A magnetization equation for non-equilibrium spin systems

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Abstract

A magnetization equation for a system of spins evolving non-adiabatically and out of equilibrium is derived without specifying the internal interactions. For relaxation processes, this equation provides a general form of magnetization damping. A special case of the spin-spin exchange interaction is considered.

Pacs numbers: 76.20.+q, 72.25.Ba.

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1 Introduction

Magnetization dynamics is conventionally described by the Landau-Lifshitz-Gilbert (LLG) equation [1],[2], which provides a plausible phenomenological model for many experimental results. Recently, the LLG equation and the Gilbert damping term have been derived from an effective Hamiltonian including the radiation-spin interaction (RSI) [3]. It has been assumed there that the spin system maintains quasi-adiabatic evolution.

Various kinds of relaxation processes are usually melded together into a single damping term. Relativistic relaxation processes result in the Gilbert damping term with one damping parameter, while for the case of both exchange and relativistic relaxation the damping term is a tensor with several damping parameters [4], [5].

The relaxation processes are specified by interactions of spins with each other and with other constituents of the magnetic system. A derivation of the damping term from first principles should therefore start with a microscopic description of the interactions. Even though such microscopic derivation of damping has been performed for some relaxation processes (for instance, [6]), a full version of derivation for the Gilbert damping term has not yet been given, and in particular for a system in non-equilibrium.

In the present talk, we aim to derive a magnetization equation for a general non-equilibrium spin system without specifying the interaction Hamiltonian and related relaxation processes. We start with a system of spins precessing in the effective magnetic field $\mathbf{H}_{\text{eff}}$ neglecting for a moment mutual interactions. Then at a fixed time later interactions in the system are switched on and influence the original precessional motion.

The interactions are assumed to be time-dependent, and the spin system evolves non-adiabatically out of equilibrium trying to relax to a new equilibrium magnetization. We perform a transformation, which is analogous to the one used in the transition to the interaction picture, to connect the density and magnetic moment operators before and after the time, when a new non-equilibrium dynamics starts, and to find an explicit expression for the interaction contribution to the magnetization equation.

2 Magnetization Equation

Let us consider a quantum spin system defined by

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}_I,$$

where $\hat{H}_0$ is the Zeeman Hamiltonian describing the interaction of spins with an effective magnetic field

$$\hat{H}_0 = -\gamma \sum_i \hat{S}_i \cdot \mathbf{H}_{\text{eff}}(t),$$

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γ being the gyromagnetic ratio and \( \hat{S}_i \) being the spin operator of the \( i \)th atom. The effective magnetic field \( \vec{H}_{\text{eff}} \) is given by the energy variational with magnetization, 
\[ \vec{H}_{\text{eff}} = -\frac{\delta E(M)}{\delta \vec{M}}, \]
where \( E(M) \) is the free energy of the magnetic system. This field includes the exchange field, the anisotropy field, and the demagnetizing field, as well as the external field, \( \vec{H}_{\text{ext}} \).

The Hamiltonian \( \hat{H}_I \) represents other possible types of interactions, which can include, for instance, higher order spin-spin interactions. The interaction terms included in \( \hat{H}_I \) are in general time-dependent, being switched on adiabatically or instantly at a fixed time \( t_0 \). The parameter \( \lambda \) in (1) can be chosen small in order to take into account the higher order effects perturbatively.

We introduce next the magnetic moment operator
\[ \hat{M} \equiv -\frac{\delta \hat{H}}{\delta \vec{H}_{\text{ext}}}, \]
which is the response of the spin system to the external field. The magnetization is defined as an ensemble average of the response
\[ \bar{M} = \langle \hat{M} \rangle \equiv \frac{1}{V} \text{Tr}\{\hat{\rho} \hat{M}\}, \]
where \( V \) is the volume of the system, while \( \hat{\rho} \) is the density operator satisfying the quantum Liouville-von Neumann (LvN) equation
\[ i\hbar \frac{\partial \hat{\rho}}{\partial t} + \{\hat{\rho}, \hat{H}\} = 0. \]

For systems in equilibrium, the Hamiltonian itself satisfies the LvN equation and the density operator is expressed in terms of the Hamiltonian. For non-equilibrium systems, the density operator is constructed by making use of the time-dependent adiabatic invariants \cite{7,8}.

