Non-equilibrium dynamics of a single spin in a tunnel junction

Henning Hammar
Abstract

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Making spintronic devices is a hot topic for future technical development. In this work the non-equilibrium dynamics of a single spin in a tunnel junction is analyzed and numerically simulated. This is done in order to understand the dynamics of e.g. a magnetic molecule between two metal contacts for future spintronic devices. The work starts with looking at the system in a many-body theory picture in order to derive the interesting properties of the system. An initial solution for the system is analytically calculated as well as for the dynamic case. The dynamic has then been numerically simulated in order to get the time evolution of the system. The results showed that the dynamics of the molecular spin induced a spin dependent charge and spin currents in the system and that the currents could be used to control the molecular spin. It showed qualitatively how different parameters, for example coupling strength, effect the system and what to consider when designing a system similar to this.
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1 Introduction

1.1 Molecular spintronics

Electronic devices and circuits are getting smaller and smaller and more effective and has for many years followed the prediction of Moore’s law [1]. Conventional electronic devices as silicon integrated circuits are now entering a level where quantum effects start to come into the picture. In order to continue this progress different kind of electronic devices is of great interest. Molecular spintronics is one of the emerging new fields where one uses the properties of magnetic molecules in order to create electronic devices. Here, one uses the spin instead of the charge of the electron when performing the operations. By using the magnetic properties of electrons instead of their charge it enables to create dissipationless electronics, as it is not longer needed to move charges. Therefore less energy is needed which is both environmental friendly and has a great impact on for example mobile devices where the need of battery reduces.

In spintronic devices the magnetic molecules can be used as nanomagnets and single-molecule magnets are among the smallest devices that could be used [2]. Molecular spintronics using single-molecule magnets has many interesting features that can be used in order to create devices for information storage and processing [3]. One of the key properties of single-molecule magnets is that they have a strong magnetic anisotropy leading to magnetic bistability which is good for making nanoscale memory cells [4]. Another key property is that they have non-trivial quantum dynamics which is good for making quantum computers [5]. Quantum computers are computers that uses the properties of a quantum state when performing computations and therefore can outperform classical computers in factoring numbers and search in databases. Because of the applications it is of great interest to understand the dynamics and properties of single-molecule magnets.

In this work the non-equilibrium dynamics of a local spin moment in a tunnel junction is analyzed. This could be a magnetic molecule between two metal contacts where one is interested in controlling either the spin polarization of the current or the magnetic moment of the molecule. This could be used for a memory cell or for performing operations on the local spin moment for quantum information processing, although here we treat the spin moment of the molecule classically.

Previous works on studying similar systems has been done. In one work the authors study what happens when pumping the spin of electrons into an excited state with a spin-polarized scanning tunneling microscope and then analyze the spin relaxation time for each excited state [6]. In another paper the authors study the magnetic anisotropy of magnetic molecules and show that higher order spin system coupled to ferromagnets can be used and controlled by electrical current in the same way as simple spin-half systems [7]. Also work has been done to analyze the non-equilibrium transport through magnetic vibrating molecules [8]. The most similar work is by Filipovic et al [9] where they analyze the spin transport and tunable Gilbert damping in a single-molecule junction using the same idealized picture and the same approach as in this work. Their conclusions was that they get that the coupling between the spin and the molecular spin induces inelastic spin currents and a Gilbert damping on the molecular spin and a modification of its frequency.

1.2 Description of the system

The system to be analyzed is a system consisting of a local spin moment in a tunnel junction interacting with the current going through the junction. In the idealized picture it is described by a quantum dot connected to two metal contacts and interacting with the local spin moment. The quantum dot is a quantum island consisting of a single level, see figure 1. When applying a voltage over the two contacts the electrons will start tunneling to the quantum dot and then to the other contact. As the electrons carries both charge and a magnetic spin this will create a charge and a spin current going through the quantum dot. The currents will then interact with the local spin moment. The local spin moment can be for example the magnetic moment
of the molecule. The local spin moment will then interact with the current going through the quantum dot. This is creating the dynamics of the system and what is going to be studied in the thesis.

1.3 Aim

The aim of the thesis is to analyze the non-equilibrium dynamics of a single spin in a tunnel junction. This includes an analytical derivation of the equations of the system from existing theory in order to numerically calculate the dynamics of the system. Here it is interesting to see how to describe such a system and where the dynamics comes from. The dynamics of the system is then calculated for different input parameters in order to understand how they affect the system and what conclusions that can be made.

2 Theory

In order to analyze the system we first need to build up the theory we need. For understanding the theory it is recommended to have an insight in quantum mechanics and solid state physics. First we will consider how to work with a many-body quantum system and what mathematical tools that can be used. Then we regard the specific system that is going to be considered. When doing so we first develop the equation of motion for the local spin moment. Then we analyze the quantum dot Green’s function and lastly the tunneling current going through the dot. The theory regarded in this section is based on previous works done by J. Fransson [10].

2.1 Many-body theory and Green’s functions

Due to the vast amount of particles treated in a solid state system we need to define some mathematical concepts in order to treat the physics of the many-body system. We start by defining an operator \( \hat{\psi} \) that acts in our system. This represents the quantization of the quantum wave function for the electron. The electrons are created at time \( t' \) by \( \hat{\psi} (t') \) and they are annihilated at time \( t \) by \( \hat{\psi}^\dagger (t) \). We then define the propagator for the electrons. The one-electron Green’s function is defined as the propagation of an electron created at time \( t' \) and annihilated at time \( t \) and is calculated for fermionic particles as

\[
G(t,t') = (-i) \langle T \hat{\psi}(t) \hat{\psi}^\dagger (t') \rangle = \begin{cases} 
  -i \langle \hat{\psi}(t) \hat{\psi}^\dagger (t') \rangle & t > t' \\
  i \langle \hat{\psi}(t) \hat{\psi}^\dagger (t') \rangle & t < t' 
\end{cases},
\]

where \( T \) is the time-ordering operator. This is propagator is defined on the complex time contour. In this work we will treat a non-equilibrium problem and need to convert our propagators into the real time domain. This is done by defining new propagators, \( G^< (t,t') \) and \( G^> (t,t') \), called the lesser and greater Green’s function respectively. The lesser/greater superscript is used to indicate if the time \( t \) is less/larger than \( t' \) on the time contour, called the Keldysh contour. We can also define the retarded/advanced Green function

\[
G^r(t,t') = \theta(t - t') \left[ G^> (t,t') - G^< (t,t') \right],
\]

\[
G^a(t,t') = \theta(t' - t) \left[ G^< (t,t') - G^> (t,t') \right],
\]

which describes the connection between the lesser and greater Green’s function.
2.2 Defining the system

The system that we want to describe is a single spin moment $S$ in a tunnel junction interacting with a single level quantum dot, see figure 1. The quantum dot is coupled through tunneling interactions to metal contacts, electron reservoirs, with the respective chemical potential $\mu_L$, $\mu_R$, where $L/R$ denotes the left/right reservoir. The Hamiltonian for the system becomes

$$H = H_L + H_R + H_T + H_{QD} + H_S + H_{int}.$$  \hspace{1cm} (4)

We write the electron operator in the reservoirs as $c^\dagger_k \sigma$ and in the quantum dot as $d^\dagger \sigma$, where $c^\dagger_k \sigma$ creates an electron in the reservoir with momentum $k$ and spin $\sigma$ and $c_k \sigma$ annihilates it. These operators are analogous to $\hat{\psi}$. The same goes for the quantum dot, but as we only have one energy level we do not need to regard the momentum and it is simplified as $d^\dagger \sigma$ and $d \sigma$. The Hamiltonian for the reservoirs thus becomes

$${\cal H}_\chi = \sum_k (\varepsilon_k - \mu_\chi) c^\dagger_k \sigma c_k \sigma$$

representing the energy for the reservoir $\chi$. Here is $\varepsilon$ the energy levels of the reservoir, $k$ denotes the momentum vector and $\sigma$ the spin. The tunneling Hamiltonian is $${\cal H}_T = {\cal H}_{TL} + {\cal H}_{TR},$$

where $${\cal H}_{T\chi} = T_\chi \sum_k \varepsilon_k c^\dagger_k \sigma d_\sigma + H.c.,$$

i.e. it creates an electron in the reservoir and annihilates it in the quantum dot and vice versa. The quantum dot is represented by $${\cal H}_{QD} = \sum_\sigma \varepsilon_\sigma d^\dagger_\sigma \sigma,$$ and the spin system by $${\cal H}_S = -g\mu_B S \cdot B,$$ where $g$ is the g-factor, $\mu_B$ the Bohr constant, $S$ the spin vector and $B$ an external magnetic field. The interactions between the spin and the quantum dot is given by $${\cal H}_{int} = -Js \cdot S,$$ where $J$ is the interacting strength and $s = \sum_\sigma \sigma' c^\dagger_\sigma \alpha c_\sigma'. 2/2$.

2.3 Equation for the local spin moment

First we want to derive the equation for the local spin moment. It is derived from the effective action. For the local spin moment we can write the effective action as

$$\mathcal{S} = \frac{1}{S^2} \int S(t) \cdot [\dot{S}(t) \times \dot{S}(t)] dt - g\mu_B B(t) \cdot S(t) + \frac{1}{e} \int S(t) \cdot \mathbf{j}(t, t') \cdot \dot{S}(t') dt dt'$$  \hspace{1cm} (5)

where the spin superscripts $q$ and $c$ denotes if the spin is fast or slow varying, respectively, depending on the frame of reference. This equation follows from previous works [10]. The current $\mathbf{j}(t, t')$ will be calculated by
We can drop the superscript and take the cross product from the left with the approximate expression

\[ j(t, t') \approx \frac{ie}{2} \theta(t - t')sp \sigma (G^<(t', t)\sigma G^>(t, t') - G^>(t', t)\sigma G^<(t, t')) \tag{6} \]

where \( G^{</>(t, t')} \) is the lesser/greater Greens function for propagation of a quantum dot electron.

