Nonequilibrium Extension of the Landau-Lifshitz-Gilbert Equation for Magnetic Systems

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Using the invariant operator method for an effective Hamiltonian including the radiation-spin interaction, we describe the quantum theory for magnetization dynamics when the spin system evolves nonadiabatically and out of equilibrium, \( \dot{\rho} \neq 0 \). It is shown that the vector parameter of the invariant operator and the magnetization defined with respect to the density operator, both satisfying the quantum Liouville equation, still obey the Landau-Lifshitz-Gilbert equation.

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I. INTRODUCTION

Magnetization dynamics has attracted much attention both in theoretical and experimental physics. In particular, the magnetic information requires a deep and fundamental understanding of the dynamics of spin system on a short time scale. The Landau-Lifshitz-Gilbert (LLG) equation provides a plausible phenomenological model for many experimental results [1]. Recently, the first three authors have derived the LLG equation from an effective Hamiltonian including the radiation-spin interaction [2]. It is assumed there that the magnetic system maintains quasi-adiabatic evolution and obeys the condition \( \dot{\rho} = 0 \). However, for a magnetic system whose Hamiltonian \( H(t) \) evolves nonadiabatically, its statistics deviates far from quasi-equilibrium. Thus the density operator does neither satisfy the condition \( \dot{\rho} = 0 \) nor is given by \( e^{-\beta H(t)} \). Instead, the density operator does satisfy the quantum Liouville equation

\[
i\hbar \frac{\partial\hat{\rho}}{\partial t} + [\hat{\rho}, \hat{H}] = 0.
\]

The main purpose of this paper is to derive the LLG equation from quantum theory for such a nonequilibrium magnetic system with the effective Hamiltonian in Ref. [2].

To find the nonadiabatic quantum states for this nonequilibrium system, we employ the invariant method developed for explicitly time-dependent Hamiltonians in the Schrödinger picture [3]. One advantage of the invariant operator method is that the eigenstates of the invariant operator satisfying the quantum Liouville equation are exact quantum states of the time-dependent Schrödinger equation up to time-dependent phase factors. Further we use this invariant operator to define the density operator \( \hat{\rho} \), in terms of which we define the magnetization. Finally we show that the magnetization satisfies the LLG equation even for nonadiabatic and nonequilibrium evolution.

II. LANDAU-LIFSHITZ EQUATION

We first consider the spin Hamiltonian without the radiation-spin interaction given by

\[
\hat{H}_0(t) = -g\mu_B \sum_{i=1}^{N} \hat{S}_i \cdot \mathbf{H}_{\text{eff}}(t),
\]

where \( g \) is the Lande’s g-factor, \( \mu_B \) is the Bohr magneton, \( N \) is the number of spins in the system, and \( \hat{S}_i \) is the \( i \)th spin operator. The effective field \( \mathbf{H}_{\text{eff}} \) includes the exchange field, the anisotropy field, and the demagnetizing field as well as the external field. As the Hamiltonian [2] has the group \( SU^N(2) \), we may look for an invariant operator with the same group \( SU^N(2) \) of the form [2]

\[
\hat{I}_0(t) = \sum_{i=1}^{N} \hat{S}_i \cdot \mathbf{R}_0(t),
\]

where \( \mathbf{R}_0 \) is a vector parameter to be determined by a dynamical equation. The invariant operator, satisfying the quantum Liouville equation [1], leads to the equation

\[
-i\hbar \sum_{i=1}^{N} \hat{S}_i \cdot \left( \frac{d\mathbf{R}_0}{dt} + g\mu_B \mathbf{R}_0 \times \mathbf{H}_{\text{eff}} \right) = 0.
\]

We thus obtain the equation for the vector parameter:

\[
\frac{d\mathbf{R}_0}{dt} = -\gamma \mathbf{R}_0 \times \mathbf{H}_{\text{eff}}
\]

with \( \gamma = g\mu_B \).

We note that the eigenstates of the invariant operator [3] are exact quantum states, up to time-dependent...
phase factors, of the time-dependent Schrödinger equation for the Hamiltonian (2). Hence the vector parameter $\mathbf{R}_0$ defines the magnetization $\mathbf{R}_0 = \mathbf{M}_0$ of the system during the nonadiabatic evolution. When the Hamiltonian $\hat{H}(t)$ explicitly depends on time, not only the states but also the operators change in the invariant method. So any physical quantity defined by $O(t) = \text{Tr}\{\hat{O}(t)\}$ has, in general, the time derivative

$$\frac{dO(t)}{dt} = \sum_n \langle \psi_n(t) | \frac{1}{i\hbar} [\hat{O}, \hat{H}] + \frac{\partial \hat{O}}{\partial t} + \rho \frac{\partial \hat{O}}{\partial t} | \psi_n(t) \rangle.$$  

$$= \text{Tr}\left\{ \frac{1}{i\hbar} [\hat{O}, \hat{H}] + \frac{\partial \hat{O}}{\partial t} \right\},$$  

where we use Eq. (1) in the last step.