To derive the magnetization equation, we proceed as follows. We perform, on \( \hat{\rho}(t) \), the transformation
\[ \hat{\rho} \rightarrow \hat{\rho}_{\text{int}} \equiv \hat{U}(t_0, t)\hat{\rho}(t)\hat{U}(t, t_0) \]
defined by the operator
\[ \hat{U}(t_0, t) \equiv T \exp\left\{ \frac{i}{\hbar} \int_{t_0}^{t} d\tau \hat{H}_0(\tau) \right\}, \]
where \( T \) denotes the time-ordering operator. For systems with \( \hat{H}_0 \) constant in time, the operator \( \hat{U}(t_0, t) = \exp\{(i/\hbar)\hat{H}_0(t - t_0)\} \) leads to the interaction picture, which proves to be very useful for all forms of interactions since it distinguishes among the interaction times. For our system with both \( \hat{H}_0 \) and \( \hat{H}_I \) dependent on time, the operator (7) plays the same role, removing the unperturbed part of the Hamiltonian from the LvN equation.
Substituting Eq. (6) into (5), yields

\[ i\hbar \frac{\partial \hat{\rho}_{\text{int}}}{\partial t} = \lambda [\hat{\mathcal{H}}_{\text{int}}, \hat{\rho}_{\text{int}}], \tag{8} \]

where

\[ \hat{\mathcal{H}}_{\text{int}}(t) \equiv \hat{U}(t_0, t)\hat{\mathcal{H}}_{\text{I}}(t)\hat{U}(t, t_0). \tag{9} \]

The magnetic moment operator and the magnetization become

\[ \hat{\mathcal{M}} = \hat{\mathcal{M}}_0 + \hat{\mathcal{M}}_I \tag{10} \]

and

\[ \vec{M} = \frac{1}{V} \text{Tr}\{\hat{\rho}_{\text{int}}(\hat{\mathcal{M}}_{0,\text{int}} + \hat{\mathcal{M}}_{I,\text{int}})\}, \tag{11} \]

where

\[ \hat{\mathcal{M}}_0 = -\frac{\delta \hat{\mathcal{H}}_0}{\delta \hat{\mathbf{H}}_{\text{ext}}} = \gamma \sum_i \hat{\mathbf{S}}_i \tag{12} \]

and

\[ \hat{\mathcal{M}}_I \equiv -\lambda \frac{\delta \hat{\mathcal{H}}_I}{\delta \hat{\mathbf{H}}_{\text{ext}}}, \tag{13} \]

while \( \hat{\mathcal{M}}_{0,\text{int}} \) and \( \hat{\mathcal{M}}_{I,\text{int}} \) are related with \( \hat{\mathcal{M}}_0 \) and \( \hat{\mathcal{M}}_I \), respectively, in the same way as \( \hat{\mathcal{H}}_{\text{int}} \) is related with \( \hat{\mathcal{H}}_{\text{I}} \). The operators \( \hat{\mathcal{M}}_a^0, a = 1, 2, 3 \), fulfill the \( SU(2) \) magnetization algebra

\[ [\hat{\mathcal{M}}_a^0, \hat{\mathcal{M}}_b^0]_\pm = i\hbar \gamma \epsilon^{abc} \hat{\mathcal{M}}_c^0, \tag{14} \]

where the summation over repeated indices is assumed.

The operators \( \hat{\mathcal{M}}_{0,\text{int}}, \hat{\mathcal{M}}_{I,\text{int}} \) are generally used to calculate the magnetic susceptibility [9]. Let us show now how these operators determine the time evolution of magnetization. The evolution in time of \( \hat{\mathcal{M}}_{0,\text{int}} \) is given by the equation

\[ \frac{\partial \hat{\mathcal{M}}_{0,\text{int}}}{\partial t} = \frac{i}{\hbar} \hat{U}(t_0, t)[\hat{\mathcal{H}}_0, \hat{\mathcal{M}}_0]_\pm \hat{U}(t, t_0) = \gamma \hat{\mathcal{M}}_{0,\text{int}} \times \vec{H}_{\text{eff}}. \tag{15} \]

It describes the magnetization precessional motion with respect to \( \vec{H}_{\text{eff}} \).

The equation for \( \hat{\mathcal{M}}_{I,\text{int}} \) describes more complex magnetization dynamics governed by the interaction Hamiltonian \( \hat{\mathcal{H}}_{\text{I}} \). However, this dynamics includes the precessional motion as well. Introducing

\[ \vec{D}_I \equiv \frac{i}{\hbar} [\hat{\mathcal{H}}_0, \hat{\mathcal{M}}_I]_\pm - \gamma \hat{\mathcal{M}}_I \times \vec{H}_{\text{eff}} \tag{16} \]
to represent deviations from the purely precessional motion, we bring the equation for $\mathcal{M}_{I,\text{int}}$ into the following form

$$\frac{\partial \mathcal{M}_{I,\text{int}}}{\partial t} = \gamma \mathcal{M}_{I,\text{int}} \times \vec{H}_{\text{eff}} + \mathcal{M}_{I,\text{int}} \times \vec{H}_{\text{eff}} + \mathcal{U}(t_0, t) \left( \frac{\partial \mathcal{M}_{I}}{\partial t} + \mathcal{D}_I \right) \mathcal{U}(t, t_0).$$