From the effective action we can derive the equation of motion. We take the functional derivative of the effective action and set it to zero as

\[ 0 = \frac{\delta \mathcal{S}}{\delta S(t)} = \frac{1}{S^2} \mathcal{S}'(t) \times \mathcal{S}'(t) - g\mu_B B(t) + \frac{1}{e} \int \mathcal{j}(t, t') \cdot \mathcal{S}'(t')dt'. \tag{7} \]

We can drop the superscript and take the cross product from the left with \( \mathcal{S}(t) \times \) to get

\[ 0 = \frac{1}{S^2} \mathcal{S}(t) \times \left[ \mathcal{S}(t) \times \dot{\mathcal{S}}(t) \right] - g\mu_B \mathcal{S}(t) \times \mathcal{B}(t) + \frac{1}{e} \int \mathcal{S}(t) \times \mathcal{j}(t, t') \cdot \mathcal{S}'(t')dt'. \tag{8} \]

Assuming that the length of the spin is constant and that we can treat it classically we can set \( \partial_t |\mathcal{S}(t)|^2 = 0 \) such that the first term can be simplified to \( -\dot{\mathcal{S}}(t) \) and moved to the left hand side. The resulting equation of motion becomes

\[ \dot{\mathcal{S}}(t) = -g\mu_B \mathcal{S}(t) \times \mathcal{B}(t) + \frac{1}{e} \int \left( \mathcal{j}^{(H)}(t, t') \mathcal{S}(t) \times \mathcal{S}(t') \right. \]
\[ \left. + \mathcal{S}(t) \times \mathcal{j}^{(I)}(t, t') \cdot \mathcal{S}'(t') - \mathcal{S}(t) \times \mathcal{j}^{(DM)}(t, t') \cdot \mathcal{S}'(t') \right) dt'. \tag{9} \]

Here, we decomposed the product \( \mathcal{S}(t) \times \mathcal{j}(t, t') \cdot \mathcal{S}'(t') \) into an isotropic Heisenberg, anisotropic Ising and anisotropic Dzyaloshinsky-Moriya (DM) like interaction according to

\[ \mathcal{S}(t) \times \mathcal{j}(t, t') \cdot \mathcal{S}'(t') = \mathcal{j}^{(H)}(t, t') \mathcal{S}(t) \times \mathcal{S}(t') + \mathcal{S}(t) \times \mathcal{j}^{(I)}(t, t') \cdot \mathcal{S}'(t') + \mathcal{S}(t) \times \mathcal{j}^{(DM)}(t, t') \times \mathcal{S}'(t'). \tag{10} \]

The interaction parameters are defined through

\[ \mathcal{j}^{(H)}(t, t') = ieJ^2 \theta(t - t') \left( G^<_0(t', t)G^<_0(t, t') - G^>_0(t', t)G^>_0(t, t') \right. \]
\[ \left. -G^<_1(t', t)G^<_1(t, t') + G^>_1(t', t)G^>_1(t, t') \right), \tag{11} \]

\[ \mathcal{j}^{(I)}(t, t') = ieJ^2 \theta(t - t') \left( G^>_1(t', t)G^<_1(t, t') - G^<_1(t', t)G^>_1(t, t') \right. \]
\[ \left. + G^>_1(t', t)G^>_1(t, t') \mathcal{G}^<_1(t, t') \right), \tag{12} \]

\[ \mathcal{j}^{(DM)}(t, t') = -eJ^2 \theta(t - t') \left( G^<_0(t', t)G^<_0(t, t') - G^>_0(t', t)G^>_0(t, t') \right. \]
\[ \left. -G^<_1(t', t)G^<_1(t, t') + G^>_1(t', t)G^>_1(t, t') \right), \tag{13} \]

where \( \mathcal{G}(t, t') = G_0(t, t')\sigma^0 + \sigma \cdot G_1(t, t') \) is the quantum dot Greens function which is separated into a spin-dependent and a spin-independent part. The quantum dot Greens function is dependent of the spin and its evolution. Thus the interaction parameters gives feedback from changes of the spin from the changes in the quantum dot Greens function. This gives a loop such that the evolution of the spin depends on the quantum dot Greens function and vice versa.
2.4 Quantum dot Greens function

We now derive the quantum dot Greens function. We start of by taking the time derivative of equation 1 which gives

$$\partial_t G_{\sigma\sigma'}(t, t') = -i \left\{ d_\sigma(t) d^\dagger_{\sigma'}(t') \right\} - i \left\{ T [d_\sigma(t), \mathcal{H}] d^\dagger_{\sigma'}(t') \right\},$$  \hspace{1cm} (14)

where $T$ is the time-ordering operator. Inserting the Hamiltonian for the quantum dot we get

$$(i\partial_t - \varepsilon_\sigma) G_{\sigma\sigma'}(t, t') = \delta_{\sigma\sigma'} \delta(t - t') + \int V_\sigma(t, \tau) G_{\sigma\sigma'}(\tau, t') d\tau - \int (S \cdot \sigma_{\sigma\sigma'}) G_{\sigma\sigma'}(t, t') d\tau,$$  \hspace{1cm} (15)

where the second term on the left hand side comes from the quantum dot Hamiltonian, the second term on the right hand side comes from the tunneling Hamiltonian and the third term from the interaction with the spin. From this operation follows that

$$V_\sigma^{</ >} (t, t') = \sum_k T^2_k g_{\kappa \sigma} (t, t'),$$  \hspace{1cm} (16)

where $g_{\kappa \sigma} (t, t') = (-i) T e^{-i\kappa_\sigma (t-t') - i\int_0^t V_\chi (\tau) d\tau}$ is the lead Greens function. Here is $e$ the elementary charge and $V_\chi (\tau)$ the applied bias voltage over the two metal contacts. We Fourier transform equation 16 and get

$$V_\sigma^{</ >} (t, t') = (\pm i) \sum_k T^2_k f(\pm \epsilon_{\kappa \sigma}) e^{-\epsilon_{\kappa \sigma} (t-t') - i\int_0^t V_\chi (\tau) d\tau}$$  \hspace{1cm} (17)

where we defined $\Gamma^\chi = \sum_k T^2_k \delta(\omega - \epsilon_{\kappa \sigma})$ and

$$I^{</ >}_\chi (t, t') = \int f(\pm \omega) e^{-i\omega (t-t') - i\int_0^t V_\chi (\tau) d\tau} \frac{d\omega}{2\pi},$$  \hspace{1cm} (18)

where $f(\omega)$ is the Fermi function and $f(-\omega) = 1 - f(\omega)$. We write the coupling matrix $V = V_0 \sigma^0 + \sigma \cdot \mathbf{v}_1$ in terms of spin-independent and spin-dependent components. Then we have

$$V_0^{</ >} (t, t') = (\pm i) \sum_{\chi \sigma} \Gamma^\chi \chi^{</ >}_\sigma (t, t') = (\pm i) \sum_{\chi \sigma} \Gamma^\chi \chi^{</ >}_\sigma (t, t'),$$  \hspace{1cm} (19)

$$V_1^{</ >} (t, t') = (\pm i) \sum_{\chi \sigma} \sigma^\chi \chi^{</ >}_\sigma (t, t') = (\pm i) \sum_{\chi \sigma} \Gamma^\chi \chi^{</ >}_\sigma (t, t'),$$  \hspace{1cm} (20)

where we have introduced the parameters $\Gamma_0 = \sum_{\sigma} \Gamma_\sigma$ and $\Gamma_S = \sum_{\sigma} \sigma^z \Gamma_\sigma \hat{\mathbf{z}}$.

We introduce a zero Greens function $g_\sigma (t, t')$ as the solution to the equation $(i\partial_t - \varepsilon_\sigma) g_\sigma (t, t') = \delta(t - t') + \int V_\sigma(t, \tau) g_\sigma (\tau, t') d\tau$. We can write the retarded/advanced zero Greens function as

$$g_\sigma^{</ >} (t, t') = (\pm i) \theta(\pm t - t') e^{-i(\varepsilon_\sigma \mp i\Gamma_\sigma)(t-t')}. $$  \hspace{1cm} (21)

Writing it in its spin-independent and spin-dependent components, $g(t, t') = g_0(t, t') \sigma^0 + \sigma \cdot g_1(t, t')$, it becomes
where we have considered the Keldysh contour.

In terms of the zero Green's function we write the approximate solution to 15 as

\[
\delta G_1^{\tau/\tau}(t, t') = (\pm i/2)\theta(\pm t + t') \sum_{\sigma} e^{-i(\varepsilon_\sigma + i\Gamma t)(t - t')},
\]

(22)

\[
g_1^{\tau/\tau}(t, t') = (\pm i/2)\theta(\pm t + t') \sum_{\sigma} \sigma_\sigma e^{-i(\varepsilon_\sigma + i\Gamma t)(t - t')} \hat{a}.
\]

(23)

The lesser/greater forms of \( \mathbf{g} \) becomes

\[
g^{<>/>}(t, t') = \int g^{\tau}(t, \tau) \mathbf{V}^{<>/>}(\tau, \tau') g^{a}(\tau', t') d\tau d\tau' = g_0^{<>/>}(t, t') \sigma_0 + \sigma g_1^{<>/>}(t, t')
\]

(24)

where we divided into the spin-independent and spin-dependent components

\[
g_0^{<>/>}(t, t') = \int \left( g_0^{<>/>}(\tau, \tau') g_0^{a} + g_0^{<>/>}(\tau, \tau') g_0^{a} + g_0^{<>/>}(\tau, \tau') g_0^{a} + g_0^{<>/>}(\tau, \tau') g_0^{a} \right) d\tau d\tau'
\]

(25)

\[
g_1^{<>/>}(t, t') = \int \left( g_1^{<>/>}(\tau, \tau') g_1^{a} + g_1^{<>/>}(\tau, \tau') g_1^{a} + g_1^{<>/>}(\tau, \tau') g_1^{a} + g_1^{<>/>}(\tau, \tau') g_1^{a} \right) d\tau d\tau'.
\]

(26)

In terms of the zero Green's function we write the approximate solution to 15 as

\[
\mathbf{G}^{<>/>}(t, t') = g^{<>/>}(t, t') - J \int g(t, \tau) \langle \mathbf{S}(\tau) \rangle \cdot \mathbf{g}(\tau, t') d\tau
\]

\[
= g_0^{<>/>}(t, t') \sigma_0 + \sigma \cdot g_1^{<>/>}(t, t') - J \int \left( g_0(t, \tau) \sigma_0 + \sigma \cdot g_1(t, \tau) \right) \langle \mathbf{S}(\tau) \rangle \cdot \sigma \mathbf{g}(\tau, t') d\tau
\]

\[
= G_0^{<>/>}(t, t') \sigma_0 + \sigma \cdot G_1^{<>/>}(t, t'),
\]

