/2} \left[\sqrt{n'} \delta_{n,n'-1} + \sqrt{n'+1} \delta_{n,n'+1} \right] \right. \\
&\quad \left. + \theta_1(n) 2^{1/2} a^{-1} \sqrt{n} \delta_{n'n-1} \right)
\end{aligned}$$

$m_{00}^{\sigma'\eta}$ and $m_{10}^{\sigma'\eta}$ are

$$\begin{aligned}
m_{00}^{\uparrow\uparrow} &= \langle 0 \uparrow | 0 \uparrow \rangle = 1 & m_{00}^{\uparrow\downarrow} &= \langle 0 \uparrow | 0 \downarrow \rangle = 0 \\
m_{00}^{\downarrow\uparrow} &= \langle 0 \downarrow | 0 \uparrow \rangle = 0 & m_{00}^{\downarrow\downarrow} &= \langle 0 \downarrow | 0 \downarrow \rangle = 1 \\
m_{10}^{\uparrow\uparrow} &= \langle 1 \uparrow | 0 \uparrow \rangle = -2^{-1/2} C_x a \alpha & m_{10}^{\uparrow\downarrow} &= \langle 1 \uparrow | 0 \downarrow \rangle = 2^{-1/2} a \alpha [1 + C_z] \\
m_{10}^{\downarrow\uparrow} &= \langle 1 \downarrow | 0 \uparrow \rangle = 2^{-1/2} a \alpha [-1 + C_z] & m_{10}^{\downarrow\downarrow} &= \langle 1 \downarrow | 0 \downarrow \rangle = 2^{-1/2} C_x a \alpha
\end{aligned}$$

The tunneling coefficients between $n = n' = 0$ states are

$$\begin{aligned}
t_{\alpha k 0}^{\uparrow\uparrow} &= \langle \alpha k \uparrow | H_T | 0 \uparrow \rangle = \sum_{n'\sigma'} t_{\alpha k n'}^{\uparrow\sigma'} m_{n'0}^{\sigma'\uparrow} \\
&= t_{\alpha k 0}^{\uparrow\downarrow} m_{00}^{\downarrow\uparrow} + t_{\alpha k 0}^{\uparrow\uparrow} m_{00}^{\uparrow\uparrow} + t_{\alpha k 1}^{\uparrow\uparrow} m_{10}^{\uparrow\uparrow} + t_{\alpha k 1}^{\uparrow\downarrow} m_{10}^{\downarrow\uparrow} \\
&= t_{\alpha k 0}^{\uparrow\uparrow} - t_{\alpha k 1}^{\uparrow\uparrow} 2^{-1/2} C_x a \alpha + t_{\alpha k 1}^{\uparrow\downarrow} [-a \alpha 2^{-1/2} + C_z a \alpha 2^{-1/2}] \\
t_{\alpha k 0}^{\downarrow\downarrow} &= \langle \alpha k \downarrow | H_T | 0 \downarrow \rangle = \sum_{n'\sigma'} t_{\alpha k n'}^{\downarrow\sigma'} m_{n'0}^{\sigma'\downarrow} \\
&= t_{\alpha k 0}^{\downarrow\uparrow} m_{00}^{\uparrow\downarrow} + t_{\alpha k 0}^{\downarrow\downarrow} m_{00}^{\downarrow\downarrow} + t_{\alpha k 1}^{\downarrow\downarrow} m_{10}^{\downarrow\downarrow} + t_{\alpha k 1}^{\downarrow\uparrow} m_{10}^{\uparrow\downarrow} \\
&= t_{\alpha k 0}^{\downarrow\downarrow} + t_{\alpha k 1}^{\downarrow\downarrow} 2^{-1/2} C_x a \alpha + t_{\alpha k 1}^{\downarrow\uparrow} [a \alpha 2^{-1/2} + C_z a \alpha 2^{-1/2}] \\
t_{\alpha k 0}^{\uparrow\downarrow} &= \langle \alpha k \uparrow | H_T | 0 \downarrow \rangle = \sum_{n'\sigma'} t_{\alpha k n'}^{\uparrow\sigma'} m_{n'0}^{\sigma'\downarrow} \\
&= t_{\alpha k 0}^{\uparrow\downarrow} m_{00}^{\downarrow\downarrow} + t_{\alpha k 0}^{\uparrow\uparrow} m_{00}^{\uparrow\downarrow} + t_{\alpha k 1}^{\uparrow\uparrow} m_{10}^{\uparrow\downarrow} + t_{\alpha k 1}^{\uparrow\downarrow} m_{10}^{\downarrow\downarrow} \\
&= t_{\alpha k 0}^{\uparrow\downarrow} + t_{\alpha k 1}^{\uparrow\uparrow} [a \alpha 2^{-1/2} + C_z a \alpha 2^{-1/2}] + t_{\alpha k 1}^{\uparrow\downarrow} 2^{-1/2} C_x a \alpha \\
t_{\alpha k 0}^{\downarrow\uparrow} &= \langle \alpha k \downarrow | H_T | 0 \uparrow \rangle = \sum_{n'\sigma'} t_{\alpha k n'}^{\downarrow\sigma'} m_{n'0}^{\sigma'\uparrow} \\
&= t_{\alpha k 0}^{\downarrow\uparrow} m_{00}^{\uparrow\uparrow} + t_{\alpha k 0}^{\downarrow\downarrow} m_{00}^{\downarrow\uparrow} + t_{\alpha k 1}^{\downarrow\downarrow} m_{10}^{\downarrow\uparrow} + t_{\alpha k 1}^{\downarrow\uparrow} m_{10}^{\uparrow\uparrow} \\
&= t_{\alpha k 0}^{\downarrow\uparrow} + t_{\alpha k 1}^{\downarrow\downarrow} [-a \alpha 2^{-1/2} + C_z a \alpha 2^{-1/2}] - t_{\alpha k 1}^{\downarrow\uparrow} 2^{-1/2} C_x a \alpha
\end{aligned}$$

If $t_{\alpha k n'}^{\sigma\sigma'}$ is independent of k , proportional to $\delta_{\sigma\sigma'}$ and also spin independent, then

$$t_{\alpha k n}^{\sigma\eta} = \sum_{n'} t_{\alpha n' m_{n'n}^{\sigma\eta}}$$

The tunneling matrix between $n = 0$ states is thus

$$\mathbf{t}_{\alpha k 0} = \begin{pmatrix} t_{\alpha k 0}^{\uparrow\uparrow} & t_{\alpha k 0}^{\uparrow\downarrow} \\ t_{\alpha k 0}^{\downarrow\uparrow} & t_{\alpha k 0}^{\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} t_{\alpha 0} - \frac{C_x a\alpha}{\sqrt{2}} t_{\alpha 1} & \frac{a\alpha}{\sqrt{2}} [1 + C_z] t_{\alpha 1} \\ \frac{a\alpha}{\sqrt{2}} [-1 + C_z] t_{\alpha 1} & t_{\alpha 0} + \frac{C_x a\alpha}{\sqrt{2}} t_{\alpha 1} \end{pmatrix} \quad (3.5)$$

Notice again that

$$a\alpha \ll 1 \text{ and } C_i \ll 1$$

If we consider a quantum dot with only one n-level, namely $n = 0$ with pseudo-spin $\eta \in \{\uparrow, \downarrow\}$, then the transition is determined by these overlaps.

3.5 Rotating the lead operators

We now focus on a single orbital, for simplicity take $n = 0$. Only virtual transitions are allowed to the other orbitals. The tunneling in and out of the $n = 0$ orbital from lead α is now described by the following tunneling term in the Hamiltonian:

$$\begin{aligned} \sum_{k\sigma\eta} t_{\alpha k 0}^{\sigma\eta} c_{\alpha k \sigma}^\dagger d_{0\eta} &= \sum_k \left[\left(t_{\alpha k 0}^{\uparrow\uparrow} d_{0\uparrow} + t_{\alpha k 0}^{\uparrow\downarrow} d_{0\downarrow} \right) c_{\alpha k \uparrow}^\dagger + \left(t_{\alpha k 0}^{\downarrow\uparrow} d_{0\uparrow} + t_{\alpha k 0}^{\downarrow\downarrow} d_{0\downarrow} \right) c_{\alpha k \downarrow}^\dagger \right] \\ &= \sum_k \left[\left(t_{\alpha k 0}^{\uparrow\uparrow} c_{\alpha k \uparrow}^\dagger + t_{\alpha k 0}^{\downarrow\uparrow} c_{\alpha k \downarrow}^\dagger \right) d_{0\uparrow} + \left(t_{\alpha k 0}^{\uparrow\downarrow} c_{\alpha k \uparrow}^\dagger + t_{\alpha k 0}^{\downarrow\downarrow} c_{\alpha k \downarrow}^\dagger \right) d_{0\downarrow} \right] \end{aligned} \quad (3.6)$$

Note that in the tunneling process any dot pseudo-spin electron (i.e. both \uparrow and \downarrow) can become a left lead electron with any spin (\uparrow and \downarrow). This differs from the trivial spin conserving form. A first attempt to deal with the tunneling Hamiltonian would be trying to rotate the operators in a way that brings the Hamiltonian on the trivial form. If it is possible to define a new set of creation and annihilation operators obeying fermion statistics that brings the Hamiltonian on the right form, then we are done. With the first line of (3.6) in mind, one could define the two brackets as some new operators and check whether they are fermion operators or not. Provided they fulfil fermion statistics, the problem is solved by expressing the Hamiltonian in terms of the new (rotated) set of operators. In this way the problem is solved by means of a rotation of the lead spin quantization axes.