In the first case of no radiation-spin interaction, the density operator may be given by

$$\hat{\rho}_0(t) = \frac{1}{Z_0} e^{-\beta Z_0(t)}, \quad Z_0 = \text{Tr}\{e^{-\beta Z_0(t)}\},$$  

where $\hat{Z}_0$ already satisfied Eq. (1). Here $\beta$ is the inverse temperature. Now we may define the magnetization per volume in the general case as

$$\mathbf{M}_0(t) = \frac{1}{V} \text{Tr}\{\hat{\rho}_0(t)\hat{M}_0\},$$  

where $V$ is the volume of the system and $\hat{M}_0$ is the magnetic moment operator defined by the external field as

$$\hat{M}_0 = -\frac{\delta \hat{H}_0}{\delta \mathbf{H}_{eff}} = g\mu_B \sum_{i=1}^{N} \hat{S}_i.$$  

Then it follows from Eq. (7) that

$$\frac{d\mathbf{M}_0}{dt} = -\gamma \mathbf{M}_0 \times \mathbf{H}_{eff}. \tag{11}$$

Note that Eq. (11) is the Landau-Lifshitz equation.

### III. LANDAU-LIFSHITZ-GILBERT EQUATION

In Ref. [2] the LLG equation is described by an effective theory including the radiation-spin interaction. The model Hamiltonian

$$\hat{H}(t) = \hat{H}_0(t) + \lambda \hat{H}_{int}(t), \tag{12}$$

with the radiation-spin interaction

$$\hat{H}_{int} = g\mu_B \sum_{i=1}^{N} \hat{S}_i \cdot (\alpha M^2 \mathbf{H}_{eff} - \mathbf{M} \times \mathbf{H}_{eff}), \tag{13}$$

is an effective theory in the sense that the Hamiltonian involves the magnetization to be determined by the theory itself. As $\hat{H}_{int}$ has the same group structure $SU^N(2)$ as $\hat{H}_0$, we still have an invariant operator of the same form

$$\hat{I}(t) = \sum_{i=1}^{N} \hat{S}_i \cdot \mathbf{R}(t). \tag{14}$$

Then the quantum Liouville equation [11] leads to the parameter vector equation

$$\frac{d\mathbf{R}}{dt} = -g\mu_B \mathbf{R} \times \left( (1 - \lambda A M^2) \mathbf{H}_{eff} + \lambda \mathbf{M} \times \mathbf{H}_{eff} \right). \tag{15}$$

Noting again that the invariant operator (14) determines exact eigenstates, we may identify $\mathbf{R} = \mathbf{M}$ for the nonadiabatic evolution. Using $\mathbf{M} \cdot d\mathbf{M}/dt = 0$ and solving for $\mathbf{M} \times d\mathbf{M}/dt$, we obtain

$$\frac{d\mathbf{M}}{dt} = -\gamma \mathbf{M} \times \mathbf{H}_{eff} + \alpha \mathbf{M} \times \frac{d\mathbf{M}}{dt}. \tag{16}$$

Thus the spin direction of the system even for the nonadiabatic evolution obeys the LLG equation.

In the nonequilibrium case, using the density operator

$$\hat{\rho}(t) = \frac{1}{Z} e^{-\beta Z(t)}, \quad Z = \text{Tr}\{e^{-\beta Z(t)}\}, \tag{17}$$

we may define the magnetization as

$$\mathbf{M}(t) = \frac{1}{V} \text{Tr}\{\hat{\rho}(t)\hat{M}(t)\}, \tag{18}$$

where $\hat{M}(t)$ is the magnetic moment operator

$$\hat{M} = -\frac{\delta \hat{H}}{\delta \mathbf{H}_{eff}} = g\mu_B \sum_{i=1}^{N} \left\{ (1 - \lambda A M^2) \hat{S}_i + \lambda \hat{S}_i \times \mathbf{M} \right\}. \tag{19}$$