(17)

Taking the time-derivative of Eq.(11) and using Eqs.(8),(15) and (17), we finally obtain

$$\frac{d\vec{M}}{dt} = -|\gamma| \vec{M} \times \vec{H}_{\text{eff}} + \vec{D},$$

(18)

where

$$\vec{D} \equiv \lambda \left( \frac{1}{i\hbar} [\mathcal{M}, \mathcal{H}_I]_\lambda \right) + \left( \frac{\partial \mathcal{M}_I}{\partial t} + \mathcal{D}_I \right).$$

(19)

Therefore, Eq.(18) is the magnetization equation for the system specified by (1). This equation is general since it is derived without specifying $\mathcal{H}_I$. The $\vec{D}$-term contains all effects that the interactions, $\mathcal{H}_I$, can have on the magnetization precession, so that Eq.(18) is complete.

The contribution of $\mathcal{H}_I$ to the $\vec{D}$-term in the magnetization equation can be divided into two parts. One is proportional to $\langle [\mathcal{M}, \mathcal{H}_I]_\lambda \rangle$ and is related to the change in the density matrix when the interactions of $\mathcal{H}_I$ are switched on. The second part $\langle \frac{\partial \mathcal{M}_I}{\partial t} + \mathcal{D}_I \rangle$ originates from the change in the magnetization itself. Which part of $\vec{D}$ is dominating depends on the nature of the interactions. For the interactions related to the relaxation processes, the $\vec{D}$-term represents a general form of magnetization damping.

### 3 Example: spin-spin interactions

The spin-spin interactions among the spins in the system introduce many body effects, which can be treated perturbatively in the weak coupling regime. In this case the $\vec{D}$-term can be expanded in powers of $\lambda$. To demonstrate this, we consider the spin-spin interactions of a specific type. The interaction between spins is usually an exchange interaction of the form

$$-2J \sum_{i,j} \hat{S}_i \hat{S}_j = -\frac{2J}{\gamma^2} \mathcal{M}_0^2,$$

(20)

the coupling constant $J$ being called the exchange integral. We generalize the ansatz given by Eq.(20) by assuming that the exchange integral depends on the magnetization and introduce the spin-spin interactions as follows

$$\lambda \mathcal{H}_I = \sum_{i,j} J^{ab} (M) \hat{S}_i^a \hat{S}_j^b,$$

(21)
where \( J^{ab} = \lambda M^a M^b \). Since \( \hat{H}_I \) does not depend explicitly on the external field, its contribution to the magnetic moment operator vanishes, \( \hat{\mathcal{M}}_I = 0 \).

The non-vanishing commutator \( [\hat{\mathcal{M}}_0, \hat{H}_I]_+ \) in Eq.(19) is the only contribution of the spin-spin interaction to the magnetization equation, resulting in

\[
\vec{D} = \frac{\lambda}{\gamma} \vec{M} \times \vec{\Omega},
\]

where

\[
\Omega^a \equiv \langle \left[ \hat{\mathcal{M}}^a_0, \hat{\mathcal{M}}^b_0 \right]_+ M^b \rangle,
\]

and

\[
[\hat{\mathcal{M}}^a_0, \hat{\mathcal{M}}^b_0]_+ \equiv \hat{\mathcal{M}}^a_0 \hat{\mathcal{M}}^b_0 + \hat{\mathcal{M}}^b_0 \hat{\mathcal{M}}^a_0.
\]

The correlation function \( G^{ab} \equiv \langle \left[ \hat{\mathcal{M}}^a_0, \hat{\mathcal{M}}^b_0 \right]_+ \rangle \) is the sum of spin correlation functions,

\[
G^{ab} = 2\gamma^2 \sum_i \sum_{j \neq i} \langle \hat{S}^a_i \hat{S}^b_j \rangle,
\]

excluding the self-interaction of spins. For the standard ansatz given in Eq.(20), \( \vec{D} = 0 \) and the magnetization equation does not change.