The left tunneling coefficient $t_{L k 0}^{\sigma\eta}$ will in general be different from the right tunneling coefficient $t_{R k 0}^{\sigma\eta}$. Thus if the dot creation and annihilation operators are rotated, there will be two distinct rotations, one associated with the left tunneling

coefficient and one with the right. Instead we want to rotate the two set of lead operators. These are distinct anyway. The result is

$$\sum_{k\sigma\eta} t_{\alpha,k0}^{\sigma\eta} c_{\alpha k\sigma}^\dagger d_{0\eta} = \sum_k \left[c_{\alpha k 0\uparrow}^\dagger d_{0\uparrow} + c_{\alpha k 0\downarrow}^\dagger d_{0\downarrow} \right]$$

where a new operator $c_{Lk0\eta}^\dagger$ has been defined as

$$\begin{aligned} c_{\alpha k 0\uparrow}^\dagger &= \left(t_{\alpha 0} - \frac{C_x a\alpha}{\sqrt{2}} t_{\alpha 1} \right) c_{\alpha k\uparrow}^\dagger + \left(\frac{a\alpha}{\sqrt{2}} [-1 + C_z] t_{\alpha 1} \right) c_{\alpha k\downarrow}^\dagger \\ c_{\alpha k 0\downarrow}^\dagger &= \left(\frac{a\alpha}{\sqrt{2}} [1 + C_z] t_{\alpha 1} \right) c_{\alpha k\uparrow}^\dagger + \left(t_{\alpha 0} + \frac{C_x a\alpha}{\sqrt{2}} t_{\alpha 1} \right) c_{\alpha k\downarrow}^\dagger \end{aligned} \quad (3.7)$$

with tunneling coefficients from (3.5). This can be interpreted as an operator creating a fermion with momentum k and pseudospin η only if the anti-commutator relations are fulfilled.

$$\begin{aligned} \{c_{\alpha k 0\uparrow}, c_{\alpha k 0\uparrow}^\dagger\} &= \left(t_{\alpha 0} - \frac{C_x a\alpha}{\sqrt{2}} t_{\alpha 1} \right)^2 \{c_{\alpha k\uparrow}, c_{\alpha k\uparrow}^\dagger\} + \left(\frac{a\alpha}{\sqrt{2}} [-1 + C_z] t_{\alpha 1} \right)^2 \{c_{\alpha k\downarrow}, c_{\alpha k\downarrow}^\dagger\} \\ &= t_{\alpha 0}^2 - \frac{C_x a\alpha}{\sqrt{2}} t_{\alpha 0} t_{\alpha 1} + O(\alpha^2, B^2) \end{aligned}$$

$$\{c_{\alpha k 0\downarrow}, c_{\alpha k 0\downarrow}^\dagger\} = t_{\alpha 0}^2 + \frac{C_x a\alpha}{\sqrt{2}} t_{\alpha 0} t_{\alpha 1} + O(\alpha^2, B^2)$$

$$\{c_{\alpha k 0\downarrow}, c_{\alpha k 0\uparrow}^\dagger\} = \sqrt{2} a\alpha C_z t_{\alpha 0} t_{\alpha 1} + O(\alpha^2, B^2)$$

$$\{c_{\alpha k 0\eta}^\dagger, c_{\alpha k 0\eta'}^\dagger\} = \{c_{\alpha k\eta}, c_{\alpha k\eta'}\} = 0$$

For $B = 0$, this is $\{c_{\alpha k 0\eta}, c_{\alpha k 0\eta'}^\dagger\} = \delta_{\eta\eta'} t_{\alpha 0}^2 + O(\alpha^2) \approx \delta_{\eta\eta'} t_{\alpha 0}^2$ and $\{c_{\alpha k 0\eta}^\dagger, c_{\alpha k 0\eta'}^\dagger\} = 0$. If $t_{\alpha 0}^2$ is absorbed into the creation and annihilation operator, then the anti-commutator relations are fulfilled to linear order in α and B . For $\mathbf{B} = (B_x, 0, B_z) \neq (0, 0, 0)$ and a non-zero SO coupling, the anti-commutation relations are not fulfilled. The anti-commutation relations hold only in the trivial case with a magnetic field along the y-axis, $\mathbf{B} = (0, B, 0)$. In that case

$$\begin{aligned} c_{\alpha k 0\uparrow}^\dagger &= t_{\alpha 0} c_{\alpha k\uparrow}^\dagger - \frac{a\alpha}{\sqrt{2}} t_{\alpha 1} c_{\alpha k\downarrow}^\dagger \\ c_{\alpha k 0\downarrow}^\dagger &= \frac{a\alpha}{\sqrt{2}} t_{\alpha 1} c_{\alpha k\uparrow}^\dagger + t_{\alpha 0} c_{\alpha k\downarrow}^\dagger \end{aligned} \quad (3.8)$$

Expressing the tunneling Hamiltonian in these fermion operators brings it on the form of a trivial, spin conserving tunneling Hamiltonian. For $B_x \neq 0 \neq B_z$ it is not possible to solve the problem by means of such a rotation. Therefore we have to deal with the tunneling Hamiltonian (3.6).

Chapter 4

Kondo model

We consider a dot Hamiltonian given by

$$\tilde{H}_D := H_d + H_Z + U n_{\uparrow} n_{\downarrow}$$

The Hamiltonian describing the system constituted by the leads and the dot is thus

$$\tilde{H} = \tilde{H}_D + H_{LR} + H_T$$

4.1 Transforming away the charge fluctuations (Schrieffer-Wolff transformation)

Following Schrieffer-Wolff[24] we want to perform a canonical transformation of the Hamiltonian that eliminates the high-energy states. The transformation should project the Hamiltonian onto a subspace with only one electron on the dot, and where excursions to the double- or single-occupied states can occur only virtually. A such transformation can be represented by means of a unitary transformation e^{iS} acting on the Hamiltonian

$$H_S = e^{iS} \tilde{H} e^{-iS}$$

such that the tunneling part is transformed away:

$$i \left[S, \tilde{H}_D + H_{LR} \right] = -H_T + O \left((t_{\alpha 0}^{\sigma \eta})^2 \right)$$

To second order in the tunneling, the rotated Hamiltonian is given by

$$H_S = e^{iS} \tilde{H} e^{-iS} \approx \tilde{H}_D + H_{LR} + \frac{i}{2} [S, H_T]$$

Such a transformation exist. Let S be given by

$$S = S^- + (S^-)^\dagger$$

with

$$S^- = -i \sum_{\alpha k \sigma \eta} \left(\frac{t_{\alpha 0}^{\sigma \eta}}{\epsilon_k - E_2 + E_1} n_{\bar{\eta}} c_{\alpha k \sigma}^\dagger d_\eta + \frac{t_{\alpha 0}^{\sigma \eta}}{\epsilon_k + E_0 - E_1} (1 - n_{\bar{\eta}}) c_{\alpha k \sigma}^\dagger d_\eta \right) = S_1^- + S_2^-$$

Then the first part of the commutator is

$$[S_1^-, H_D + H_{LR}] = i \sum_{\alpha k \sigma \eta} t_{\alpha 0}^{\sigma \eta} n_{\bar{\eta}} c_{\alpha k \sigma}^\dagger d_\eta$$

where we have used that $n_{\bar{\eta}}^2 = n_{\bar{\eta}}$ and $E_2 - E_1 = U + \epsilon_\eta$. Similarly $[S_2^-, H_D + H_{LR}] = i \sum_{\alpha k \sigma \eta} t_{\alpha 0}^{\sigma \eta} (1 - n_{\bar{\eta}}) c_{\alpha k \sigma}^\dagger d_\eta$ and hence

$$[S^-, H_D + H_{LR}] = i \sum_{\alpha k \sigma \eta} t_{\alpha 0}^{\sigma \eta} c_{\alpha k \sigma}^\dagger d_\eta$$

Using $[S^-, H_D + H_{LR}] + [S^+, H_D + H_{LR}] = [S^-, H_D + H_{LR}] - [S, H_D + H_{LR}]^\dagger$, we see that the first commutator in the Baker-Campbell-Hausdorff expansion cancels out the tunneling hamiltonian:

$$i [S, H_D + H_{LR}] = - \left(\sum_{\alpha k \sigma \eta} t_{\alpha 0}^{\sigma \eta} c_{\alpha k \sigma}^\dagger d_\eta + \sum_{\alpha k \sigma \eta} t_{\alpha 0}^{\sigma \eta *} c_{\alpha k \sigma} d_\eta^\dagger \right) = -H_T$$

Calculation of $H_S^{(2)} = \frac{i}{2} [S, H_T]$:

$$\begin{aligned} [S, H_T] &= [S^-, H_T^+] + [S^+, H_T^-] + [S^-, H_T^-] + [S^+, H_T^+] \\ &\approx [S^-, H_T^+] + [S^+, H_T^-] \\ &= [S^-, H_T^+] + [(S^-)^\dagger, (H_T^+)^\dagger] \\ &= [S^-, H_T^+] - [S^-, H_T^+]^\dagger \\ &= 2i \operatorname{Im} ([S^-, H_T^+]) \end{aligned} \tag{4.1}$$

$$\begin{aligned} [S_1^-, H_T^+] &= -i \sum_{\substack{\alpha k \sigma \eta \\ \alpha' k' \sigma' \eta'}} \frac{t_{\alpha 0}^{\sigma \eta} t_{\alpha' 0}^{\sigma' \eta' *} }{\xi_{\alpha k} - E_2 + E_1} \left[n_{\bar{\eta}} c_{\alpha k \sigma}^\dagger d_\eta, d_{\eta'}^\dagger c_{\alpha' k' \sigma'} \right] \\ &= -i \sum_{\substack{\alpha k \sigma \eta \\ \alpha' k' \sigma' \eta'}} \frac{t_{\alpha 0}^{\sigma \eta} t_{\alpha' 0}^{\sigma' \eta' *} }{\xi_{\alpha k} - E_2 + E_1} c_{\alpha k \sigma}^\dagger c_{\alpha' k' \sigma'} d_\eta d_{\eta'}^\dagger \end{aligned}$$

where we have used that $n_{\bar{\eta}} d_\eta = 0$ and $n_{\bar{\eta}} d_\eta d_{\eta'}^\dagger = d_\eta d_{\eta'}^\dagger$ when acting on a dot occupied by one electron (in \uparrow or \downarrow state). $[S_2^-, H_T^+]$ is calculated similarly.

If $\xi_{\alpha k} \ll E_2 - E_1$, $E_0 - E_1$, the dependence on $\xi_{\alpha k}$ in the denominator can be neglected[4]. Using the relation $d_\eta d_{\eta'}^\dagger = \delta_{\eta\eta'} - d_{\eta'}^\dagger d_\eta$, the commutator reads

$$\begin{aligned}
 [S^-, H_T^+] \approx & -i \sum_{\substack{\alpha k \sigma \eta \\ \alpha' k' \sigma' \eta'}} t_{\alpha 0}^{\sigma \eta} t_{\alpha' 0}^{\sigma' \eta'} \left\{ \left(\frac{1}{E_2 - E_1} + \frac{1}{E_0 - E_1} \right) c_{\alpha k \sigma}^\dagger c_{\alpha' k' \sigma'} d_{\eta'}^\dagger d_\eta \right. \\
 & - \left(\frac{1}{E_2 - E_1} \right) \delta_{\eta\eta'} c_{\alpha k \sigma}^\dagger c_{\alpha' k' \sigma'} \\
 & \left. - \left(\frac{1}{E_0 - E_1} \right) \delta_{\alpha k \sigma, \alpha' k' \sigma'} d_{\eta'}^\dagger d_\eta \right\}
 \end{aligned} \tag{4.2}$$

Letting \mathbf{s} (\mathbf{S}) denote the spin on the lead (dot), one can define spin operators by[4, p. 172]

$$\begin{aligned}
 \mathbf{s}_{\alpha' k' \alpha k} &= \sum_{\sigma \sigma'} \frac{1}{2} c_{\alpha' k' \sigma'}^\dagger \boldsymbol{\tau}_{\sigma' \sigma} c_{\alpha k \sigma} \\
 \mathbf{S} &= \sum_{\eta \eta'} \frac{1}{2} d_{\eta'}^\dagger \boldsymbol{\tau}_{\eta' \eta} d_\eta
 \end{aligned}$$

where $\boldsymbol{\tau}_{\sigma' \sigma} = \langle \sigma' | \tau^x, \tau^y, \tau^z | \sigma \rangle$. In addition we define

$$\begin{aligned}
 s_{\alpha' k' \alpha k}^0 &= c_{\alpha k \uparrow}^\dagger c_{\alpha' k' \uparrow} + c_{\alpha k \downarrow}^\dagger c_{\alpha' k' \downarrow} \\
 S^0 &= d_{\uparrow}^\dagger d_{\uparrow} + d_{\downarrow}^\dagger d_{\downarrow} = \mathbb{I}
 \end{aligned}$$