(27)

where we defined \( G_0^{<>/>}(t, t') = g_0^{<>/>}(t, t') + \delta G_0^{<>/>}(t, t') \) and \( G_1^{<>/>}(t, t') = g_1^{<>/>}(t, t') + \delta G_1^{<>/>}(t, t') \). Here is

\[
\delta G_0^{<>/>}(t, t') = -J \int \left( \mathbf{g}_1^{<>/>}(t, \tau) \cdot \langle \mathbf{S}(\tau) \rangle \right) \left( \mathbf{g}_1^{<>/>}(\tau, t') + g_0^{<>/>}(t, \tau) \cdot \langle \mathbf{S}(\tau) \rangle \right) \mathbf{g}_1^{a}(\tau, t')
\]

\[
+ \mathbf{g}_1^{<>/>}(t, \tau) \cdot \langle \mathbf{S}(\tau) \rangle \left( \mathbf{g}_1^{<>/>}(\tau, t') + g_0^{<>/>}(t, \tau) \cdot \langle \mathbf{S}(\tau) \rangle \right) g_0^{a}(\tau, t')
\]

\[
+ i \left[ \mathbf{g}_1(t, \tau) \times \langle \mathbf{S}(\tau) \rangle \right] \mathbf{g}_1^{<>/>}(\tau, t') + i \left[ \mathbf{g}_1^{<>/>}(t, \tau) \times \langle \mathbf{S}(\tau) \rangle \right] \mathbf{g}_1^{a}(\tau, t') d\tau,
\]

(28)

\[
\delta G_1^{<>/>}(t, t') = -J \int \left( \mathbf{g}_1(t, \tau) \cdot \langle \mathbf{S}(\tau) \rangle \right) g_0^{<>/>}(t, \tau) + g_0^{<>/>}(t, \tau) \cdot \langle \mathbf{S}(\tau) \rangle g_0^{a}(\tau, t')
\]

\[
+ i \left[ \mathbf{g}_1(t, \tau) \times \langle \mathbf{S}(\tau) \rangle \right] g_0^{<>/>}(\tau, t') + i \left[ \mathbf{g}_1^{<>/>}(t, \tau) \times \langle \mathbf{S}(\tau) \rangle \right] g_0^{a}(\tau, t')
\]

\[
+ i \left[ \mathbf{g}_1(t, \tau) \times \langle \mathbf{S}(\tau) \rangle \right] \times \left[ \mathbf{g}_1^{<>/>}(\tau, t') + i \left[ \mathbf{g}_1^{<>/>}(t, \tau) \times \langle \mathbf{S}(\tau) \rangle \right] \mathbf{g}_1^{a}(\tau, t') \right] d\tau.
\]

(29)

where we have considered the Keldysh contour.


2.5 Tunneling current

The tunneling current flowing between the electrodes represents the change of particles in the two contacts. We begin from the charge current in the left electrode, \( I_L^C(t) = -e \partial_t \left( \sum_{p,\sigma} n_{p\sigma} \right) = i \epsilon \sigma \partial_t \sum_p \mathcal{E}_p(t, t') \), which leads to the expression

\[
I_L^C(t) = \frac{-2e}{\hbar} \text{Im} \Gamma^L \int_{-\infty}^{t} \left( I_L^C(t) G^<(t', t) + I_L^C(t) G^>(t', t) \right) dt'
\]

where \( \Gamma^x = \Gamma_0^x \sigma^0 + \sigma \cdot \Gamma_S^x \) and

\[
I_L^C(t) = \frac{-4e}{\hbar} I m \int_{-\infty}^{t} \left( I_L^C(t) \Gamma_0^L G_0^L(t', t) + I_L^C(t) \Gamma_0^L G_0^L(t', t) \right) dt',
\]

\[
I_L^C(t) = \frac{-4e}{\hbar} I m \int_{-\infty}^{t} \left( I_L^C(t) \Gamma_0^L dt \right) + I_L^C(t) \Gamma_0^L G_0^L(t', t) \right) dt'.
\]

The spin current follows from \( I_L^S(t) = -e \partial_t \left( \sum_{p,\sigma,\sigma'} c_{p\sigma}^\dagger \sigma \cdot \Gamma_S^x \sigma' \right) c_{p\sigma'} \) which leads to the expression

\[
I_L^S(t) = \frac{-2e}{\hbar} \text{Im} \sigma \cdot \Gamma^L \int_{-\infty}^{t} \left( I_L^S(t) G^<(t', t) + I_L^S(t) G^>(t', t) \right) dt'
\]

where

\[
I_L^S(t) = \frac{-4e}{\hbar} I m \int_{-\infty}^{t} \left( I_L^S(t) \Gamma_0^L G_1^L(t', t) + I_L^S(t) \Gamma_0^L G_1^L(t', t) \right) dt',
\]

\[
I_L^S(t) = \frac{-4e}{\hbar} I m \int_{-\infty}^{t} \left( I_L^S(t) \Gamma_0^L G_0^L(t', t) + i \Gamma_S^L \times G_1^L(t', t) \right) + I_L^S(t) \left( \Gamma_0^L G_0^L(t', t) + i \Gamma_S^L \times G_1^L(t', t) \right) \right) dt'.
\]

3 Analysis

The aim of the project is to solve the time evolution of the system regarded in the theory section numerically. This is done by solving the ordinary differential equation in equation 9. To do this we need to first find an initial solution for a time \( t_0 \) and then find the dependence \( \mathbf{S}(t, \mathbf{S}) \) for each time step. This is done by solving the Greens function for the initial case and the dynamic case, regarded in the following subsections. The final product of the calculation is the tunneling currents which is derived from the Greens function for the initial and dynamic case.
3.1 Initial solution

First we solve the Greens functions for the system without any applied voltage and solve it in equilibrium. We regard the symmetric case where there is no \( \chi \) dependence and we write the tunneling parameters as

\[
\Gamma_S = \beta \Gamma_0 \quad \text{where} \quad \beta = 1-p.
\]

We do the same for the electron level of the quantum dot and write it as

\[
\varepsilon = \varepsilon_0, \quad \varepsilon_\perp = \frac{\varepsilon_0}{\varepsilon_0 + \varepsilon_\perp} (1+p) \quad \text{and} \quad \varepsilon_\parallel = \frac{\varepsilon_0}{\varepsilon_\perp} (1-p). \]

As we have no applied voltage we can simplify \( \Lambda_S \) and we write the zero Greens function as

\[
G_{0}(t', t) = \frac{1}{2} \int \mathcal{L}_{0}(\omega) f(\pm \omega) e^{-i \omega (t - t')} \frac{d \omega}{2 \pi}, \quad (36)
\]

where

\[
\mathcal{L}_{0}(\omega) = \frac{i}{2} \left( \frac{1}{\Gamma_0 \left( \Gamma_0^2 + (\omega - \varepsilon_\perp)^2 \right) + \Gamma_\parallel^2 + (\omega - \varepsilon_\parallel)^2} \right) + \frac{1}{\Gamma_S \left( \Gamma_0^2 + (\omega - \varepsilon_\perp)^2 \right) + \Gamma_\parallel^2 + (\omega - \varepsilon_\parallel)^2}, \quad (38)
\]

and

\[
\mathcal{L}_{1}(\omega) = \frac{i}{2} \left( \frac{1}{\Gamma_S \left( \Gamma_0^2 + (\omega - \varepsilon_\perp)^2 \right) + \Gamma_\parallel^2 + (\omega - \varepsilon_\parallel)^2} \right) + \frac{1}{\Gamma_0 \left( \Gamma_0^2 + (\omega - \varepsilon_\perp)^2 \right) + \Gamma_\parallel^2 + (\omega - \varepsilon_\parallel)^2}. \quad (39)
\]

From this we can derive the Greens function and its components, \( G_i(t', t) = G_{0}(t', t) \sigma^i + \sigma \cdot G_{1}(t', t) \). In order to do this we need to solve the equation for the spin. We solve equation 9 assuming a constant magnetic field in the \( z \)-direction, \( B = Bz \), and no interaction. This gives the spin components \( S_x = S_{xy} \sin(\omega_L t), S_y = S_{xy} \cos(\omega_L t) \) and \( S_z = S_z \) where \( S^2 = S_{xy}^2 + S_z^2 \) and \( \omega_L = g \mu_B |B| \). The components for the Greens function thus becomes

\[
G_{0i}(t', t) = \mp \int f(\pm \omega) e^{-i \omega (t - t')} \left( \mathcal{L}_{0}(\omega) + \frac{J}{2} \mathcal{S}_i \mathcal{C}_0(\omega) \right) \frac{d \omega}{2 \pi}, \quad (40)
\]

\[
G_{1i}(t', t) = \pm \frac{i}{2} J S_{xy} \int f(\pm \omega) e^{-i \omega (t - t')} \left( A(\omega) e^{i \omega_L t} - A^*(\omega) e^{-i \omega_L t'} + B(\omega) e^{-i \omega_L t} - B^*(\omega) e^{i \omega_L t'} \right) \frac{d \omega}{2 \pi}, \quad (41)
\]

\[
G_{1i}(t', t) = \mp \frac{i}{2} J S_{xy} \int f(\pm \omega) e^{-i \omega (t - t')} \left( A(\omega) e^{i \omega_L t} + A^*(\omega) e^{-i \omega_L t'} - B(\omega) e^{-i \omega_L t} - B^*(\omega) e^{i \omega_L t'} \right) \frac{d \omega}{2 \pi}, \quad (42)
\]

\[
G_{1i}(t', t) = \pm \frac{i}{2} J S_{xy} \int f(\pm \omega) e^{-i \omega (t - t')} \left( A(\omega) e^{i \omega_L t} + A^*(\omega) e^{-i \omega_L t'} - B(\omega) e^{-i \omega_L t} - B^*(\omega) e^{i \omega_L t'} \right) \frac{d \omega}{2 \pi}, \quad (43)
\]

where
\begin{equation}
A(\omega) = \frac{\Lambda_1(\omega) - \Lambda_0(\omega)}{\varepsilon_\uparrow - \omega + \omega_L - i\Gamma_\uparrow},
\end{equation}
\begin{equation}
B(\omega) = \frac{\Lambda_1(\omega) + \Lambda_0(\omega)}{\varepsilon_\downarrow - \omega - \omega_L - i\Gamma_\downarrow},
\end{equation}
\begin{equation}
C_0(\omega) = 2 \left( \Lambda_0(\omega) \left( \frac{\omega - \varepsilon_\uparrow}{\Gamma_\uparrow^2 + (\omega - \varepsilon_\uparrow)^2} - \frac{\omega - \varepsilon_\downarrow}{\Gamma_\downarrow^2 + (\omega - \varepsilon_\downarrow)^2} \right) + \Lambda_1(\omega) \left( \frac{\omega - \varepsilon_\uparrow}{\Gamma_\uparrow^2 + (\omega - \varepsilon_\uparrow)^2} + \frac{\omega - \varepsilon_\downarrow}{\Gamma_\downarrow^2 + (\omega - \varepsilon_\downarrow)^2} \right) \right),
\end{equation}
\begin{equation}
C_1(\omega) = 2 \left( \Lambda_0(\omega) + \Lambda_1(\omega) \right) \left( \frac{\omega - \varepsilon_\uparrow}{\Gamma_\uparrow^2 + (\omega - \varepsilon_\uparrow)^2} + \frac{\omega - \varepsilon_\downarrow}{\Gamma_\downarrow^2 + (\omega - \varepsilon_\downarrow)^2} \right).
\end{equation}