If the spin-spin interactions are turned on at \( t = t_0 \), so that \( \hat{\rho}(t_0) = \hat{\rho}_0(t_0) \), then, integrating both sides of Eq.(8), we find

\[
\hat{\rho}_\lambda(t) = \hat{\rho}_0(t_0) + \frac{\lambda}{i\hbar} \int_{t_0}^t d\tau \left[ \hat{H}_\lambda(\tau), \hat{\rho}_\lambda(\tau) \right]_-.
\]

Substituting Eq.(26) into the definition of \( G^{ab} \), yields the equation

\[
G^{ab}(t) = G^{ab}_0(t_0)
+ \frac{1}{\gamma} \int_{t_0}^t d\tau J^{cd}(\tau) \left( \varepsilon^{ace} G^{ebd}(\tau) + \varepsilon^{bce} G^{aecd}(\tau) \right),
\]

where

\[
G^{ab}_0 \equiv \langle \left[ \hat{\mathcal{M}}^a_0, \hat{\mathcal{M}}^b_0 \right]_+ \rangle_0,
\]

which relates \( G^{ab} \) to the third order correlation function, i.e. the correlation function of the product of three magnetic moment operators,

\[
G^{abc} \equiv \langle \left[ \hat{\mathcal{M}}^a_0, \hat{\mathcal{M}}^b_0 \right]_+, \hat{\mathcal{M}}^c_0 \rangle_+.
\]

The correlation function \( G^{abc} \), in turn, is related to the fourth order correlation function and etc., and we have therefore an infinite number of coupled equations for spin correlation functions. For any practical calculation this infinite hierarchy has to be truncated. That then defines the approximation scheme which may be considered
on the basis of the physical requirements for the system. The approximation scheme will depend on the physical properties such as density and on the strength of the interactions.

If the Hamiltonian $\hat{H}_1$ is a small perturbation to the original $\hat{H}_0$, we can solve Eq.(26) perturbatively. In the lowest, zeroth order in $\lambda$, we replace $\hat{\rho}_\lambda(t)$ by $\hat{\rho}_0(t_0)$, so that $G^{ab} \approx G_0^{ab}(t_0)$. We choose the initial value for $G^{ab}$ as

$$\sum_i \sum_{j \neq i} \langle \hat{S}_i^a \hat{S}_j^b \rangle_0 = I^{ab}$$  \hspace{1cm} (30)

with $I^{xx} = I^{yy} = 0$, $I^{zz} = I$ and $I^{ab} = 0$ for $a \neq b$. We also define again the $z$-direction as the direction of the effective magnetic field that is chosen uniform and static. Then the $\vec{D}$-term becomes, in component form,

$$D_x = 2\lambda \gamma I M_y M_z, \hspace{1cm} (31)$$
$$D_y = -2\lambda \gamma I M_x M_z, \hspace{1cm} (32)$$
$$D_z = 0. \hspace{1cm} (33)$$

producing two effects in the magnetization equation: the magnetization is now precessing with respect to $(H_z - 2\lambda I M_z)$, its $z$-component remaining constant in time, $(d/dt)M_z = 0$, and the frequency of the precession is

$$\omega_0 \equiv \omega_0 \left(1 - \frac{2IM_z}{H_z}\right). \hspace{1cm} (34)$$

Therefore, in the lowest order of perturbations, when the $\vec{D}$ is linear in $\lambda$, it shifts the direction and the frequency of the precessional motion without introducing damping effects. To find a role of the higher powers of $\lambda$ in $\vec{D}$ and to determine how they affect the magnetization equation, a truncation of the chain of spin correlation equations is needed. This would require a consistent perturbation approach to the hierarchy of the coupled equations for the correlation functions.

4 Conclusion

We have derived a general form of magnetization equation for a system of spins precessing in an effective magnetic field without specifying the internal interactions. It can be applied in the study of magnetization dynamics of any type, including non-equilibrium and nonlinear effects, provided the interaction of individual spins with each other and with other degrees of freedom of the system is specified.

The $\vec{D}$-term in the magnetization equation has been obtained without using any approximation scheme. It is exact, accumulates all effects of the internal interactions on the magnetization precessional motion and can be a starting point for practical calculations. For the spin-spin interactions, it is determined by the spin correlation
functions, which fulfil an infinite chain of equations. A further analysis of the $\vec{D}$-term requires an approximation scheme to truncate the chain in a consistent approach to higher order calculations.

In our talk, we have considered a specific type of the spin-spin interactions, which do not contribute to the algebra of magnetic moment operators. However, if spin-spin interactions depend explicitly on the external field, the form of the algebra can change. In this case, the total magnetic moment operator becomes nonlinear in $\hat{M}_0$, and this results in the magnetization algebra with an infinite chain of commutation relations. The chain has to be truncated in a way consistent with the truncation of the chain of equations for the spin correlation functions in the same approximation scheme.

Numerical computations along the lines developed in [10] can provide a further insight into the problem. This talk is based on the work [11] where an extended list of references can be found.

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