Note that since we are in the Kondo regime where the quantum dot is populated by exactly one electron in either the \uparrow or the \downarrow state, S^0 is simply the identity operator. The creation and annihilation operators expressed in terms of spin operators are given by

$$\begin{aligned}
 c_{\alpha k \uparrow}^\dagger c_{\alpha' k' \uparrow} &= \frac{1}{2} \left(c_{\alpha k \uparrow}^\dagger c_{\alpha' k' \uparrow} + c_{\alpha k \downarrow}^\dagger c_{\alpha' k' \downarrow} \right) + \frac{1}{2} \left(c_{\alpha k \uparrow}^\dagger c_{\alpha' k' \downarrow} - c_{\alpha k \downarrow}^\dagger c_{\alpha' k' \uparrow} \right) = \frac{1}{2} s_{\alpha k \alpha' k'}^0 + s_{\alpha k \alpha' k'}^z \\
 c_{\alpha k \downarrow}^\dagger c_{\alpha' k' \downarrow} &= \frac{1}{2} s_{\alpha k \alpha' k'}^0 - s_{\alpha k \alpha' k'}^z \\
 c_{\alpha k \uparrow}^\dagger c_{\alpha' k' \downarrow} &= s_{\alpha k \alpha' k'}^+ = s_{\alpha k \alpha' k'}^x + i s_{\alpha k \alpha' k'}^y \\
 c_{\alpha k \downarrow}^\dagger c_{\alpha' k' \uparrow} &= s_{\alpha k \alpha' k'}^- = s_{\alpha k \alpha' k'}^x - i s_{\alpha k \alpha' k'}^y
 \end{aligned}$$

for the lead operators $\alpha \in \{L, R\}$ and for the dot:

$$\begin{aligned}
 d_{\uparrow}^\dagger d_{\uparrow} &= \frac{1}{2} \left(d_{\uparrow}^\dagger d_{\uparrow} + d_{\downarrow}^\dagger d_{\downarrow} \right) + \frac{1}{2} \left(d_{\uparrow}^\dagger d_{\uparrow} - d_{\downarrow}^\dagger d_{\downarrow} \right) = \frac{1}{2} S_0 + S_z \\
 d_{\downarrow}^\dagger d_{\downarrow} &= \frac{1}{2} S_0 - S_z \\
 d_{\uparrow}^\dagger d_{\downarrow} &= S^+ = S_x + i S_y \\
 d_{\downarrow}^\dagger d_{\uparrow} &= S^- = S_x - i S_y
 \end{aligned}$$

Expressing (4.2) in components of the spin operators gives

$$\begin{aligned}
[S^-, H_T^+] \approx & -i \sum_{\alpha k \alpha' k'} \left\{ \left(\frac{1}{E_2 - E_1} + \frac{1}{E_0 - E_1} \right) \right. \\
& \times \left[t_{\alpha 0}^{11} t_{\alpha' 0}^{11*} \left(\frac{1}{4} s_{\alpha k \alpha' k'}^0 S^0 + \frac{1}{2} s_{\alpha k \alpha' k'}^z S^0 + \frac{1}{2} s_{\alpha k \alpha' k'}^0 S^z + s_{\alpha k \alpha' k'}^z S^z \right) \right. \\
& + t_{\alpha 0}^{22} t_{\alpha' 0}^{22*} \left(\frac{1}{4} s_{\alpha k \alpha' k'}^0 S^0 - \frac{1}{2} s_{\alpha k \alpha' k'}^z S^0 - \frac{1}{2} s_{\alpha k \alpha' k'}^0 S^z + s_{\alpha k \alpha' k'}^z S^z \right) \\
& + t_{\alpha 0}^{12} t_{\alpha' 0}^{12*} \left(\frac{1}{4} s_{\alpha k \alpha' k'}^0 S^0 + \frac{1}{2} s_{\alpha k \alpha' k'}^z S^0 - \frac{1}{2} s_{\alpha k \alpha' k'}^0 S^z - s_{\alpha k \alpha' k'}^z S^z \right) \\
& + t_{\alpha 0}^{21} t_{\alpha' 0}^{21*} \left(\frac{1}{4} s_{\alpha k \alpha' k'}^0 S^0 - \frac{1}{2} s_{\alpha k \alpha' k'}^z S^0 + \frac{1}{2} s_{\alpha k \alpha' k'}^0 S^z - s_{\alpha k \alpha' k'}^z S^z \right) \\
& + t_{\alpha 0}^{11} t_{\alpha' 0}^{21*} s_{\alpha k \alpha' k'}^+ \left(\frac{1}{2} S^0 + S^z \right) + t_{\alpha 0}^{12} t_{\alpha' 0}^{11*} \left(\frac{1}{2} s_{\alpha k \alpha' k'}^0 + s_{\alpha k \alpha' k'}^z \right) S^+ \\
& + t_{\alpha 0}^{12} t_{\alpha' 0}^{22*} s_{\alpha k \alpha' k'}^+ \left(\frac{1}{2} S^0 - S^z \right) + t_{\alpha 0}^{22} t_{\alpha' 0}^{21*} \left(\frac{1}{2} s_{\alpha k \alpha' k'}^0 - s_{\alpha k \alpha' k'}^z \right) S^+ \\
& + t_{\alpha 0}^{21} t_{\alpha' 0}^{11*} s_{\alpha k \alpha' k'}^- \left(\frac{1}{2} S^0 + S^z \right) + t_{\alpha 0}^{11} t_{\alpha' 0}^{12*} \left(\frac{1}{2} s_{\alpha k \alpha' k'}^0 + s_{\alpha k \alpha' k'}^z \right) S^- \\
& + t_{\alpha 0}^{22} t_{\alpha' 0}^{12*} s_{\alpha k \alpha' k'}^- \left(\frac{1}{2} S^0 - S^z \right) + t_{\alpha 0}^{21} t_{\alpha' 0}^{22*} \left(\frac{1}{2} s_{\alpha k \alpha' k'}^0 - s_{\alpha k \alpha' k'}^z \right) S^- \\
& + t_{\alpha 0}^{11} t_{\alpha' 0}^{22*} s_{\alpha k \alpha' k'}^+ S^- + t_{\alpha 0}^{12} t_{\alpha' 0}^{21*} s_{\alpha k \alpha' k'}^+ S^+ \\
& \left. + t_{\alpha 0}^{22} t_{\alpha' 0}^{11*} s_{\alpha k \alpha' k'}^- S^+ + t_{\alpha 0}^{21} t_{\alpha' 0}^{12*} s_{\alpha k \alpha' k'}^- S^- \right] \\
& - \left(\frac{1}{E_2 - E_1} \right) \left[\left(t_{\alpha 0}^{11} t_{\alpha' 0}^{11*} + t_{\alpha 0}^{12} t_{\alpha' 0}^{12*} \right) \left(\frac{1}{2} s_{\alpha k \alpha' k'}^0 + s_{\alpha k \alpha' k'}^z \right) \right. \\
& + \left(t_{\alpha 0}^{21} t_{\alpha' 0}^{21*} + t_{\alpha 0}^{22} t_{\alpha' 0}^{22*} \right) \left(\frac{1}{2} s_{\alpha k \alpha' k'}^0 - s_{\alpha k \alpha' k'}^z \right) \\
& + \left(t_{\alpha 0}^{11} t_{\alpha' 0}^{21*} + t_{\alpha 0}^{12} t_{\alpha' 0}^{22*} \right) s_{\alpha k \alpha' k'}^+ \\
& \left. + \left(t_{\alpha 0}^{21} t_{\alpha' 0}^{11*} + t_{\alpha 0}^{22} t_{\alpha' 0}^{12*} \right) s_{\alpha k \alpha' k'}^- \right] \\
& - \left(\frac{1}{E_0 - E_1} \right) \left[\left(t_{\alpha 0}^{11} t_{\alpha' 0}^{11*} + t_{\alpha 0}^{21} t_{\alpha' 0}^{21*} \right) \left(\frac{1}{2} S^0 + S^z \right) \right. \\
& + \left(t_{\alpha 0}^{12} t_{\alpha' 0}^{12*} + t_{\alpha 0}^{22} t_{\alpha' 0}^{22*} \right) \left(\frac{1}{2} S^0 - S^z \right) \\
& + \left(t_{\alpha 0}^{12} t_{\alpha' 0}^{11*} + t_{\alpha 0}^{22} t_{\alpha' 0}^{21*} \right) S^+ \\
& \left. + \left(t_{\alpha 0}^{11} t_{\alpha' 0}^{12*} + t_{\alpha 0}^{21} t_{\alpha' 0}^{11*} \right) S^- \right]
\end{aligned} \tag{4.3}$$

where again S^0 is really the unit operator, just kept here to remind ourselves where it came from.

The types of terms in (4.3) are $s_{\alpha k \alpha' k'}^i$, S^i , $s_{\alpha k \alpha' k'}^j S^i$, $s_{\alpha k \alpha' k'}^i S^0$, $s_{\alpha k \alpha' k'}^0 S^i$ and $s_{\alpha k \alpha' k'}^0 S^0$ for $ij \in \{x, y, z\}$. Subtracting the hermitian conjugate in (4.1) gives a

Hamiltonian on the general form:

$$\begin{aligned}
H_S^{(2)} = & \sum_{\alpha\alpha'kk'} \sum_{ij \in \{x,y,z\}} J_{\alpha\alpha'}^{ij} s_{\alpha k \alpha' k'}^j S^i + \sum_{\alpha\alpha'kk'} (v_{\alpha\alpha'} s_{\alpha k \alpha' k'}^0 + V_{\alpha\alpha'} S^0) \\
& + \sum_{\alpha\alpha'kk'} \omega_{\alpha\alpha'} s_{\alpha k \alpha' k'}^0 S^0 + \sum_{\alpha\alpha'kk'} \sum_{i \in \{x,y,z\}} (w_{\alpha\alpha'}^i s_{\alpha k \alpha' k'}^i S^0 + W_{\alpha\alpha'}^i s_{\alpha k \alpha' k'}^0 S^i) \\
& + \sum_{\alpha\alpha'kk'} \sum_{i \in \{x,y,z\}} (L_{\alpha\alpha'}^i s_{\alpha k \alpha' k'}^i + M_{\alpha\alpha'}^i S^i)
\end{aligned}$$

or inserting that $S^0 = \mathbb{I}$:

$$\begin{aligned}
H_S^{(2)} = & \sum_{\alpha\alpha'kk'} \sum_{ij \in \{x,y,z\}} J_{\alpha\alpha'}^{ij} s_{\alpha k \alpha' k'}^j S^i + \sum_{\alpha\alpha'kk'} \sum_{i \in \{x,y,z\}} K_{\alpha\alpha'}^i s_{\alpha k \alpha' k'}^0 S^i \\
& + \sum_{\alpha\alpha'kk'} \sum_{i \in \{x,y,z\}} (L_{\alpha\alpha'}^i s_{\alpha k \alpha' k'}^i + M_{\alpha\alpha'}^i S^i) + \sum_{\alpha\alpha'kk'} N_{\alpha\alpha'} s_{\alpha k \alpha' k'}^0 + \sum_{\alpha\alpha'kk'} O_{\alpha\alpha'}
\end{aligned} \tag{4.4}$$

All of the energies J,K,L...,O contain an energy prefactor, e.g. $\left(\frac{1}{E_2-E_1} + \frac{1}{E_0-E_1}\right)$. In the following j,k,l,...,o shall denote the energies J,K,L,...,O without these prefactors.