### 3.2 The dynamic Greens function

At time zero we apply a constant voltage \( V \) between the two contacts and turn on the interaction. When extending our analysis from a constant spin to a changing discrete spin we need to make use of an approximation. It is that for sufficiently small time steps the expectation value of the spin in the integral in equation 27 can be assumed to be a constant value, which is the spin calculated from the previous time step, \( \langle S(t) \rangle = S_{k-1} \). Then equation 27 simplifies to integrals over the zero Greens functions, as for the initial solution.

When performing the integral over time, as when calculating the current, we need to regard the correct time ordering. In order to do so we need to divide equation 18 into three parts, no applied voltage and where \( t \) and \( t' \) is less than \( t_0 \), with applied voltage and where \( t' \) is less than \( t_0 \) and then one part with applied voltage and where both \( t \) and \( t' \) is greater than \( t_0 \). Then equation 18 becomes

\begin{equation}
I^{<~/>}(t, t') = \begin{cases}
\int f(\pm\omega)e^{-i\omega(t-t')} \frac{d\omega}{2\pi} & t' < t < t_0 \\
\int f(\pm\omega)e^{-i\omega(t-t')-ieVt} \frac{d\omega}{2\pi} & t' < t_0 < t \\
\int f(\pm\omega)e^{-i(\omega+eV)t} \frac{d\omega}{2\pi} & t_0 < t < t'
\end{cases}
\end{equation}

The first part is already derived as the initial solution while we need to regard the second and third part when we extend the analysis for the dynamic case. We simplify the derivation assuming the symmetric case \( V = V_L = V_R \). For the case where \( t' \) is less than \( t_0 \) we get the zero Green functions

\begin{equation}
g^{<~/>}_0(t, t') = \mp \int \alpha_0(\omega)f(\pm\omega)e^{-i\omega(t-t')-ieVt} \frac{d\omega}{2\pi},
\end{equation}
\begin{equation}
g^{<~/>}_1(t, t') = \mp \int \alpha_1(\omega)f(\pm\omega)e^{-i\omega(t-t')-ieVt} \frac{d\omega}{2\pi}
\end{equation}

where
\[
\alpha_0(\omega) = -\frac{i}{4} \left( \Gamma_0 \left( \frac{1}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} + \frac{1}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} \right) \left( \frac{1}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} + \frac{1}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right) 
  + \Gamma_S \left( \frac{1}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} + \frac{1}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} \right) \left( \frac{1}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} + \frac{1}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right) \right), \tag{51}
\]

\[
\alpha_1(\omega) = -\frac{i}{4} \left( \Gamma_S \left( \frac{1}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} + \frac{1}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} \right) \left( \frac{1}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} + \frac{1}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right) 
  + \Gamma_0 \left( \frac{1}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} + \frac{1}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} \right) \left( \frac{1}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} + \frac{1}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right) \right). \tag{52}
\]

When we go to the case where \( t' \) is greater than \( t_0 \) we get the zero Green functions

\[
g_{0}^{<>/}(t, t') = \mp \int \beta_0(\omega) f(\pm \omega) e^{-i(\omega + eV)(t-t')} \frac{d\omega}{2\pi}, \tag{53}
\]

\[
g_{1}^{<>/}(t, t') = \mp \int \beta_1(\omega) f(\pm \omega) e^{-i(\omega + eV)(t-t')} \frac{d\omega}{2\pi}, \tag{54}
\]

where

\[
\beta_0(\omega) = -\frac{i}{2} \left( \Gamma_0 \left( \frac{1}{\Gamma_\uparrow^2 + (\omega + eV - \epsilon_\uparrow)^2} + \frac{1}{\Gamma_\downarrow^2 + (\omega + eV - \epsilon_\downarrow)^2} \right) 
  + \Gamma_S \left( \frac{1}{\Gamma_\uparrow^2 + (\omega + eV - \epsilon_\uparrow)^2} - \frac{1}{\Gamma_\downarrow^2 + (\omega + eV - \epsilon_\downarrow)^2} \right) \right), \tag{55}
\]

\[
\beta_1(\omega) = -\frac{i}{2} \left( \Gamma_S \left( \frac{1}{\Gamma_\uparrow^2 + (\omega + eV - \epsilon_\uparrow)^2} + \frac{1}{\Gamma_\downarrow^2 + (\omega + eV - \epsilon_\downarrow)^2} \right) 
  + \Gamma_0 \left( \frac{1}{\Gamma_\uparrow^2 + (\omega + eV - \epsilon_\uparrow)^2} - \frac{1}{\Gamma_\downarrow^2 + (\omega + eV - \epsilon_\downarrow)^2} \right) \right). \tag{56}
\]

This in turn will give the total Green function. For the case where \( t' \) is less than \( t_0 \) we get
\[
G_0^{<\!/>(t,t')} = \mp \int f(\pm \omega)e^{-i(\omega(t-t') - eVt)} \left( \alpha_0(\omega) + S_z(t) \frac{J}{2} D_0(\omega) \right) \frac{d\omega}{2\pi},
\]
\[
G_{1x}^{<\!/>(t,t')} = \mp J \int f(\pm \omega)e^{-i(\omega(t-t') - eVt)} D_x(\omega,t) \frac{d\omega}{2\pi},
\]
\[
G_{1y}^{<\!/>(t,t')} = \mp J \int f(\pm \omega)e^{-i(\omega(t-t') - eVt)} D_y(\omega,t) \frac{d\omega}{2\pi},
\]
\[
G_{1z}^{<\!/>(t,t')} = \pm \int f(\pm \omega)e^{-i(\omega(t-t') - eVt)} D_z(\omega,t) \frac{d\omega}{2\pi},
\]

where

\[
D_0(\omega) = \alpha_0 \left( \frac{1}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} - \frac{1}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} + \frac{1}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} - \frac{1}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right) + \alpha_1 \left( \frac{1}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} + \frac{1}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} + \frac{1}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} + \frac{1}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right),
\]

\[
D_x(\omega,t) = \frac{1}{2} \left( \frac{(\alpha_0 - \alpha_1)(S_x(t) - iS_y(t))}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} + \frac{(\alpha_0 + \alpha_1)(S_x(t) + iS_y(t))}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} + \frac{(\alpha_0 - \alpha_1)(S_x(t) + iS_y(t))}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} + \frac{(\alpha_0 + \alpha_1)(S_x(t) - iS_y(t))}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right),
\]

\[
D_y(\omega,t) = \frac{1}{2} \left( \frac{(\alpha_0 - \alpha_1)(S_y(t) - iS_x(t))}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} + \frac{(\alpha_0 + \alpha_1)(S_y(t) + iS_x(t))}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} + \frac{(\alpha_0 - \alpha_1)(S_y(t) + iS_x(t))}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} + \frac{(\alpha_0 + \alpha_1)(S_y(t) - iS_x(t))}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right),
\]

\[
D_z(\omega,t) = \alpha_1 + \frac{J}{2} S_z(t) \left( \frac{1}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} - \frac{1}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} + \frac{1}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} - \frac{1}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right) + \alpha_1 \left( \frac{1}{\omega + eV - \epsilon_\uparrow + i\Gamma_\uparrow} + \frac{1}{\omega + eV - \epsilon_\downarrow + i\Gamma_\downarrow} + \frac{1}{\omega - \epsilon_\uparrow - i\Gamma_\uparrow} + \frac{1}{\omega - \epsilon_\downarrow - i\Gamma_\downarrow} \right).
\]

For the case where \( t' \) is greater than \( t_0 \) we get

\[
G_0^{<\!/>(t,t')} = \mp \int f(\pm \omega)e^{-i(\omega + eV)(t-t')} \left( \beta_0(\omega) + S_z(t) \frac{J}{2} E_0(\omega) \right) \frac{d\omega}{2\pi},
\]

\[
G_{1x}^{<\!/>(t,t')} = \mp J \int f(\pm \omega)e^{-i(\omega + eV)(t-t')} E_x(\omega,t) \frac{d\omega}{2\pi},
\]

\[
G_{1y}^{<\!/>(t,t')} = \mp J \int f(\pm \omega)e^{-i(\omega + eV)(t-t')} E_y(\omega,t) \frac{d\omega}{2\pi},
\]
When deriving the equations for the tunneling current, we need to divide our derivation into first taking the case when \( t < t_0 \), with no applied voltage, and then derive the current for \( t > t_0 \), with applied voltage. For the case when \( t < t_0 \), when we have no applied current, we get

\[
I_0^C(t) = -\frac{4e}{\hbar} \Gamma_0 \text{Im} \int \frac{i(f(\omega) - f(\omega')) (\Lambda_0(\omega') + \frac{i}{2} S_z(t) C_0(\omega'))}{\omega' - \omega + i\delta} \frac{d\omega \, d\omega'}{2\pi^2},  
\]

\[
I_1^C(t) = -\frac{4e}{\hbar} \Gamma_S \text{Im} \int \frac{i(f(\omega) - f(\omega')) C_z(\omega', t)}{\omega' - \omega + i\delta} \frac{d\omega \, d\omega'}{2\pi^2},  
\]

\[
I_{0x}^S(t) = -\frac{4e}{\hbar} J \Gamma_0 \text{Im} \int \frac{i(f(\omega) - f(\omega')) C_x(\omega', t)}{\omega' - \omega + i\delta} \frac{d\omega \, d\omega'}{2\pi^2},  
\]