The magnetization can be written as

$$\mathbf{M} = (1 - \lambda A M^2) \mathbf{M}_1 + \lambda \mathbf{M}_1 \times \mathbf{M}, \tag{20}$$

where

$$\mathbf{M}_1(t) = \frac{1}{V} \text{Tr}\{\hat{\rho}(t)\hat{M}_0\}. \tag{21}$$

It should be noted that $\mathbf{M}_0$ and $\mathbf{M}_1$ are weighted with $\hat{\rho}_0$ and $\hat{\rho}$, respectively. Taking the cross product of Eq. (20) with $\mathbf{M}_1$ and rearranging $\mathbf{M}_1 \times (\mathbf{M}_1 \times \mathbf{M})$, we find that $\mathbf{M}$ is parallel to $\mathbf{M}_1$:

$$\mathbf{M} = \frac{(1 - \lambda A M^2) + \lambda^2 (\mathbf{M}_1 \cdot \mathbf{M})}{1 + \lambda M_1^2} \mathbf{M}_1. \tag{22}$$

Hence the last term in Eq. (20) drops out, and we get

$$\mathbf{M} = (1 - \lambda A M^2) \mathbf{M}_1. \tag{23}$$
The magnetic moment may depend on time through $M$. From Eq. (7) follows the time derivative of $M$, which is given by

$$\frac{dM}{dt} = i\hbar \text{Tr}\{\hat{\rho}[\hat{H}, \hat{M}]\} + \frac{1}{V} \text{Tr}\{\hat{\rho} \frac{\partial \hat{M}}{\partial t}\}. \quad (24)$$

Note that Eq. (24) is quite a general result, valid in all circumstances, including nonequilibrium evolution. Furthermore, it has the same form as Eq. (15) of Ref. [2], where the static limit $d\hat{\rho}/dt = 0$ was assumed. Evaluating Eq. (24), we finally obtain the LLG equation

$$\frac{dM}{dt} = -\gamma M \times H_{\text{eff}} + \alpha M \times \frac{dM}{dt}. \quad (25)$$

In deriving Eq. (25) from Eq. (24) we have used $M \cdot \frac{dM}{dt} = 0$, which can be checked self-consistently in Eq. (25).

A few comments are in order. The Gilbert damping term in Eq. (25) has the effect of slowing down the precession of magnetization and leads to a final constant value. Thus the final state is a thermal state with the constant magnetization. Then the vector parameter in Eq. (15) would have the final value

$$R(t = \infty) = -g\mu_B \left(1 - \lambda \alpha M^2\right)H_{\text{eff}} + \alpha M \times H_{\text{eff}}. \quad (26)$$

The invariant operator settles down to the Hamiltonian itself, $\hat{I}(\infty) = \hat{H}(\infty)$. Thus the system, after undergoing a nonequilibrium evolution, reaches a thermalization process towards the final equilibrium with $\hat{\rho}(\infty) = e^{-\beta\hat{H}(\infty)}/Z$.

**IV. CONCLUSION**

In this paper we derived the Landau-Lifshitz-Gilbert equation for the magnetic system with an effective Hamiltonian including the radiation-spin interaction in Ref. [2]. The time-evolving magnetization enters the Hamiltonian as a parameter and the Hamiltonian thus provides an effective theory. When the magnetization proceeds rapidly, the system evolves nonadiabatically and out of equilibrium. To treat such a nonequilibrium evolution, we employed the invariant method to find the equation for magnetization.

The invariant operator, satisfying the quantum Liouville equation, provides exact quantum states, up to time-dependent phase factors, of the time-dependent Schrödinger equation. Due to the group structure of the effective Hamiltonian [13], we were able to find the invariant operator, $\hat{I}(t)$ in Eq. (14), whose vector parameter defines the magnetization. We further used the invariant operator to introduce the density operator [17], in terms of which the magnetization, $M(t) = \text{Tr}[e^{-\beta\hat{I}(t)\hat{M}(t)}]/Z$, is defined for nonequilibrium evolution. We showed that the dynamical equation for nonequilibrium magnetization satisfies the same equation as for the equilibrium case and, therefore, the Landau-Lifshitz-Gilbert equation is valid in all cases of time development. The nonequilibrium definition of the magnetization in this paper has the following physical meaning. After the magnetization reaches a final value, the invariant operator reduces to the Hamiltonian itself, $\hat{I}(\infty) = \hat{H}(\infty)$, and the magnetization with respect to the density operator, $e^{-\beta\hat{I}}$, is nothing but a thermal ensemble average of the magnetic moment operator.

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