4.2 The Kondo Hamiltonian

We shall now focus on the exchange-like term

$$[S^-, H_T^+]_K = -2i \sum_{\alpha\alpha'kk'} \left(\frac{1}{E_2-E_1} + \frac{1}{E_0-E_1} \right) \sum_{ij} j_{\alpha\alpha'}^{ij} s_{\alpha k \alpha' k'}^j S^i$$

with the complex matrix given by (4.6). In order to find

$$H_K^{(2)} = \frac{i}{2} [S, H_T]_K \approx \frac{i}{2} \left([S^-, H_T^+]_K - [S^-, H_T^+]_K^\dagger \right)$$

one needs the hermitian conjugate of the products $j_{\alpha\alpha'}^{ij} s_{\alpha k \alpha' k'}^j S^i$. The matrix element $j_{\alpha\alpha'}^{ij}$ is a complex number (and not an operator or a pseudoscalar), hence $j_{\alpha\alpha'}^{ij\dagger} = j_{\alpha\alpha'}^{ij*}$. By writing the spin operators in terms of the creation and annihilation operators and using the fact that dot operators anti-commutes with lead operators, one finds that $(s_{\alpha k \alpha' k'}^j S^i)^\dagger = s_{\alpha' k' \alpha k}^j S^i$ for all $i, j \in \{x, y, z\}$. The term to subtract is thus

$$[S^-, H_T^+]_K^\dagger = +2i \sum_{\alpha\alpha'kk'} \left(\frac{1}{E_2-E_1} + \frac{1}{E_0-E_1} \right) \sum_{ij} j_{\alpha\alpha'}^{ij*} s_{\alpha' k' \alpha k}^j S^i$$

and since $j_{\alpha'\alpha}^{ij} = j_{\alpha\alpha'}^{ij*}$ the "sum" is

$$H_K^{(2)} = \sum_{\alpha\alpha'kk'} \left(\frac{1}{E_2 - E_1} + \frac{1}{E_0 - E_1} \right) \sum_{ij} (j_{\alpha\alpha'}^{ij} s_{\alpha k \alpha' k'}^j + j_{\alpha'\alpha}^{ij} s_{\alpha' k' \alpha k}^j) S^i$$

The Kondo Hamiltonian is

$$H_K^{(2)} = \sum_{\alpha\alpha'kk'} 2 \left(\frac{1}{E_2 - E_1} + \frac{1}{E_0 - E_1} \right) \sum_{ij} j_{\alpha\alpha'}^{ij} s_{\alpha k \alpha' k'}^j S^i \quad (4.5)$$

with

$$j_{\alpha\alpha} = \begin{pmatrix} t_{\alpha 0}^2 & 0 & -2\gamma t_{\alpha 0} t_{\alpha 1} \\ 0 & t_{\alpha 0}^2 & 0 \\ 2\gamma t_{\alpha 0} t_{\alpha 1} & 0 & t_{\alpha 0}^2 \end{pmatrix}_{ij}$$

$$j_{\alpha\alpha'} = \begin{pmatrix} t_{\alpha 0} t_{\alpha' 0} & iC_x \gamma (t_{\alpha 1} t_{\alpha' 0} - t_{\alpha' 1} t_{\alpha 0}) & -\gamma (t_{\alpha 1} t_{\alpha' 0} + t_{\alpha' 1} t_{\alpha 0}) \\ -iC_x \gamma (t_{\alpha 1} t_{\alpha' 0} - t_{\alpha' 1} t_{\alpha 0}) & t_{\alpha 0} t_{\alpha' 0} & -iC_z \gamma (t_{\alpha 1} t_{\alpha' 0} - t_{\alpha' 1} t_{\alpha 0}) \\ \gamma (t_{\alpha 1} t_{\alpha' 0} + t_{\alpha' 1} t_{\alpha 0}) & iC_z \gamma (t_{\alpha 1} t_{\alpha' 0} - t_{\alpha' 1} t_{\alpha 0}) & t_{\alpha 0} t_{\alpha' 0} \end{pmatrix}_{ij} \quad (4.6)$$

where

$$\gamma = -2^{-1/2} a \alpha$$

Note that the alpha in γ is the SO coupling strength unlike the labels on M that numbers the leads. The Rashba Hamiltonian was transformed away only to linear order in the coupling (see (3.3)). The Shrieffer-Wolff transformation is valid only to linear order in the tunneling coefficients. Therefore we have neglected higher-order terms in the the above.

In the absence of spin-orbit interaction the Kondo Hamiltonian is isotropic:

$$J_{\alpha\alpha'} \sum_i s_{\alpha k \alpha' k'}^i S^i$$

An anisotropic form would be

$$\sum_i J_{\alpha\alpha'}^i s_{\alpha k \alpha' k'}^i S^i = \sum_i J_{\perp} (s_{\alpha k \alpha' k'}^+ S^- + s_{\alpha k \alpha' k'}^- S^+) + J_{\parallel} s_{\alpha k \alpha' k'}^z S^z$$

In the case of a Rashba SO interaction, the Kondo Hamiltonian is even more complex. The Kondo Hamiltonian thus has very low symmetry. For magnetic field, $\mathbf{B} = (0, B_y, 0)$, the $\alpha\alpha$ -contribution to the Kondo Hamiltonian is

$$\sum_{ij} (j_{\alpha\alpha}^{ij} s_{\alpha\alpha}^j) S^i = t_{\alpha 0}^2 \underbrace{\begin{pmatrix} 1 & 0 & \theta_{\alpha} \\ 0 & 1 & 0 \\ -\theta_{\alpha} & 0 & 1 \end{pmatrix}}_{R_y(\theta_{\alpha}) + O(\theta_{\alpha}^2)} \mathbf{s}_{\alpha} \cdot \mathbf{S} \approx t_{\alpha 0}^2 (R^y(\theta_{\alpha}) \mathbf{s}_{\alpha}) \cdot \mathbf{S}$$

where $\theta_{\alpha} = \sqrt{2} (t_{\alpha 1} / t_{\alpha 0}) a \alpha$. These terms are on the form of a dot product between a rotation of $\mathbf{s}_{\alpha\alpha}$ and \mathbf{S} . The anisotropy can be understood as a rotation of an isotropic system.

4.3 Current

In a system described by the Kondo Hamiltonian, a transition from left to right is due to

$$j_{RL}^{ij} c_{R\tilde{k}'\tilde{\sigma}'}^\dagger \tau_{\tilde{\sigma}'\tilde{\sigma}}^j c_{L\tilde{k}\tilde{\sigma}} S^i$$

The transition rate $\Gamma_{\eta'\eta}^{Rk'\sigma'Lk\sigma}$ is between an initial state $|i\rangle = |i_L\rangle|i_R\rangle|\eta\rangle$ fulfilling

$$\begin{aligned} c_{Lk\sigma}^\dagger c_{Lk\sigma} |i_L\rangle &= |i_L\rangle \\ c_{Rk'\sigma'}^\dagger c_{Rk'\sigma'} |i_R\rangle &= 0 \end{aligned}$$

and a final state

$$|f\rangle = c_{R,k',\sigma'}^\dagger d_{\eta'}^\dagger d_{\eta} c_{L,k\sigma} |i\rangle = c_{R,k',\sigma'}^\dagger c_{L,k\sigma} |i_L\rangle |i_R\rangle |\eta'\rangle$$

Here the lead eigenstates $|i_\alpha\rangle$ are N-particle basis states in the occupation number representation.

If one is only interested in what happens on the dot, one can define a transition $\Gamma_{\eta'\eta}^{RL}$ as the sum over all possible initial and final states of the transition, each weighted by a thermal distribution function W . Going a step further and summing over all directions of currents gives $\Gamma_{\eta'\eta}$, the transition for the process of the dot spin changing from η to $\eta' \in \{\eta, \bar{\eta}\}$. In general this is[4]

$$\begin{aligned} \Gamma_{\eta'\eta}^{\alpha'k'\sigma'\alpha k\sigma} &= \frac{2\pi}{\hbar} |\langle f|H_T|i\rangle|^2 \delta(E_f - E_i) \\ \Gamma_{\eta'\eta}^{\alpha'\alpha} &= \sum_{kk'\sigma\sigma'} \sum_i \Gamma_{\eta'\eta}^{\alpha'k'\sigma'\alpha k\sigma} W^{i_{\alpha'}} W^{i_\alpha} \\ \Gamma_{\eta'\eta} &= \sum_{\alpha\alpha'} \Gamma_{\eta'\eta}^{\alpha'\alpha} \end{aligned}$$

The transition $\Gamma_{\eta'\eta}^{RL}$ is between an initial state $|i\rangle = |i_L\rangle|i_R\rangle|\eta\rangle$ and a final state

$$|f\rangle = c_{R,k',\sigma'}^\dagger d_{\eta'}^\dagger d_{\eta} c_{L,k\sigma} |i\rangle = c_{R,k',\sigma'}^\dagger c_{L,k\sigma} |i_L\rangle |i_R\rangle |\eta'\rangle$$

The transition rate from $|i\rangle$ to $|f\rangle$ is given by Fermi's Golden Rule:

$$\begin{aligned} \Gamma_{\eta'\eta}^{RL} &= 2\pi \sum_{f_L, f_R} \sum_{i_L, i_R} \left| \langle \eta' | \langle f_R | \langle f_L | H_T | i_L \rangle | i_R \rangle | \eta \rangle \right|^2 W_{i_L} W_{i_R} \\ &\quad \times \delta[E_{f_L} + E_{f_R} + E_{\eta'} - E_{i_L} - E_{i_R} - E_\eta] \end{aligned}$$