\[
I_{0y}^S(t) = -\frac{4e}{\hbar} J \Gamma_0 \text{Im} \int \frac{i(f(\omega) - f(\omega')) C_y(\omega', t)}{\omega' - \omega + i\delta} \frac{d\omega \, d\omega'}{2\pi^2}.  
\]
\[ I_0^C(t) = -\frac{4e}{\hbar} \Gamma_0 \text{Im} \int \frac{i(f(\omega) - f(\omega')) C_z(\omega', t) \, d\omega \, d\omega'}{\omega' - \omega + i\delta}, \quad (78) \]

\[ I_1^S(t) = -\frac{4e}{\hbar} \Gamma_S \text{Im} \int \frac{i(f(\omega) - f(\omega')) C_y(\omega', t) \, d\omega \, d\omega'}{\omega' - \omega + i\delta}, \quad (79) \]

\[ I_1^S(t) = \frac{4e}{\hbar} \Gamma_S \text{Im} \int \frac{i(f(\omega) - f(\omega')) C_z(\omega', t) \, d\omega \, d\omega'}{\omega' - \omega + i\delta}, \quad (80) \]

\[ I_1^S(t) = -\frac{4e}{\hbar} \Gamma_S \text{Im} \int \frac{i(f(\omega) - f(\omega')) C_z(\omega', t) \, d\omega \, d\omega'}{\omega' - \omega + i\delta}, \quad (81) \]

where \( \delta \) is an infinitesimal constant and

\[ C_x(\omega, t) = (\Lambda_0(\omega) - \Lambda_1(\omega)) \frac{S_x(t)(\omega - \xi_t) + S_y(t)\Gamma_1}{\Gamma_1 + (\omega - \xi_t)^2} + (\Lambda_0(\omega) + \Lambda_1(\omega)) \frac{S_x(t)(\omega - \xi_t) - S_y(t)\Gamma_1}{\Gamma_1 + (\omega - \xi_t)^2}, \quad (82) \]

\[ C_y(\omega, t) = (\Lambda_0(\omega) - \Lambda_1(\omega)) \frac{S_y(t)(\omega - \xi_t) + S_z(t)\Gamma_1}{\Gamma_1 + (\omega - \xi_t)^2} + (\Lambda_0(\omega) + \Lambda_1(\omega)) \frac{S_y(t)(\omega - \xi_t) - S_z(t)\Gamma_1}{\Gamma_1 + (\omega - \xi_t)^2}, \quad (83) \]

\[ C_z(\omega, t) = \Lambda_1(\omega) + JS_z(t) \left( (\Lambda_0(\omega) - \Lambda_1(\omega)) \frac{\omega - \xi_t}{\Gamma_1^2 + (\omega - \xi_t)^2} + (\Lambda_0(\omega) + \Lambda_1(\omega)) \frac{\omega - \xi_t}{\Gamma_1^2 + (\omega - \xi_t)^2} \right). \quad (84) \]

When calculating the current for the case \( t > t_0 \), with an applied constant voltage, we need to have in mind the cases where \( t' < t_0 \) and \( t' > t_0 \) which yields different Green functions. By doing so we get the currents for \( t > t_0 \)

\[ I_0^C(t) = -\frac{4e}{\hbar} \Gamma_0 \text{Im} \int i(f(\omega) - f(\omega')) \left[ \frac{\beta_0(\omega') + \frac{1}{2} S_z(t) E_0(\omega')}{\omega' - \omega + i\delta} \right. \]

\[ + \left. \left( \frac{\alpha_0(\omega') + \frac{1}{2} S_z(t) D_0(\omega')}{\omega' - \omega + eV + i\delta} e^{-i\omega V(t-t_0)} - \frac{\beta_0(\omega') + \frac{1}{2} S_z(t) E_0(\omega')}{\omega' - \omega + i\delta} \right) e^{-i(\omega - \omega')(t-t_0)} \right] \frac{d\omega \, d\omega'}{2\pi \, 2\pi}, \quad (85) \]

\[ I_1^C(t) = -\frac{4e}{\hbar} \Gamma_S \text{Im} \int i(f(\omega) - f(\omega')) \left[ \frac{E_z(\omega', t)}{\omega' - \omega + i\delta} \right. \]

\[ + \left. \left( \frac{D_z(\omega', t)}{\omega' - \omega + eV + i\delta} e^{-i\omega V(t-t_0)} - \frac{E_z(\omega', t)}{\omega' - \omega + i\delta} \right) e^{-i(\omega - \omega')(t-t_0)} \right] \frac{d\omega \, d\omega'}{2\pi \, 2\pi}, \quad (86) \]

\[ I_0^S(t) = -\frac{4e}{\hbar} \Gamma_0 \text{Im} \int i(f(\omega) - f(\omega')) \left[ \frac{E_x(\omega', t)}{\omega' - \omega + i\delta} \right. \]

\[ + \left. \left( \frac{D_x(\omega', t)}{\omega' - \omega + eV + i\delta} e^{-i\omega V(t-t_0)} - \frac{E_x(\omega', t)}{\omega' - \omega + i\delta} \right) e^{-i(\omega - \omega')(t-t_0)} \right] \frac{d\omega \, d\omega'}{2\pi \, 2\pi}, \quad (87) \]
The main problem to solve numerically is the ordinary differential equation (ODE) in equation 9 and the integrals over the energies \( \omega \) and \( \omega' \) for each time step. The solution need to converge and solved in a reasonable time frame. The calculations were done in MATLAB. We divide our analysis into two parts, the ODE and the integrals.

4 Method

The problem at hand is to numerically solve the ordinary differential equation (ODE) in equation 9 and the integrals over the energies \( \omega \) and \( \omega' \) for each time step. The solution need to converge and solved in a reasonable time frame. The calculations were done in MATLAB. We divide our analysis into two parts, the ODE and the integrals.

4.1 Ordinary differential equation

The main problem to solve numerically is the ordinary differential equation in equation 9. We solve over time, starting from our initial solution in section 2.6. The basic problem to solve is

\[
\frac{dS}{dt} = f(t, S), \ t_0 \leq t
\]
with the initial condition \( S(t_0) \) given by the Green functions in section 2.6. There are several methods to use for solving the ODE and the most straightforward method is Euler's method. It is defined by

\[
S_{k+1} = S_k + hf(t_k, S_k), \quad k = 0, 1, ..., N - 1,
\]

(95)

where \( h \) is the step size and \( k \) is the step indices. This gives a global discretization error of \( O(h) \). This is a rather slow method as the step size needs to be small in order for it to converge. For improving the rate of convergence we look at higher order methods as the second order Runge-Kutta method. It is called Heun's method and defined as

\[
S_{k+1} = S_k + \frac{h}{2} [f(t_k, S_k) + f(t_{k+1}, S_k + hf(t_k, S_k))]
\]

(96)

which is an average of \( f \) at two points forward in time. This gives a global discretization error of \( O(h^2) \) and yields faster convergence than Euler's method [11]. We could go to even higher order methods, but it is not needed as the step size will be to big to show all the features in the graphs.

### 4.2 Integrals

The built-in function trapz in MATLAB was used for solving the integrals over the energies \( \omega \) and \( \omega' \) for each time step. The function is based on trapezoidal numerical integration where the integration value is the one over the trapezoid

\[
I(f) = \frac{(b - a)}{2} [f(a) - f(b)],
\]

where \( f \) is the function and \( a \) and \( b \) is the integration boundaries for each step [11]. The built-in function yielded a much faster result than coding the same method with a for-loop.

### 4.3 Resources

The simulations were done in MATLAB and on the departments UPPMAX resources. In order to be able to perform the simulations more efficient on the computer cluster the program needed to be run on parallel processor cores. This was done by using the built-in function parfor in MATLAB. The parfor-function runs the for-loops in parallel on the designated CPUs. This yielded several times faster results than running the simulation on a single core and a converging solution could be found within hours of computations.

### 5 Results

The simulations gave several interesting results when evaluating different parameters. The units used for energies are eV. Time and current are in arbitrary units (a.u.). The parameter of interest are the parameters that can be controlled when performing an experiment. The parameters that can be externally controlled in an experiment is the bias voltage, eV, and the energy level of the quantum dot, \( \varepsilon_0 \). When designing the system the tunneling constant \( \Gamma_0 \) and the coupling strength \( J \) between the electrons and spin may be of interest. Also the polarization factor for the tunneling constant, \( p \), and for the energy level of the quantum dot, \( p' \), are of interest. All these parameters have been regarded in this work and presented in this section. For the parameters a set of standard values was used, where we set \( eV = 1 \) eV, \( \varepsilon_0 = 0.5 \) eV, \( p' = 0.5 \), \( \Gamma_0 = 1 \) eV, \( p = 0.5 \) and \( J = 0.1 \). The spin is set to have the initial value of \( S_{xy} = \sin(45^\circ) \) and \( S_z = \cos(45^\circ) \). For the code, see Appendix A.1.
First we regard the case with the standard parameters. For a maximum time of 15 time units we get the evolution of the xyz-components of the spin in figure 2. We see that the spin start to change when we turn on the interactions and apply a bias voltage. This is due to the damping that the current performs on the spin. For the z-component we see that it takes some time for the line to become straight. This comes from the dynamics of the system, as we integrate over the previous spins in equation 9. Note that the step functions in the interaction parameters makes the integral in the spin equation of motion to become an integral over all previous spins.

The resulting charge and spin currents are shown in figure 3. We see a jump in the currents at time $t_0$ when the bias voltage is turned on and that they start to oscillate. This follows from the second term in the equations for the current, equation 85-93, which creates a step function at $t = t_0$. As $eV = 1$ we see that the frequency of the charge current and the spin current in the z-direction follows the frequency of the spin. The oscillations in the currents are induced currents from the rotating spin, making it oscillate but without a net current in either direction.

Extending the time frame to a maximum time of 200 time units we get the spin evolution in figure 4 and the charge and spin currents in figure 5. We see that the spin goes to a constant value and aligns with the external magnetic field in the z-direction, as could be expected when having an outer magnetic field in the same direction. The spin currents start to decrease in the x- and y-directions and get an overtone, a behavior with a lower frequency. The spin currents decrease because of that the spin aligns in the z-direction, making the $S_x$ and $S_y$ component decrease. This can be seen in the equations for the spincurrents which is showed in equation 70 and 71. The spin currents gets an overtone and the frequency of the overtone increases drastically for higher voltages, see 9. We also see that the charge current goes slightly towards to oscillate around zero.

If we increase the tunneling parameter $\Gamma_0$ to 10 eV we get the results in figure 6 and 7. We get that the
Figure 3: The charge current $I_C$ and the xyz-components of the spin current $I_s$ for the initial case, 15 time units.

Figure 4: The xyz-components of the spin for the initial case, 200 time units.
spin instead go in negative z-direction. The disturbance at $t = t_0$ is also not as apparent as well. This could be because of the faster process when more electrons tunnel through the quantum dot, as we divide by $\Gamma$ in for example equation 65 and 69. The charge current increases significantly and spin current in z-direction more than doubles, which can be expected as more electrons tunnel through the dot. The spin currents in x- and y-directions decreases significantly by the same reason. In the y-direction the currents also become negative.

We get the results shown in figure 8 and 9 when increasing the voltage, $eV$, to $2 \, eV$. Here we see an overtone in the currents, with an frequency much higher than in the case where $eV = 1$. The spin gets less damped but changes more abruptly, as we do not see as big bump at $t_0$. The charge current becomes positive and we also note that the frequency in the currents doubles. This is quite interesting that we first have a negative current for low applied voltages, which then turns positive when increasing the bias voltage. The fact that we get a higher frequency comes from the exponential factor in for example equation 85. The overtone we see here, as well as the overtone for the standard parameters, is hard to see where it comes from in the equations and what it depends on. Presumably it depends on the bias voltage as the frequency increases drastically when doubling it. This is an interesting phenomena that can be investigated further.

When setting both the bias voltage and the energy level of the quantum dot to zero we get the results in figure 10 and 11. We see that we get a small bump in the charge current (note the scale on the y-axis) and in the z-component of the spin current that is caused by turning on the interaction. Interesting to note is that the bump is negative. Here we also see that we have an oscillating spin current in the x- and y-direction even without any feedback, which behaviour continue without any applied bias voltage. The spin z-component decreases and we see a small bump because of the turning on of the interactions.

We can choose to only allow spin up or spin down electrons through the quantum dot. To only allow spin up electrons we set the polarization factor $p = 0$. This could for example represent having two ferromagnetic
Figure 6: The components of the spin for $\Gamma_0 = 10$ eV.

Figure 7: The charge and spin current for $\Gamma_0 = 10$ eV.
Figure 8: Spin evolution with a bias voltage of 2 eV applied at $t_0$.

Figure 9: Charge and spin currents when bias voltage of 2 eV is applied at $t_0$. 
Figure 10: Spin evolution when there is no applied bias voltage.

Figure 11: Charge and spin currents with no applied bias voltage.
Figure 12: The spin independent and dependent currents for only spin up electrons.

Figure 13: Spin evolution for the double coupling strength J between the electrons and the local spin moment.
metals as contacts. We then get the spin independent and dependent currents that can be seen in figure 12. We see that we get no spin dependent currents in this case as expected as we have only have spin up electrons.

When doubling the coupling strength between electrons and local spin moment we get the results in figure 13 and 14. We see that the spin changes more rapidly as well as the amplitude of the spin currents in the x- and y-direction, as expected. We also see that the spin currents has higher amplitude as they have a stronger coupling to the local spin moment.

6 Discussion

Regarding all simulations we can make some conclusions about the behaviour of the system. First we see that the current going through the quantum dot effect the evolution of the local spin moment and that the local spin moment creates oscillations in the current. We see that the frequency of the charge and spin current depends on the bias voltage. We also see a connection between the dynamics of the system, how rapidly things evolve, and the coupling constant between the quantum dot and the local spin moment. This coupling constant also effect the amplitude of the spin currents. We see as well a connection between the currents and the tunneling constant as it increases and decreases the amplitude of the currents.

There are some interesting phenomena that rises new questions. Why do we get an overtone in the x- and y-components of the spin currents and what does it depend on? Why is the current negative for small bias voltages? Is it because of that the numerical approximation causes the bump in the case when the bias voltage is zero? This questions leaves it open that there are still a lot of interesting phenomena that can be further investigated in order to better understand the system.
For applications it could be of interest to use the current to control the local spin moment of the molecule. We see from our results that it could be done by applying a bias voltage. For the initial spin that was studied in this work the spin will go into the negative direction when there is no applied bias voltage. For positive bias voltage it will increase. For higher voltages the process is slower. We also see that the evolution of the spin depends on the coupling constant, such that for higher coupling constants the spin changes the direction it will evolve. A more throughout analysis of how to control the local spin moment of the molecule by the currents could be performed in order to better understand it. Here it could be interesting to see how the spin polarization of the current will effect the evolution of the spin.

In the theory part some approximations and simplifications were done. In order to extend this analysis we can add properties that were not considered. One of those is to separate the two metal contacts, in this analysis they were considered to have the same properties. In this case we could for example study cases where one contact is ferromagnetic and the other one not. Another case that we could take into consideration is to apply a sinusoidal bias voltage at \( t_0 \) and see the response to such a function.

7 Conclusion

In this work the non-equilibrium dynamics of a local spin moment coupled to a quantum dot have been considered. Starting from many body theory, equations have been derived for the local spin moment and the currents going through the quantum dot. In order to numerically simulate the equations, different numerical methods have been considered such that it could be done efficiently with small errors. The results showed qualitatively the effect of changing different parameters on the local spin moment and the currents. The results showed that the currents oscillate because of the rotation of the local spin moment and that the currents effect the evolution of the local spin moment. Here we see that the local spin moment of a molecule can be controlled using currents. For future work a more complex system can be considered, where more properties could be added to the system, as well as different bias voltages. Some interesting phenomena appear that can be investigated further. It would also be interesting to compare the simulations to experimental results.
References


A Appendix

A.1 Code

Listing 1: main.m

```matlab
% This program will loop a numerical solution of the current in a system
% of a quantum dot, connected to two leads and interacting with a magnetic spin

matlabpool open

clear

tic

% initial values
kB = 8.6173324*10^-5; % Boltzmann constant, in eV*K^-1
T=1; % temperature in K
beta=1/(kB*T); % beta value
e=1.602176665*10^-19; % elementary charge
hbar=1; % normalized Planck's constant
hbar1=6.626197323*10^-27; % Planck's constant in eV*S
p=0.5; % Polarization of gamma_up and gamma_down
```
\begin{verbatim}
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17 gama0 = 1;  \% Gamma 0 in eV
18 gammaS = p * gama0;  
19 gamma_up = gama0 / 2 * (1 + p);  
20 gamma_down = gama0 / 2 * (1 - p);  
21 epsilon0 = 0.5;  
22 p2 = 0.5;  
23 epsilon_up = epsilon0 / 2 * (1 + p2);  
24 epsilon_down = epsilon0 / 2 * (1 - p2);  
25 g = 2;  \% g-factor
26 myB = 1;  \% Bohr magneton
27 B = 1;  \% Magnetic field
28 J = 0.1;  \% Coupling strength
29 Sz0 = 0.70710678118664752440084436210485;  \% Initial Sz value
30 Sxy = 0.70710678118664752440084436210485;  \% Initial Sxy value
31 Wl-g=4yB*B;  \% Frequency
32 delta = 10^-6;  \% Delta in current equations
33 eV = 1;  \% Voltage after t0
34 t0 = 0;
35 tmin = -5;
36 tmax = 15;
37 timestep = 0.025;  \% Time steps size
38 timestep2 = 0.025;
39 tback = 200;  \% How many steps back for -inf time integration
40 t = [t0 : timestep2 : tmax];
41 t0_length = length(t);
42 tprime = [tmin : timestep : t0];
43 tprimeless = zeros(1, t0_length + length(t));
44 timestep = 0.05;  \% Energy steps size
45 w1 = [-5 : step : 5];
46 w2 = [-5 : step : 5];
47 \% Get omega functions (constants depending on omega)
48 [lambda01, lambda11] = lambda(w1, hbar, gamma0, gammaS, gamma_up, ...
49   gamma_down, epsilon_up, epsilon_down);
50 [a11, b11, b21, c01, c11, d01, e01] = omegafunct(w1, hbar, ...  
51   w, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, eV);
52 [lambda02, lambda12] = lambda(w2, hbar, gamma0, gammaS, gamma_up, ...
53   gamma_down, epsilon_up, epsilon_down);
54 [a12, b12, b22, c02, c12, d02, e02] = omegafunct(w2, hbar, ...  
55   w, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, eV);
56 \% Fermi functions
57 fermi1 = 1. / (1+exp(beta*w1));
58 fermi2 = 1. / (1+exp(beta*w2));
59 \% Initial Solution
60 \% Calculating the initial solution
61 initialsolution
62 oldJ = [jH; jIX; jIY; jIZ; jDMX; jDMY; jDMZ];
63 \% Solving the spin equation of motion
64 \% Loop from t0 to t with numerically solving the system of equations
65 for j = 2:length(t)
66   tprime = [tprime, t(j)];
\end{verbatim}
if(t(j) == floor(t(j)))
    timestep = t(j);
    timeused = toc;
    disp(['Timestep: ' num2str(timestep)])
    disp(['Timeused: ' num2str(timeused)])
end

Sz(j) = Sz(j-1) + timestep * real(dSz);
Sy(j) = Sy(j-1) + timestep * real(dSy);
Sz(j) = Sz(j-1) + timestep * real(dSz);

% New Sz at t
Sz1 = Sz(j);
Sy1 = Sy(j);
Sz1 = Sz(j);
SxT = [SxT, Sz1];
SyT = [SyT, Sy1];
SxT = [SxT, Sz1];

% Calculate S(S)
[dSx1, dSy1, dSz1, oldJ, tprimeless, tprime, t0, tback, Sx1, Sy1, Sz1, beta, J, gamma0, 
gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, fermi, 
fermi2, lambda01, lambda02, c01, c02, d01, d02, e01, e02, SxT, 
SyT, SxT, g, myB, B, oldJ, eV);

% Calculate dS(S+h*dS(S))
Sx2 = Sx1 + timestep * dSx1;
Sy2 = Sy1 + timestep * dSy1;
Sz2 = Sz1 + timestep * dSz1;
SxT2 = [SxT, Sx2];
SyT2 = [SyT, Sy2];
SxT2 = [SxT, Sz2];
t2 = t(j) + timestep;