Neglecting everything but the first term in $H_K^{(2)}$, the transition rate from $|i\rangle$ to $|f\rangle$ is given by

$$\begin{aligned}
\Gamma_{\eta'\eta}^{RL} &= 2\pi \sum_{k\sigma k'\sigma'} \sum_{i_L, i_R} \left| \langle i | c_{L,k\sigma}^\dagger d_{\eta'}^\dagger c_{R,k'\sigma'} \frac{4}{U/2} \sum_{ij\tilde{k}\tilde{k}'} \left(j_{RL}^{ij} s_{R\tilde{k}',L\tilde{k}}^j \right) S^i | i \rangle \right|^2 \\
&\quad \times W_{i_L} W_{i_R} \delta[\xi_{Rk'\sigma'} + \xi_{\eta'} - (\xi_{Lk\sigma} + \xi_\eta)] \\
&= \sum_{k\sigma k'\sigma'} \frac{128\pi}{U^2} \left| \sum_{ij} \frac{j_{RL}^{ij}}{4} \tau_{\sigma'\sigma}^j \tau_{\eta'\eta}^i \right|^2 \left(\sum_{i_L} W_{i_L} \langle i_L | c_{Lk\sigma}^\dagger c_{Lk\sigma} | i_L \rangle \right) \\
&\quad \times \left(\sum_{i_R} W_{i_R} \langle i_R | c_{Rk'\sigma'}^\dagger c_{Rk'\sigma'} | i_R \rangle \right) \left(\sum_{\tilde{\eta}\tilde{\eta}'} \langle \eta' | d_{\tilde{\eta}}^\dagger d_{\tilde{\eta}'} | \eta \rangle \right) \\
&\quad \times \delta[\xi_{k'\sigma'} + \xi_{\eta'} - (\xi_{k\sigma} + \xi_\eta)] \\
&= \sum_{\sigma\sigma'} \frac{8\pi}{U^2} \left| \sum_{ij} j_{RL}^{ij} \tau_{\sigma'\sigma}^j \tau_{\eta'\eta}^i \right|^2 \sum_{kk'} n_F(\xi_{Lk\sigma} - \mu_L) [1 - n_F(\xi_{Rk'\sigma'} - \mu_R)] \\
&\quad \times \delta[\xi_{k'\sigma'} + \xi_{\eta'} - (\xi_{k\sigma} + \xi_\eta)]
\end{aligned}$$

with $n_F(\xi_{Lk\sigma} - \mu_L)$ being the Fermi-Dirac distribution function

$$n_F(\xi_{Lk\sigma} - \mu_L) = \frac{1}{\exp[(\xi_{Lk\sigma} - \mu_L)/k_B T] + 1}$$

Here we have used that $\langle i_L | c_{Lk\sigma}^\dagger c_{L\tilde{k}\tilde{\sigma}} | i_L \rangle \propto \delta_{k\tilde{k}} \delta_{\sigma\tilde{\sigma}}$ and likewise for the inner products concerning the right lead and the dot. Assuming that the lead energies are independent of spin, that is $\xi_{\alpha k\sigma} = \xi_{\alpha k}$, the Fermi distribution functions and the delta function can be taken outside the spin sum. In an isotropic Kondo model ($j_{RL}^{ij} \propto \delta_{ij}$), the product of Pauli matrices is simply

$$\begin{aligned}
\sum_{\sigma\sigma'} \left| \sum_{ij} j_{RL}^{ij} \delta_{ij} \tau_{\sigma'\sigma}^j \tau_{\eta'\eta}^i \right|^2 &= \sum_{kj} j_{RL}^{jj} j_{RL}^{kk*} \sum_{\sigma\sigma'} \tau_{\sigma'\sigma}^j \tau_{\sigma'\sigma}^{k\dagger} \tau_{\eta'\eta}^j \tau_{\eta'\eta}^{k\dagger} \\
&= \sum_{kj} j_{RL}^{jj} j_{RL}^{kk*} \underbrace{\text{Tr}[\tau^j \tau^k]}_{2\delta_{jk}} \tau_{\eta'\eta}^j \tau_{\eta'\eta}^k = 2\theta_{\eta'\eta}^{RL}
\end{aligned}$$

where theta has been defined as

$$\theta_{\eta'\eta}^{RL} := \sum_j (j_{RL}^{jj})^2 \tau_{\eta'\eta}^j \tau_{\eta'\eta}^j$$

Here hermiticity of the Pauli matrices ($\tau^{i\dagger} = \tau^i$) have been used to find $\tau_{\sigma'\sigma}^{i*} = \langle \sigma' | \tau^i | \sigma \rangle^* = \langle \sigma | \tau^i | \sigma' \rangle = \tau_{\sigma\sigma'}^i$. In the anisotropic case the product of Pauli matrices

is

$$\begin{aligned}
\sum_{\sigma\sigma'} \left| \sum_{ij} j_{RL}^{ij} \tau_{\sigma'\sigma}^j \tau_{\eta'\eta}^i \right|^2 &= \sum_{\sigma\sigma'} \sum_{ij} j_{RL}^{ij} \tau_{\sigma'\sigma}^j \tau_{\eta'\eta}^i \sum_{kl} \tau_{\eta'\eta}^{kl*} \tau_{\sigma'\sigma}^l j_{RL}^{kl*} \\
&= \sum_{ijkl} j_{RL}^{ij} j_{RL}^{kl*} \left(\sum_{\sigma\sigma'} \tau_{\sigma'\sigma}^j \tau_{\sigma\sigma'}^l \right) \tau_{\eta'\eta}^i \tau_{\eta\eta'}^k \\
&= 2 \sum_{ijk} j_{RL}^{ij} j_{RL}^{kj*} \tau_{\eta'\eta}^i \tau_{\eta\eta'}^k \\
&= 2 \sum_{ik} \tau_{\eta'\eta}^i A_{ik}^{RL} \tau_{\eta\eta'}^k := 2\theta_{\eta'\eta}^{RL}
\end{aligned}$$

with $A_{ik}^{RL} = \sum_j j_{RL}^{ij} j_{RL}^{kj*}$. Because of the continuous density of states, we replace sums by integrals:

$$\sum_{\alpha k} \rightarrow \int_{-\infty}^{\infty} d\xi_{\alpha k} g(\xi_{\alpha k})$$

for $\alpha = L, R$. Assuming that $g(\xi_{Lk})g(\xi_{Rk'})$ is constant in the relevant energy range and hence can be taken outside the energy integrals, we obtain the transition rate

$$\begin{aligned}
\Gamma_{\eta'\eta}^{RL} &= \frac{16\pi}{U^2} \theta_{\eta'\eta}^{RL} g_L g_R \int_{-\infty}^{\infty} d\xi_{Rk'} \int_{-\infty}^{\infty} d\xi_{Lk} n_F(\xi_{Lk} - \mu_L) \\
&\quad \times [1 - n_F(\xi_{Rk'} - \mu_R)] \delta[\xi_{Rk'} + \xi_{\eta'} - (\xi_{Lk} + \xi_{\eta})] \\
&= \frac{16\pi (t_R t_L)^2}{U^2} \theta_{\eta'\eta}^{RL} g_L g_R \int_{-\infty}^{\infty} d\xi_{Rk'} n_F(\xi_{Rk'} + \xi_{\eta'} - \xi_{\eta} - \mu_L) [1 - n_F(\xi_{Rk'} - \mu_R)] \\
&= \frac{16\pi}{U^2} \theta_{\eta'\eta}^{RL} g_L g_R n_B(\xi_{\eta'} - \xi_{\eta} - \mu_L + \mu_R) \\
&\quad \times \int_{-\infty}^{\infty} d\xi_{Rk'} [n_F(\xi_{Rk'} - \mu_R) - n_F(\xi_{Rk'} + \xi_{\eta'} - \xi_{\eta} - \mu_L)] \\
&= 16\pi U^{-2} g_L g_R \theta_{\eta'\eta}^{RL} (\xi_{\eta'} - \xi_{\eta} - \mu_L + \mu_R) n_B(\xi_{\eta'} - \xi_{\eta} - \mu_L + \mu_R)
\end{aligned}$$

A transition from right to left, $\Gamma_{\eta'\eta}^{LR}$, is given by initial and final states $|f\rangle = c_{Lk\sigma}^\dagger d_{\eta'}^\dagger d_{\eta} c_{Rk'\sigma'} |i\rangle$ and the Kondo Hamiltonian $j_{LR}^{ij} c_{L\tilde{k}\tilde{\sigma}}^\dagger \tau_{\tilde{\sigma}\tilde{\sigma}'}^j c_{R\tilde{k}'\tilde{\sigma}'} S^i$. With the substitutions $(R, L, \sigma, \sigma') \hookrightarrow (L, R, \sigma', \sigma)$, the calculation runs like the above.

$$\begin{aligned}
\Gamma_{\eta'\eta}^{LR} &= \sum_{\sigma\sigma'} \frac{8\pi}{U^2} \left| \sum_{ij} j_{LR}^{ij} \tau_{\sigma\sigma'}^j \tau_{\eta'\eta}^i \right|^2 \sum_{kk'} n_F(\xi_{RL'\sigma'} - \mu_R) [1 - n_F(\xi_{Lk\sigma} - \mu_L)] \delta[\dots] \\
&= 16\pi U^{-2} g_L g_R \theta_{\eta'\eta}^{LR} (\xi_{\eta'} - \xi_{\eta} - \mu_R + \mu_L) n_B(\xi_{\eta'} - \xi_{\eta} - \mu_R + \mu_L)
\end{aligned}$$

with

$$\theta_{\eta'\eta}^{LR} = \sum_{ijk} j_{LR}^{ij} j_{LR}^{kj*} \tau_{\eta'\eta}^i \tau_{\eta\eta'}^k$$

Note that the relation $j_{\alpha\alpha'}^{ij*} = j_{\alpha'\alpha}^{ij}$ ($\alpha \neq \alpha'$) is not sufficient to ensure identical thetas:

$$\theta_{\eta'\eta}^{LR} := \sum_{ijk} j_{LR}^{ij} j_{LR}^{kj*} \tau_{\eta'\eta}^i \tau_{\eta\eta'}^k = \sum_{ijk} j_{RL}^{ij*} j_{RL}^{kj} \tau_{\eta'\eta}^i \tau_{\eta\eta'}^k \neq \sum_{ijk} j_{RL}^{ij} j_{RL}^{kj*} \tau_{\eta'\eta}^i \tau_{\eta\eta'}^k = \theta_{\eta'\eta}^{RL}$$

Similar calculations leads to $\Gamma_{\eta'\eta}^{\alpha\alpha}$, $\alpha \in \{L, R\}$. In these cases the transition is described by initial and final states $|f\rangle = c_{\alpha k\sigma}^\dagger d_\eta^\dagger c_{\alpha k'\sigma'} |i\rangle$ and the Kondo Hamiltonian $j_{\alpha\alpha}^{ij} c_{\alpha\tilde{k}\tilde{\sigma}}^\dagger \tau_{\tilde{\sigma}\tilde{\sigma}'}^j c_{\alpha\tilde{k}'\tilde{\sigma}'} S^i$.

$$\begin{aligned} \Gamma_{\eta'\eta}^{\alpha\alpha} = 2\pi \sum_{k\sigma k'\sigma'} \sum_{i_\alpha} & \left| \langle i | c_{\alpha, k\sigma}^\dagger d_\eta^\dagger c_{\alpha, k'\sigma'} \frac{4}{U/2} \sum_{ij\tilde{k}'\tilde{k}} \left(j_{\alpha\alpha}^{ij} s_{\alpha\tilde{k}', \alpha\tilde{k}}^j \right) S^i | i \rangle \right|^2 \\ & \times W_{i_\alpha} \delta[\xi_{\alpha k'\sigma'} + \xi_{\eta'} - (\xi_{\alpha k\sigma} + \xi_\eta)] \end{aligned}$$

Since only one lead is involved, the initial state $|i_\alpha\rangle$ is sandwiched between not only one annihilation and one creation operator, but between two of each, all with different momenta and spins. The inner product is

$$\begin{aligned} \sum_{\tilde{k}\tilde{k}'\tilde{\sigma}\tilde{\sigma}'} \langle i_\alpha | c_{\alpha k'\sigma'}^\dagger c_{\alpha k\sigma} c_{\alpha\tilde{k}\tilde{\sigma}}^\dagger c_{\alpha\tilde{k}'\tilde{\sigma}'} | i_\alpha \rangle &= \sum_{\tilde{k}\tilde{k}'\tilde{\sigma}\tilde{\sigma}'} \langle i_\alpha | c_{\alpha k'\sigma'}^\dagger c_{\alpha k\sigma} c_{\alpha\tilde{k}\tilde{\sigma}}^\dagger c_{\alpha\tilde{k}'\tilde{\sigma}'} | i_\alpha \rangle \delta_{\tilde{k}\tilde{k}'} \delta_{\tilde{k}'\tilde{k}'} \delta_{\tilde{\sigma}\tilde{\sigma}'} \delta_{\tilde{\sigma}'\tilde{\sigma}'} \\ &= \langle i_\alpha | c_{\alpha k'\sigma'}^\dagger c_{\alpha k\sigma} c_{\alpha\tilde{k}\tilde{\sigma}}^\dagger c_{\alpha\tilde{k}'\tilde{\sigma}'} | i_\alpha \rangle \\ &= \langle i_\alpha | c_{\alpha k'\sigma'}^\dagger c_{\alpha k\sigma} \left(\delta_{\tilde{k}\tilde{k}'} \delta_{\tilde{\sigma}\tilde{\sigma}'} - c_{\alpha k'\sigma'} c_{\alpha k\sigma}^\dagger \right) | i_\alpha \rangle \\ &= \langle i_\alpha | c_{\alpha k'\sigma'}^\dagger c_{\alpha k\sigma} c_{\alpha\tilde{k}\tilde{\sigma}}^\dagger c_{\alpha\tilde{k}'\tilde{\sigma}'} | i_\alpha \rangle \\ &= \sum_{j_\alpha} \langle i_\alpha | c_{\alpha k'\sigma'}^\dagger c_{\alpha k\sigma} | j_\alpha \rangle \langle j_\alpha | c_{\alpha k\sigma} c_{\alpha\tilde{k}\tilde{\sigma}}^\dagger | i_\alpha \rangle \\ &= \langle i_\alpha | c_{\alpha k'\sigma'}^\dagger c_{\alpha k\sigma} | i_\alpha \rangle \langle i_\alpha | c_{\alpha k\sigma} c_{\alpha\tilde{k}\tilde{\sigma}}^\dagger | i_\alpha \rangle \end{aligned}$$

Each of these inner products equals zero or one. Therefore

$$\begin{aligned} \sum_{kk'} \sum_{i_\alpha} |\langle i_\alpha | \dots | i_\alpha \rangle|^2 W_{i_\alpha} &= \sum_{kk'} \sum_{i_\alpha} \langle i_\alpha | c_{\alpha k'\sigma'}^\dagger c_{\alpha k\sigma} | i_\alpha \rangle \langle i_\alpha | c_{\alpha k\sigma} c_{\alpha\tilde{k}\tilde{\sigma}}^\dagger | i_\alpha \rangle W_{i_\alpha} \\ &= \sum_{kk'} n_F(\xi_{\alpha k'\sigma'} - \mu_\alpha) [1 - n_F(\xi_{\alpha k\sigma} - \mu_\alpha)] \end{aligned}$$

The transition rate is

$$\Gamma_{\eta'\eta}^{\alpha\alpha} = 16\pi U^{-2} g_\alpha^2 \theta_{\eta'\eta}^{\alpha\alpha} (\xi_{\eta'} - \xi_\eta) n_B(\xi_{\eta'} - \xi_\eta)$$

with $\theta_{\eta'\eta}^{\alpha\alpha} = \sum_{ijk} j_{\alpha\alpha}^{ij} j_{\alpha\alpha}^{kj} \tau_{\eta'\eta}^i \tau_{\eta\eta'}^k$. All transition rates $\alpha', \alpha \in \{L, R\}$ are on the same form:

$$\Gamma_{\eta'\eta}^{\alpha'\alpha} = 16\pi U^{-2} g_{\alpha'} g_\alpha \theta_{\eta'\eta}^{\alpha'\alpha} (\xi_{\eta'} - \xi_\eta - \mu_\alpha + \mu_{\alpha'}) n_B(\xi_{\eta'} - \xi_\eta - \mu_\alpha + \mu_{\alpha'}) \quad (4.7)$$

with

$$\theta_{\eta'\eta}^{\alpha'\alpha} = \sum_{ijk} j_{\alpha'\alpha}^{ij} j_{\alpha'\alpha}^{kj} {}^* \tau_{\eta'\eta}^i \tau_{\eta\eta'}^k = \sum_{ijk} j_{\alpha'\alpha}^{ij} j_{\alpha\alpha'}^{kj} \tau_{\eta'\eta}^i \tau_{\eta\eta'}^k$$

A transition between dot states η and η' can happen in a process where an electron tunnels from lead $\alpha \in \{L, R\}$ to lead $\alpha' \in \{L, R\}$. In other words, if one is only interested in the net process on the dot, a transition rate $\Gamma_{\eta'\eta}$ is defined by

$$\Gamma_{\eta'\eta} = \Gamma_{\eta'\eta}^{RL} + \Gamma_{\eta'\eta}^{LR} + \Gamma_{\eta'\eta}^{LL} + \Gamma_{\eta'\eta}^{RR}$$

We can now determine the nonequilibrium occupation numbers $P(\eta)$. This is done by solving the following master equations:

$$\begin{aligned} \frac{dP(\uparrow)}{dt} &= -\Gamma_{\downarrow\uparrow} P(\uparrow) + \Gamma_{\uparrow\downarrow} P(\downarrow) \\ \frac{dP(\downarrow)}{dt} &= -\Gamma_{\uparrow\downarrow} P(\downarrow) + \Gamma_{\downarrow\uparrow} P(\uparrow) \end{aligned}$$

with the constraint that $P(\uparrow) + P(\downarrow) = 1$. In a steady state ($dP(\eta)/dt = 0$), the master equations give

$$0 = -\Gamma_{\uparrow\downarrow} P(\downarrow) + \Gamma_{\downarrow\uparrow} P(\uparrow) = -\Gamma_{\uparrow\downarrow} + (\Gamma_{\uparrow\downarrow} + \Gamma_{\downarrow\uparrow}) P(\uparrow)$$

and hence

$$P(\uparrow) = \frac{\Gamma_{\uparrow\downarrow}}{\Gamma_{\uparrow\downarrow} + \Gamma_{\downarrow\uparrow}}, \quad P(\downarrow) = \frac{\Gamma_{\downarrow\uparrow}}{\Gamma_{\uparrow\downarrow} + \Gamma_{\downarrow\uparrow}} \quad (4.8)$$

Inserting the transitions rates in the above relations yields $P(\eta)$. To calculate the current through the junction, one needs the transition between all states within the Kondo regime:

$$\begin{aligned} I &= (-e) \sum_{\eta\eta'} (\Gamma_{\eta'\eta}^{RL} - \Gamma_{\eta\eta'}^{LR}) P(\eta) \\ &= (-e) 16\pi U^{-2} g_R g_L \sum_{\eta\eta'} \left[(\xi_{\eta'} - \xi_{\eta} - V) n_B(\xi_{\eta'} - \xi_{\eta} - V) \theta_{\eta'\eta}^{RL} \right. \\ &\quad \left. - (\xi_{\eta'} - \xi_{\eta} + V) n_B(\xi_{\eta'} - \xi_{\eta} + V) \theta_{\eta'\eta}^{LR} \right] P(\eta) \end{aligned} \quad (4.9)$$

where the potential V has been defined as $V := \mu_L - \mu_R$. Note that also $P(\eta)$ depends on $\xi_{\eta'}, \xi_{\eta}$ and V through the transitions $\Gamma_{\eta'\eta}$.

A mathematica-calculation of the differential conductance as function of bias-voltage is displayed in fig. 4.1. See the code in Appendix. A similar mathematica-calculation of the conductance in the case of a vanishing magnetic field do not show a Kondo peak. This is due to the fact that higher order contributions have been neglected. These become increasingly important as the magnetic field is decreased.

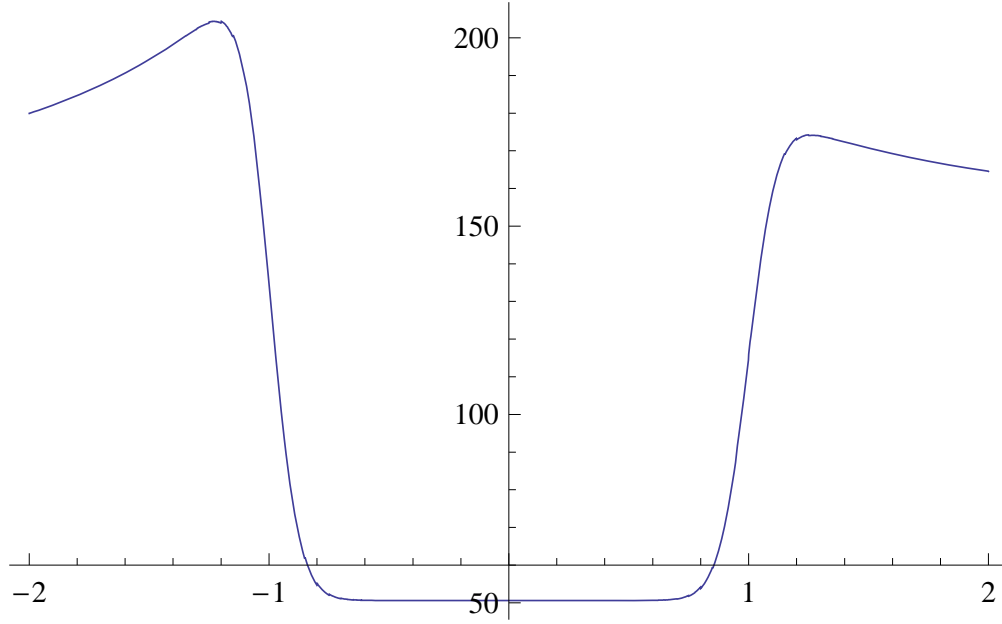


Figure 4.1: Differential Conductance dI/dV plotted against V for the values: $C_x = 0.4$, $C_z = 0.1$, $\gamma = -2^{-1/2}a\alpha = 0.1$, $t_{L0} = 1, t_{R0} = 1, t_{R1} = -1$, $T = 0.4$, $B = 1.0$. Notice the strong asymmetry in the peaks at $V = \pm 1.2$. By zooming out it is possible to see that dI/dV converges to the same value in $V = \pm\infty$