% The total dS
[dSx2, dSy2, dSz2, oldJ2, tprimeless, 
tprime, t0, tprime, Sx2, Sy2, Sz2, beta, J, gamma0, 
gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, fermi, 
fermi2, lambda01, lambda02, c01, c02, d01, d02, e01, e02, SxT2, 
SyT2, SxT2, g, myB, B, oldJ, eV);

% The total current
current = toc;

save simulationX.mat
\[ G_{1 z \text{ great}} = (1 - \text{fermi}_1) \cdot \frac{1}{2 \pi} \cdot \exp \left( -i \cdot w_1 \cdot (t_{\text{prime}}(i) - t_0) \cdot \frac{\hbar}{\omega_L} \right) \cdot (\lambda_{11} + J/2 \cdot c_{11}) \]

\[ G_{1 z \text{ less}} = -\text{fermi}_1 \cdot \frac{1}{2 \pi} \cdot \exp \left( -i \cdot w_1 \cdot (t_{\text{prime}}(i) - t_0) \cdot \frac{\hbar}{\omega_L} \right) \cdot (\lambda_{11} + J/2 \cdot c_{11}) \]

\[ G_{1 y \text{ great}} = J/2 \cdot S_{xy} \cdot (1 - \text{fermi}_2) \cdot \frac{1}{2 \pi} \cdot \exp \left( -i \cdot w_2 \cdot (t_0 - t_{\text{prime}}(i)) \cdot \frac{\hbar}{\omega_L} \right) \cdot (\lambda_{12} + J/2 \cdot c_{12}) \]

\[ G_{1 y \text{ less}} = -J/2 \cdot S_{xy} \cdot \text{fermi}_2 \cdot \frac{1}{2 \pi} \cdot \exp \left( -i \cdot w_2 \cdot (t_0 - t_{\text{prime}}(i)) \cdot \frac{\hbar}{\omega_L} \right) \cdot (\lambda_{12} + J/2 \cdot c_{12}) \]

\[ G_{0 \text{ great}} = (1 - \text{fermi}_2) \cdot \frac{1}{2 \pi} \cdot \exp \left( -i \cdot w_2 \cdot (t_0 - t_{\text{prime}}(i)) \cdot \frac{\hbar}{\omega_L} \right) \cdot (\lambda_{02} + S_{z0} \cdot J/2 \cdot c_{02}) \]

\[ G_{0 \text{ less}} = -\text{fermi}_2 \cdot \frac{1}{2 \pi} \cdot \exp \left( -i \cdot w_2 \cdot (t_0 - t_{\text{prime}}(i)) \cdot \frac{\hbar}{\omega_L} \right) \cdot (\lambda_{02} + S_{z0} \cdot J/2 \cdot c_{02}) \]
% Interaction parameters

\[ \begin{align*}
\text{d}j_H &= t \cdot (G_0 \text{l}ess^1 \cdot \text{G}1 \text{less}^2 \cdot \text{G}1 \text{great}^2 \cdot \text{G}1 \text{less}^1 \cdot \text{G}1 \text{great}^1 \cdot \text{G}1 \text{great}^2 \cdot \text{G}1 \text{less}^2) \\
\text{d}j_{Ix} &= 2 \cdot t \cdot (G_1 \text{less}^1 \cdot \text{G}1 \text{great}^2 - \text{G}1 \text{great}^1 \cdot \text{G}1 \text{less}^2) \\
\text{d}j_{Iy} &= 2 \cdot t \cdot (G_1 \text{less}^1 \cdot \text{G}1 \text{great}^2 - \text{G}1 \text{great}^1 \cdot \text{G}1 \text{less}^2) \\
\text{d}j_{Iz} &= 2 \cdot t \cdot (G_1 \text{less}^1 \cdot \text{G}1 \text{great}^2 - \text{G}1 \text{great}^1 \cdot \text{G}1 \text{less}^2) \\
\text{d}j_{DMx} &= -J^2 \cdot (G_0 \text{l}ess^1 \cdot \text{G}1 \text{great}^2 - G_0 \text{great}^1 \cdot \text{G}1 \text{less}^2 - \text{G}1 \text{less}^1 \cdot G_0 \text{great}^2 + \text{G}1 \text{great}^1 \cdot G_0 \text{l}ess^2) \\
\text{d}j_{DMy} &= -J^2 \cdot (G_0 \text{l}ess^1 \cdot \text{G}1 \text{great}^2 - G_0 \text{great}^1 \cdot \text{G}1 \text{less}^2 - \text{G}1 \text{less}^1 \cdot G_0 \text{great}^2 + \text{G}1 \text{great}^1 \cdot G_0 \text{l}ess^2) \\
\text{d}j_{DMz} &= -J^2 \cdot (G_0 \text{l}ess^1 \cdot \text{G}1 \text{great}^2 - G_0 \text{great}^1 \cdot \text{G}1 \text{less}^2 - \text{G}1 \text{less}^1 \cdot G_0 \text{great}^2 + \text{G}1 \text{great}^1 \cdot G_0 \text{l}ess^2) \\
\end{align*} \]

\[ j_H(i) = \text{trapz}(w_2, \text{trapz}(w_1, \text{d}j_H)) \]
\[ j_{Ix}(i) = \text{trapz}(w_2, \text{trapz}(w_1, \text{d}j_{Ix})) \]
\[ j_{Iy}(i) = \text{trapz}(w_2, \text{trapz}(w_1, \text{d}j_{Iy})) \]
\[ j_{Iz}(i) = \text{trapz}(w_2, \text{trapz}(w_1, \text{d}j_{Iz})) \]
\[ j_{DMx}(i) = \text{trapz}(w_2, \text{trapz}(w_1, \text{d}j_{DMx})) \]
\[ j_{DMy}(i) = \text{trapz}(w_2, \text{trapz}(w_1, \text{d}j_{DMy})) \]
\[ j_{DMz}(i) = \text{trapz}(w_2, \text{trapz}(w_1, \text{d}j_{DMz})) \]

Listing 3: spinfunctions.m

function [dSx, dSy, dSz, newJ, tprimeless] = spinfunctions(w1, w2, hbar, t, tprime, tback, t0, tprimeless, Sx, Sy, Sz, beta, J, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, fermi1, fermi2, lambda01, lambda02, c01, c02, d01, d02, e01, e02, Sx, Sy, Sz, g, myB, B, oldJ, ev)
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\[ \beta_{01}, \beta_{11} = \text{betafunc}(w_2, \hbar, \gamma_{0}, \gamma_{S}, \gamma_{up}, \gamma_{down}, \epsilon_{up}, \epsilon_{down}, ev) \];

\[ \beta_{02}, \beta_{12} = \text{betafunc}(w_2, \hbar, \gamma_{0}, \gamma_{S}, \gamma_{up}, \gamma_{down}, \epsilon_{up}, \epsilon_{down}, ev) \];

t_start = length(tprime) - tback;

\[ jH = \text{oldJ}(1,:) \];

\[ jI_x = \text{oldJ}(2,:) \];

\[ jI_y = \text{oldJ}(3,:) \];

\[ jI_z = \text{oldJ}(4,:) \];

\[ jDM_x = \text{oldJ}(5,:) \];

\[ jDM_y = \text{oldJ}(6,:) \];

% Loop for \(-\infty\) to \(t\)
parfor i = tstart:length(tprime)

% Greens functions depending on time to initiate current
if t <= t0
  G0less1 = -fermi1 ./ (2*pi) .* exp(-i.*w1.*(tprime(i)-t)/hbar).* (lambda01 + Sz*J/2.*c01);
  G0great1 = -(1-fermi1) ./ (2*pi) .* exp(-i.*w1.*(tprime(i)-t)/hbar).* (lambda01 + Sz*J/2.*c01);
  G0less2 = -fermi2 ./ (2*pi) .* exp(-i.*w2.*(t-tprime(i))/hbar).* (lambda02 + Sz*J/2.*c02);
  G0great2 = -(1-fermi2) ./ (2*pi) .* exp(-i.*w2.*(t-tprime(i))/hbar).* (lambda02 + Sz*J/2.*c02);
end

if tprime(i) <= t0
  G0less1 = -fermi1 ./ (2*pi) .* exp(-i.*w1.*(tprime(i)-t)/hbar).* (alpha01 + Sz*J/2.*d01);
  G0great1 = -(1-fermi1) ./ (2*pi) .* exp(-i.*w1.*(tprime(i)-t)/hbar).* (alpha01 + Sz*J/2.*d01);
  G0less2 = -fermi2 ./ (2*pi) .* exp(-i.*w2.*(t-tprime(i))/hbar).* (alpha02 + Sz*J/2.*d02);
  G0great2 = -(1-fermi2) ./ (2*pi) .* exp(-i.*w2.*(t-tprime(i))/hbar).* (alpha02 + Sz*J/2.*d02);
end

% Greens functions 1

G0less1 = -fermi1 ./ (2*pi) .* exp(-i.*w1.*(tprime(i)-t)/hbar).* (beta01 + Sz*J/2.*e01);
G0great1 = -(1-fermi1) ./ (2*pi) .* exp(-i.*w1.*(tprime(i)-t)/hbar).* (beta01 + Sz*J/2.*e01);
G0less2 = -fermi2 ./ (2*pi) .* exp(-i.*w2.*(t-tprime(i))/hbar).* (beta02 + Sz*J/2.*e02);
G0great2 = -(1-fermi2) ./ (2*pi) .* exp(-i.*w2.*(t-tprime(i))/hbar).* (beta02 + Sz*J/2.*e02);

end

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Listing 4: greensfunctions.m

```matlab
function [G1less1, G1yless1, G1zless1, G1great1, G1ygreat1, G1zgreat1]=greensfunctions2(w1, hbar, t, tprime(i), Sx, Sy, Sz, beta, J, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, ev);

end

Interaction parameters

djH(1) = -1. * J^2. * (G0less1 .* G1great2 - G0great1 .* G1less2);
djH(2) = -1. * J^2. * (G1less1 .* G1great2 - G1yless1 .* G1great1 - G1great2 .* G1yless1);
djI(1) = 2. * 1i. * J^2. * (G1xless1 .* G1xless2 - G1xless1 .* G1xgrea2);
djI(2) = 2. * 1i. * J^2. * (G1yless1 .* G1yless2 - G1yless1 .* G1ygrea2);
djDМ_I(1) = - J^2. * (G0less1 .* G1xgrea2 - G0great1 .* G1xless2);
djDМ_I(2) = - J^2. * (G0less1 .* G1ygrea2 - G0great1 .* G1yless2);
djDМ_I(3) = - J^2. * (G0less1 .* G1zgrea2 - G0great1 .* G1zless2);
```