4.3.1 Differential conductance for $|V| \gg |B|$

The energy of state $|0, \uparrow / \downarrow\rangle$ is to linear order in B given by

$$\xi_\eta = \eta g \mu_B B / 2$$

Then $(\xi_{\eta'} - \xi_\eta) \propto B$ so the condition $|V| \gg |\xi_{\eta'} - \xi_\eta|$ is equivalent to $|V| \gg |B|$. The probability $P(\eta)$ is a rather complicated expression of the energies and the bias-voltage. The transition rate $\Gamma_{\eta\bar{\eta}}$ that enters $P(\eta)$ contains terms linear in V and terms linear in B . Neglecting all terms linear in B yields the transition rate in the case of $|V| \gg |B|$:

$$\Gamma_{\eta\bar{\eta}} \approx I_0 [\theta_{\eta\bar{\eta}}^{RL}(-V) n_B(-V) + \theta_{\eta\bar{\eta}}^{LR} V n_B(V)]$$

with $I_0 := (-e) 16\pi U^{-2} g_R g_L$, so

$$P(\eta) \approx \frac{\theta_{\eta\bar{\eta}}^{RL}(-V) n_B(-V) + \theta_{\eta\bar{\eta}}^{LR} V n_B(V)}{[\theta_{\eta\bar{\eta}}^{RL}(-V) n_B(-V) + \theta_{\eta\bar{\eta}}^{LR} V n_B(V)] + [\theta_{\bar{\eta}\eta}^{RL}(-V) n_B(-V) + \theta_{\bar{\eta}\eta}^{LR} V n_B(V)]}$$

In this case the only difference between $P(\uparrow)$ and $P(\downarrow)$ are the thetas in the numerator. For a bias-voltage much larger than the temperature, that is $V \gg$

$k_B T$, the product of the bias-voltage with the Bose-Einstein distribution function is approximately linear in V . Introducing a step function $\theta(x)$, the product is

$$(\pm V) n_B(\pm V) = \frac{\pm V}{e^{\pm V/k_B T} - 1} \approx |V| \theta(\mp V)$$

For $V \gg k_B T$ (and still for $|V| \gg |B|$) the occupation is

$$P(\eta) \approx \begin{cases} \theta_{\eta\bar{\eta}}^{RL} / (\theta_{\eta\bar{\eta}}^{RL} + \theta_{\bar{\eta}\eta}^{RL}) & \text{for } V > 0 \\ \theta_{\eta\bar{\eta}}^{LR} / (\theta_{\eta\bar{\eta}}^{LR} + \theta_{\bar{\eta}\eta}^{LR}) & \text{for } V < 0 \end{cases}$$

The differential conductance is given by

$$dI/dV \approx \begin{cases} I_0 \sum_{\eta\eta'} \theta_{\eta'\eta}^{RL} \theta_{\eta\bar{\eta}}^{RL} / (\theta_{\eta\bar{\eta}}^{RL} + \theta_{\bar{\eta}\eta}^{RL}) & \text{for } V > 0 \\ I_0 \sum_{\eta\eta'} \theta_{\eta'\eta}^{LR} \theta_{\eta\bar{\eta}}^{LR} / (\theta_{\eta\bar{\eta}}^{LR} + \theta_{\bar{\eta}\eta}^{LR}) & \text{for } V < 0 \end{cases} \quad (4.10)$$

If there is no spin-orbit coupling, then $j_{\alpha'\alpha}^{ij} = \delta_{ij}$ for all $\alpha', \alpha \in \{L, R\}$, hence $\theta_{\eta'\eta}^{\alpha'\alpha} = \sum_i \tau_{\eta'\eta}^i \tau_{\eta\eta'}^i = \theta_{\eta'\eta}^{\alpha\alpha'}$. In this case (4.10) shows that the differential conductance will be equal in $\pm V$ (for $|V| \gg \tau$). In other words, there is a symmetry in left and right, such that by flipping a large bias-voltage V the current will maintain its magnitude and shift direction. With a finite Rashba-coupling $\theta_{\eta'\eta}^{\alpha\alpha'} \neq \theta_{\eta'\eta}^{\alpha'\alpha}$, e.g.

$$\theta_{\uparrow\downarrow}^{LR} - \theta_{\uparrow\downarrow}^{RL} = 4C_x(t_{L1}t_{R0} - t_{L0}t_{R1})\gamma(-2t_{L0}t_{R0} + t_{L1}t_{R0}\gamma + t_{L0}t_{R1}\gamma) \quad (4.11)$$

which in general is non-zero. Here $\gamma = -2^{-1/2}a\alpha$ and we shall remember that the expression is only valid up to linear order in the gammas and magnetic field, hence we shall only look at the terms linear in these:

$$\theta_{\uparrow\downarrow}^{LR} - \theta_{\uparrow\downarrow}^{RL} = -8C_x(t_{L1}t_{R0} - t_{L0}t_{R1})t_{L0}t_{R0}(-2^{-1/2}a\alpha) \quad (4.12)$$

By expressing all thetas in terms of gammas and C's, one finds that

$$\theta_{\eta'\eta}^{RL} \theta_{\eta\bar{\eta}}^{RL} / (\theta_{\eta\bar{\eta}}^{RL} + \theta_{\bar{\eta}\eta}^{RL}) = \theta_{\eta'\eta}^{LR} \theta_{\eta\bar{\eta}}^{LR} / (\theta_{\eta\bar{\eta}}^{LR} + \theta_{\bar{\eta}\eta}^{LR})$$

and the differential conductance (4.10) is thus equal in $\pm V$ (for $|V| \gg \tau$).

4.3.2 Differential conductance for $V = \pm B$

For a bias-voltage V in the neighbourhood of $\pm B$, there is a difference in diff. conductance for $\pm V$. For $-B < V < B$ only the ground state (\downarrow) can be occupied, hence the only transition allowed is the spin-preserving one $\Gamma_{\downarrow\downarrow}$. For $|V| > B$, spin-flip processes $\Gamma_{\uparrow\downarrow}$ and $\Gamma_{\downarrow\uparrow}$ are possible since the potential difference

”delivers the energy needed to flip the spin”. By turning up the bias-voltage from $|V| < B$ to $V = \pm B$ there must be a step in dI/dV where the first spin flips, that is where the transition $\Gamma_{\uparrow\downarrow}$ becomes possible. Here, the current is given by

$$I = I_0 \left[(\xi_{\uparrow} - \xi_{\downarrow} - V) n_B (\xi_{\uparrow} - \xi_{\downarrow} - V) \theta_{\uparrow\downarrow}^{RL} \right. \\ \left. - (\xi_{\uparrow} - \xi_{\downarrow} + V) n_B (\xi_{\uparrow} - \xi_{\downarrow} + V) \theta_{\uparrow\downarrow}^{LR} \right. \\ \left. + (-V) n_B (-V) \theta_{\downarrow\downarrow}^{RL} - (+V) n_B (+V) \theta_{\downarrow\downarrow}^{LR} \right] P(\downarrow)$$

For $B = (\xi_{\uparrow} - \xi_{\downarrow}) = -V$ the differential conductance is:

$$\frac{dI}{dV_-} \approx -I_0 \frac{d}{dV} [(B + V) n_B (B + V)] \Big|_{B=-V} \theta_{\uparrow\downarrow}^{LR}$$

and for $B = V$:

$$\frac{dI}{dV_+} \approx I_0 \frac{d}{dV} [(B - V) n_B (B - V)] \Big|_{B=V} \theta_{\uparrow\downarrow}^{RL}$$

and hence

$$\frac{dI/dV_+}{dI/dV_-} \approx \frac{\theta_{\uparrow\downarrow}^{RL}}{\theta_{\uparrow\downarrow}^{LR}} \quad (4.13)$$

The difference (4.12) is to linear order in the Rashba coupling given by

$$(\theta_{\uparrow\downarrow}^{LR} - \theta_{\uparrow\downarrow}^{RL}) = 4\sqrt{2}C_x(t_{L1}t_{R0} - t_{L0}t_{R1})t_{L0}t_{R0}a\alpha$$

Taylor expanding (4.13) as a function of the Rashba spin-orbit coupling α around $\alpha = 0$ gives (to linear order in α)

$$\frac{dI/dV_+}{dI/dV_-} = \frac{\theta_{\uparrow\downarrow}^{RL}}{\theta_{\uparrow\downarrow}^{RL} + (\theta_{\uparrow\downarrow}^{LR} - \theta_{\uparrow\downarrow}^{RL})} \approx 1 - \frac{(\theta_{\uparrow\downarrow}^{LR} - \theta_{\uparrow\downarrow}^{RL})}{\theta_{\uparrow\downarrow}^{RL} \Big|_{\alpha=0}}$$

Using

$$\theta_{\uparrow\downarrow}^{LR} = t_{L0}^2 t_{R0}^2 - 2\sqrt{2} (t_{L0}^2 t_{R0} t_{R1} - t_{R0}^2 t_{L0} t_{L1}) a C_x \alpha$$

yields the result

$$\frac{dI/dV_+}{dI/dV_-} = 1 - 4\sqrt{2} \left(\frac{t_{L1}}{t_{L0}} - \frac{t_{R1}}{t_{R0}} \right) \frac{g\mu_B B_x}{\hbar\omega_0} \frac{a}{\lambda_{SO}} \quad (4.14)$$

where $\lambda_{SO} = \alpha^{-1}$ is the Rashba spin-orbit length. Hence the peaks in differential conductance at $V = \pm B$ are equal only if

$$\frac{t_{L1}}{t_{L0}} = \frac{t_{R1}}{t_{R0}} \quad (4.15)$$

or if either the spin-orbit coupling or the x-component of the magnetic field is zero. The tunneling coefficient $t_{\alpha n} = t_{\alpha k n}^{\sigma\sigma'} := \langle \alpha k \sigma | H_T | n \sigma' \rangle$ which we have assumed independent of spins and momentum is the tunneling coefficient between a metallic lead and a dot described by oscillator eigenstates (without SO-interaction) with harmonic oscillator length a . If the tunneling coefficients fulfill $t_{L1}/t_{L0} \neq t_{R1}/t_{R0}$ and if a Rashba spin-orbit interaction is present, then the magnetic field \mathbf{B} is a handle for controlling the asymmetry of the differential conductance.