Equation of motion at t

```matlab
iSx = jH.* (Sx.*SyT-Sz.*SxT)+(Sy.*jIz.*SxT.*SyT)-Sx.+(jDMX.*SxT-jDMy.*SxT)+Sz.+(jDMy.*SxT-jDMX.*SxT);
dx = (-g * mb * B * Sy * trapz(tprime).*Sx) .* hbar;
iSy = jH.* (Sz.*SxT-Sx.*SzT)+(Sx.*jIz.*SxT.*SzT)-Sx.+(jDMy.*SxT-jDMX.*SyT)+Sz.+(jDMX.*SxT-jDMy.*SyT);
dy = (g * mb * B * Sx * trapz(tprime).*Sy) .* hbar;
iSz = jH.* (Sx.*SyT-Sy.*SxT)+(Sy.*jIz.*SyT.*SxT)-Sy.+(jDMy.*SyT-jDMX.*SzT)+Sz.+(jDMX.*SyT-jDMy.*SzT);
dz = -trapz(tprime).*Sz) .* hbar;
end
```

fnew = [jH; jI; jDMy; jDM];
Listing 5: greensfunctions1.m

```matlab
function [G1xless, G1xgreat, G1yless, G1ygreat, G1zless, G1zgreat] = greensfunctions1(w, hbar, t1, t2, Sx, Sy, Sz, beta, J, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, eV)
    [alpha0, alpha1] = alpha(w, hbar, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, eV);
    fermi = 1./(1+exp(beta*w));
    Dx = 0.5*(((alpha0-alpha1).*((Sx-1i*Sy)./(w+epsilon_up+1i*gamma_up)+(alpha0+alpha1).*((Sx+1i*Sy)./(w+epsilon_down+1i*gamma_down))));
    Dy = 0.5*(((alpha0-alpha1).*((Sx+1i*Sy)./(w+epsilon_up+1i*gamma_up)+(alpha0+alpha1).*((Sx-1i*Sy)./(w+epsilon_down+1i*gamma_down))));
    Dz = alpha1 + Sz.*J/2.*((alpha0-alpha1)./(w+epsilon_up+1i*gamma_up)+(alpha0+alpha1)./(w+epsilon_down+1i*gamma_down));
end
```

Listing 6: greensfunctions2.m

```matlab
function [G1xless, G1xgreat, G1yless, G1ygreat, G1zless, G1zgreat] = greensfunctions2(w, hbar, t1, t2, Sx, Sy, Sz, beta, J, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, eV)
    [beta0, beta1] = betafunc(w, hbar, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, eV);
end
```
Listing 7: current.m

```matlab
% Calculating the current
Ic0 = zeros(1, length(t));
Ic1 = zeros(1, length(t));
Is0x = zeros(1, length(t));
Is0y = zeros(1, length(t));
Is0z = zeros(1, length(t));
Is1x = zeros(1, length(t));
Is1y = zeros(1, length(t));
Is1z = zeros(1, length(t));

[alpha01, alpha11] = alpha(w1, hbar, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, ev);
[alpha02, alpha12] = alpha(w2, hbar, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, ev);
[beta01, beta11] = betafunc(w1, hbar, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, ev);
[beta02, beta12] = betafunc(w2, hbar, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, ev);

for j = 1:length(tprime)
    Ic0tot = zeros(1, length(w2));
    Ic1tot = zeros(1, length(w2));
    Is0xtot = zeros(1, length(w2));
    Is0ytot = zeros(1, length(w2));
    Is0ztot = zeros(1, length(w2));
    Is1xtot = zeros(1, length(w2));
    Is1ytot = zeros(1, length(w2));
    Is1ztot = zeros(1, length(w2));

    if j <= t0length
        Cx2 = (lambda02 - lambda12) .* (SyT(j) .* (w2 - epsilon_up) + SyT(j) .* gamma_up) ./ ((w2 - epsilon_up) .* 2 + (lambda02 + lambda12) .* (SyT(j) .* (w2 - epsilon_down) - SyT(j) .* gamma_down) ./ ((w2 - epsilon_down) .* 2));
```
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```plaintext
for i=1:length(w2)
    Iz0bare(i) = -(fermi1 - fermi2(i)).*(lambda02(i)+1i)*Sx(i).*gamma0.*imag(trapz(w1,Iz0bare(i)));
    Iz0t0t(i) = -4*e/hbar1/gamma0.*imag(trapz(w1,Iz0bare(i)));
    Iz0bare(i) = (fermi1 - fermi2(i)).*(Cz(i) + 1i).*gamma_up.*imag(trapz(w1,Iz0bare(i)));
    Iz0t0t(i) = -4*e/hbar1/gamma0.*imag(trapz(w1,Iz0bare(i)));
    Iz0ybare(i) = (fermi1 - fermi2(i)).*(Cz(i) + 1i).*gamma_down.*imag(trapz(w1,Iz0bare(i)));
    Iz0yt0t(i) = -4*e/hbar1/gamma0.*imag(trapz(w1,Iz0bare(i)));
    Iz0xbare(i) = (fermi1 - fermi2(i)).*(Cz(i) + 1i).*gamma_down.*imag(trapz(w1,Iz0bare(i)));
    Iz0xt0t(i) = -4*e/hbar1/gamma0.*imag(trapz(w1,Iz0bare(i)));
end
else
    Dx2 = -0.5.*(alpha12.*SyT(j) - 1i.*SyT(j) + w2.*epsilon_up + 1i.*gamma_up) + (SyT(j) + 1i.*SyT(j) + w2.*epsilon_down + 1i.*gamma_down);
    Dy2 = -0.5.*(alpha12.*SyT(j) - SyT(j) + w2.*epsilon_up + 1i.*gamma_up) + (SyT(j) + 1i.*SyT(j) + w2.*epsilon_down + 1i.*gamma_down);
    Dz2 = (alpha12.*SyT(j) + w2.*epsilon_up + 1i.*gamma_up) + (alpha12.*SyT(j) + w2.*epsilon_down + 1i.*gamma_down);
    Ex2 = (beta12.*beta12.*SyT(j) + w2.*epsilon_up + 1i.*gamma_up) + (w2.*epsilon_down + 1i.*gamma_down); 
    Ey2 = (beta12.*beta12.*SyT(j) + w2.*epsilon_up + 1i.*gamma_up) + (w2.*epsilon_down + 1i.*gamma_down); 
    Ez2 = (beta12.*beta12.*SyT(j) + w2.*epsilon_up + 1i.*gamma_up) + (w2.*epsilon_down + 1i.*gamma_down); 
end

for i=1:length(w2)
```

```plaintext
```
Listing 8: omegafunctions.m

function [a1, a2, b1, b2, c0, c1, d0, e0] = omegafunctions(w, hbar, wL, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, eV)

end

Listing 9: Listing 8: omegafunctions.m
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Listing 9: alpha.m

```matlab
function [alpha0, alpha1] = alpha(w, hbar, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, ev)
alpha0 = -hbar^2/4*gamma0*(1/(w+ev+1i*gamma_up-epsilon_up)+1/(w+ev+1i*gamma_down-epsilon_down)).*(1/(w+1i*gamma_up-epsilon_up)+1/(w+1i*gamma_down-epsilon_down)).*(1/(w+ev+1i*gamma_up-epsilon_up)+1/(w+ev+1i*gamma_down-epsilon_down)).*(1/(w+1i*gamma_up-epsilon_up)+1/(w+1i*gamma_down-epsilon_down)).*(1/(w+ev+1i*gamma_up-epsilon_up)+1/(w+ev+1i*gamma_down-epsilon_down)).*(1/(w+1i*gamma_up-epsilon_up)+1/(w+1i*gamma_down-epsilon_down)).*(1/(w+ev+1i*gamma_up-epsilon_up)+1/(w+ev+1i*gamma_down-epsilon_down)).*(1/(w+1i*gamma_up-epsilon_up)+1/(w+1i*gamma_down-epsilon_down)).*(1/(w+ev+1i*gamma_up-epsilon_up)+1/(w+ev+1i*gamma_down-epsilon_down)).*(1/(w+1i*gamma_up-epsilon_up)+1/(w+1i*gamma_down-epsilon_down));
alpha1 = -hbar^2/4*gammaS*(1/(w+ev+1i*gamma_up-epsilon_up)+1/(w+ev+1i*gamma_down-epsilon_down)).*(1/(w+1i*gamma_up-epsilon_up)+1/(w+1i*gamma_down-epsilon_down)).*(1/(w+ev+1i*gamma_up-epsilon_up)+1/(w+ev+1i*gamma_down-epsilon_down)).*(1/(w+1i*gamma_up-epsilon_up)+1/(w+1i*gamma_down-epsilon_down)).*(1/(w+ev+1i*gamma_up-epsilon_up)+1/(w+ev+1i*gamma_down-epsilon_down)).*(1/(w+1i*gamma_up-epsilon_up)+1/(w+1i*gamma_down-epsilon_down)).*(1/(w+ev+1i*gamma_up-epsilon_up)+1/(w+ev+1i*gamma_down-epsilon_down)).*(1/(w+1i*gamma_up-epsilon_up)+1/(w+1i*gamma_down-epsilon_down));
end
```

Listing 10: betafunc.m

```matlab
function [beta0, beta1] = betafunc(w, hbar, gamma0, gammaS, gamma_up, gamma_down, epsilon_up, epsilon_down, ev)
beta0 = -hbar^2/2*(gamma0*1/(gamma_up^2+epsilon_up-w-ev)+1/(gamma_down^2+epsilon_down-w-ev)+gammaS*1/(gamma_up^2+epsilon_up-w-ev)+1/(gamma_down^2+epsilon_down-w-ev));
end
```
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beta1 = \( hbar^2 \times 1i / 2 \times (\gamma_S \times (1 / (\gamma_{up}^2 + (\epsilon_{up} w_e V)^2) + 1 / (\gamma_{down}^2 + (\epsilon_{down} w_e V)^2)) + \gamma_0 \times (1 / (\gamma_{up}^2 + (\epsilon_{up} w_e V)^2) - 1 / (\gamma_{down}^2 + (\epsilon_{down} w_e V)^2)) \right) ;

end