In the g-factor g enters in its original form. This is due to the neglect of higher order terms in the transformation (3.3). The quadratic term $\frac{1}{2} [S, H_{Ra}]$ contains an anisotropic correction to g . Carrying out the transformation to higher order (infinitely high order) will thus lead to a renormalization of the g-factor.

A recent measurement by Csonka et al. have shown an asymmetry in the Zeeman-split Kondo zero bias anomaly [5](see fig. 4.2). Other experiments such as the one by Park [19](see fig 4.3) have showed a slight asymmetry. This

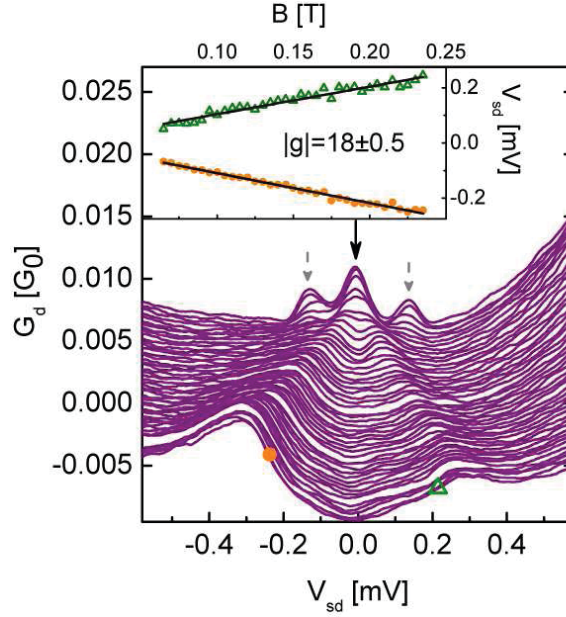


Figure 4.2: Magnetic field splitting of the Kondo zero bias anomaly. (main panel): Differential conductance vs. source drain voltage at different perpendicular magnetic field values $B = 0, 5, 10, \dots, 240$ mT (back to front). Measured at $V_{bg} = -2.64$ V and $V_{tg} = 0.08$ V. The curves are shifted for clarity. The two side peaks (gray arrows) are superconducting features induced by the Ti/Al electrodes. (inset): The position of the inflection points of the $G_d(V_{sd})$ curves from the main panel (orange dot and green triangle) as a function of the magnetic field. Linear fit (line) with the extracted $|g|$ -factor. [5]

asymmetry cannot be explained by a Kondo model that does not take into account spin-orbit interactions. The model examined in this thesis offers an explanation, namely that for a given a, α and \mathbf{B} the asymmetry is determined by the tunneling

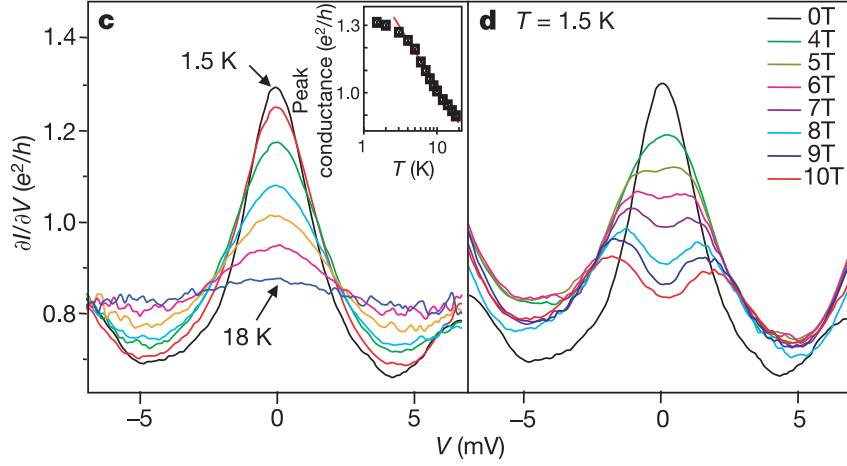


Figure 4.3: Right: Magnetic-field dependence of the Kondo peak. The peak splitting varies linearly with magnetic field. Notice the slight asymmetry. [19]

coefficients t_{L1} , t_{L0} , t_{R1} , t_{R0} . The result will be modified by contributions of higher order in the coupling and in the magnetic field. However, this simple approach is sufficient to describe the characteristics of the asymmetry.

4.3.3 The spin-orbit coupling constant α

The relation (4.3.2) can be used to determine the coupling α . Say that we have a mesoscopic quantum dot that can be described by a harmonic potential with a certain oscillator (or frequency) length a (ω_0) that is known. We apply a fixed external magnetic field B_x and measure the current through the junction as a function of applied voltage. In order to determine α one has to find a way to evaluate the fractions (t_{L1}/t_{L0}) and (t_{R1}/t_{R0}) .

Typical values of the spin-orbit length $\lambda_{SO} = 1/\alpha$ are 50 – 200 nm. Fasth et al. have measured the spin-orbit length in an InAs nanowire quantum dot of length 46 nm and width 18 nm to be $\lambda_{SO} \approx 127$ nm [6]. For unconfined electrons in similar InAs wires, Hansen et al. have found a spin-orbit length of $\lambda_{SO} \approx 200$ nm [10]. In a recent experiment P.D. Nissen have estimated the spin-orbit length in InAs nanowire quantum dots of length 220–250 nm and width 75–90 nm to $\lambda_{SO} \approx 80 \pm 20$ nm [18].

4.4 Potential Scattering Terms

The other contributions in (4.4) are calculated similarly to the Kondo Hamiltonian. Collecting terms of the same type in (4.2) and using that

- $(s_{\alpha k \alpha' k'}^i)^\dagger = s_{\alpha' k' \alpha k}^i$, $(S^i)^\dagger = S^i$ and $[s_{\alpha k \alpha' k'}^i, S^j] = 0$ for $i, j \in \{0, x, y, z\}$
- the prefactor $p \in \{k, l, \dots, o\}$ multiplying the concerning term fulfills $(p_{\alpha \alpha'}^i)^* = p_{\alpha' \alpha}^i$
- $H_S^{(2)} = \frac{i}{2} [S, H_T] \approx \frac{i}{2} ([S^-, H_T^+] - [S^-, H_T^+]^\dagger)$

yields

$$\begin{aligned}
H_S^{(2)} = & \sum_{\alpha \alpha' k k'} \sum_{i j \in \{x, y, z\}} J_{\alpha \alpha'}^{ij} s_{\alpha k \alpha' k'}^j S^i + \sum_{\alpha \alpha' k k'} \sum_{i \in \{x, y, z\}} K_{\alpha \alpha'}^i s_{\alpha k \alpha' k'}^0 S^i \\
& + \sum_{\alpha \alpha' k k'} \sum_{i \in \{x, y, z\}} (L_{\alpha \alpha'}^i s_{\alpha k \alpha' k'}^i + M_{\alpha \alpha'}^i S^i) + \sum_{\alpha \alpha' k k'} N_{\alpha \alpha'} s_{\alpha k \alpha' k'}^0 + \sum_{\alpha \alpha' k k'} O_{\alpha \alpha'}
\end{aligned}$$

with the energies

$$\begin{aligned}
K_{\alpha \alpha'} &= \left(\frac{1}{E_2 - E_1} + \frac{1}{E_0 - E_1} \right) \frac{a\alpha}{\sqrt{2}} \begin{pmatrix} C_z (t_{\alpha' 0} t_{\alpha 1} + t_{\alpha 0} t_{\alpha' 1}) \\ i (t_{\alpha' 0} t_{\alpha 1} - t_{\alpha 0} t_{\alpha' 1}) \\ C_x (t_{\alpha' 0} t_{\alpha 1} + t_{\alpha 0} t_{\alpha' 1}) \end{pmatrix}_i \\
L_{\alpha \alpha'} &= \left(\frac{1}{E_2 - E_1} - \frac{1}{E_0 - E_1} \right) \frac{a\alpha}{\sqrt{2}} \begin{pmatrix} -C_z (t_{\alpha' 0} t_{\alpha 1} + t_{\alpha 0} t_{\alpha' 1}) \\ -i (t_{\alpha' 0} t_{\alpha 1} - t_{\alpha 0} t_{\alpha' 1}) \\ C_x (t_{\alpha' 0} t_{\alpha 1} + t_{\alpha 0} t_{\alpha' 1}) \end{pmatrix}_i \\
M_{\alpha \alpha'} &= \left(\frac{1}{E_0 - E_1} \right) \frac{2a\alpha}{\sqrt{2}} \begin{pmatrix} -C_z (t_{\alpha' 0} t_{\alpha 1} + t_{\alpha 0} t_{\alpha' 1}) \\ -i (t_{\alpha' 0} t_{\alpha 1} - t_{\alpha 0} t_{\alpha' 1}) \\ C_x (t_{\alpha' 0} t_{\alpha 1} + t_{\alpha 0} t_{\alpha' 1}) \end{pmatrix}_i \\
N_{\alpha \alpha'} &= \left(\frac{1}{E_2 - E_1} - \frac{1}{E_0 - E_1} \right) \frac{(-t_{\alpha 0} t_{\alpha' 0})}{2} \\
O_{\alpha \alpha'} &= \left(\frac{1}{E_0 - E_1} \right) (-t_{\alpha 0} t_{\alpha' 0})
\end{aligned} \tag{4.16}$$

In the particle-hole symmetric point $L_{\alpha \alpha'} = N_{\alpha \alpha'} = 0$. In the absence of spin-orbit interactions the only terms beside the Kondo term are the constant term $O_{\alpha \alpha'}$ and the potential scattering contribution $N_{\alpha \alpha'}$. For a nonvanishing SO coupling there are two additional contributions (again in the particle-hole symmetric point), $K_{\alpha \alpha'}$ and $M_{\alpha \alpha'}$. This is not potential scattering in its traditional sense. However, it is fundamentally different from the Kondo term in that it is not an exchange scattering. The Kondo Hamiltonian describes that the spin of the lead electrons can change if, at the same time, the spin of the dot changes. The terms $K_{\alpha \alpha'}$ and $M_{\alpha \alpha'}$ do not have a such exchange. It is the still Kondo term that is responsible for the interesting physics.

Chapter 5

Summary and Outlook

Starting from the Anderson model for a quantum dot, with Rashba type spin-orbit interactions, coupled to two metallic electrodes, we have derived a Kondo-model. The model has a very low symmetry and the resulting Zeeman-split Kondo peak in the conductance has an asymmetry controlled by the coupling to the leads. In a quantum dot where the coupling to one lead is different from the coupling to the other, the Zeeman split Kondo peak will be asymmetric. This model offers an explanation of why a Kondo-effect is observed in materials that has substantial spin-orbit coupling. Moreover, it can explain the asymmetry in the Zeeman-split Kondo peak that has been observed by Csonka [5].

Solving the Kondo problem for this Kondo-model is outside the scope of this thesis. An approach could be to make a 'poor man's scaling', inspired by Anderson's solution of the original Kondo problem[2].

Appendix A

Mathematica code

See the next page.

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