

Postprint: On the General Form of the Spin Semiclassical Langevin Equation

Authors: Li Dezhang, Lu Zhiwei, Zhao Yujun, Yang Xiaobao, Yang Xiaobao

Date: 2023-08-25T00:00:00+00:00

Abstract

At finite temperatures, the stochastic dynamical behavior of spin semiclassical systems is typically described by the stochastic Landau-Lifshitz equation. Within the framework of Langevin stochastic differential equations, this paper derives the general form of an effective Langevin equation and the expression for its corresponding Fokker-Planck equation. This effective Langevin equation can correctly describe the statistical physical properties of spin semiclassical systems in the canonical ensemble, and reduces to the spin semiclassical equation of motion when the damping and stochastic terms vanish; therefore, it represents a generalization of the stochastic Landau-Lifshitz equation. In both Cartesian and spherical coordinate systems, we present explicit expressions for the general form of the effective Langevin equation and the corresponding Fokker-Planck equation. In the spherical coordinate system, we discuss the longitudinal field effect in the Langevin equation and provide a criterion for determining whether the longitudinal field effect is included based on the form the equation takes. Finally, the effective Langevin equation is applied to a system of a single spin in a constant external magnetic field. By adopting a specific form of the equation, we obtain a straightforward solution and successfully derive the Boltzmann steady-state distribution, which also verifies the accuracy of the effective Langevin equation.

Full Text

Study of the General Form of Spin Semiclassical Langevin Equation*

Li De-Zhang¹⁾, Lu Zhi-Wei²⁾, Zhao Yu-Jun¹⁾, Yang Xiao-Bao^{1)†}

¹⁾ School of Physics and Optoelectronics, South China University of Technology, Guangzhou 510640, China

²⁾ Department of Applied Physics, School of Engineering Sciences, KTH Royal Institute of Technology, Stockholm SE-10691, Sweden

The stochastic dynamics of spin semiclassical systems at finite temperature is usually described by the stochastic Landau-Lifshitz equation. Within the framework of Langevin stochastic differential equations, this paper derives the general form of an effective Langevin equation and the corresponding Fokker-Planck equation. This effective Langevin equation correctly describes the statistical physical properties of spin semiclassical systems in the canonical ensemble, and reduces to the spin semiclassical equation of motion when the damping and stochastic terms vanish, thus representing a generalization of the stochastic Landau-Lifshitz equation. Explicit expressions for the effective Langevin equation and the corresponding Fokker-Planck equation are presented in both Cartesian and spherical coordinates. In spherical coordinates, the longitudinal field effect in the Langevin equation is discussed, and criteria for determining whether the longitudinal field effect is included are provided based on the form of the equation. Finally, the effective Langevin equation is applied to a system of a single spin in a constant external magnetic field. By adopting a specific form of the equation, a straightforward solution is obtained and the Boltzmann stationary distribution is successfully derived, which also verifies the accuracy of the effective Langevin equation.

Keywords: stochastic Landau-Lifshitz equation, Langevin equation, Fokker-Planck equation, Boltzmann distribution

PACS: 05.20.-y, 05.10.Gg, 02.30.Jr

*Project supported by Guangdong Basic and Applied Basic Research Foundation (Grant No. 2021A1515010328), Key-Area Research and Development Program of Guangdong Province (Grant No. 2020B010183001) and National Natural Science Foundation of China (Grant No. 12074126).

† Corresponding author. E-mail: scxbyang@scut.edu.cn

First author. E-mail: lidezhang907@163.com

1 Introduction

Spin is an intrinsic property of particles that emerges from quantum mechanics. For magnetic materials and magnetic systems, spin is an essential element of study. Whether in theoretical analysis, experimental observation, or computational simulations driven by the rapid development of computer technology, spin effects must be considered in magnetic research. This paper does not study spin effects and magnetic properties in magnetic systems from the perspective of quantum mechanics, but rather examines spin systems from the viewpoint of statistical physics. Spin has no classical counterpart, although it shares similarities with angular momentum in classical mechanics. Therefore, within the framework of semiclassical approximation, this paper considers the statistical physical properties of spin semiclassical systems. In this framework, spin is treated as a semiclassical mechanical quantity. For spin semiclassical systems,

the statistical distribution studied in this paper is the classical Boltzmann distribution in the canonical ensemble, with the primary tool being the Langevin stochastic differential equation for spin semiclassical systems.

The spin variable in a semiclassical system is represented by a three-dimensional vector $\mathbf{S}$. The semiclassical equation of motion for the system is [?]:

$$\frac{d\mathbf{S}}{dt} = -\gamma \mathbf{S} \times \mathbf{H}_{\text{eff}} \quad (1)$$

Here we adopt Cartesian coordinate notation. In the equation, $H(\mathbf{S})$ is the Hamiltonian of the system, $\mathbf{H}_{\text{eff}} = \partial H / \partial \mathbf{S}$ is the effective field vector for spin $\mathbf{S}$, γ is the gyromagnetic ratio, and $\times$ denotes the vector cross product. This equation can be derived and understood through various methods, such as derivations based on fundamental principles of quantum mechanics [?, ?], derivations using semiclassical approximations of Poisson brackets [?], and descriptions employing magnetic torque analogous to the relationship between angular momentum and torque in classical mechanics [?], among others, which will not be discussed in detail here.

At finite temperature, the most commonly used tool for describing the stochastic motion of spin systems is the stochastic Landau-Lifshitz equation [?]:

$$d\mathbf{S} = -\gamma \mathbf{S} \times \mathbf{H}_{\text{eff}} dt + \lambda \mathbf{S} \times (\mathbf{S} \times \mathbf{H}_{\text{eff}}) dt + \mathbf{S} \times \mathbf{h}_{\text{th}} dt \quad (2)$$

This is a Langevin stochastic differential equation that adds damping and stochastic terms to the semiclassical equation of motion. Here λ is the damping factor, and $\mathbf{h}_{\text{th}}$ is a Gaussian white noise random vector satisfying:

$$\langle h_{\text{th},i}(t) \rangle = 0, \quad \langle h_{\text{th},i}(t) h_{\text{th},j}(t') \rangle = 2\mu \delta_{ij} \delta(t - t') \quad (3)$$

or equivalently:

$$\langle \mathbf{h}_{\text{th}}(t) \mathbf{h}_{\text{th}}^T(t') \rangle = 2\mu \mathbf{1} \delta(t - t') \quad (4)$$

where $\mathbf{1}$ is the identity matrix. The coefficient $S\mu$ preceding the stochastic process generally must satisfy the fluctuation-dissipation relation:

$$\mu = \frac{\lambda k_B T}{\gamma} \quad (5)$$

to ensure that the Boltzmann distribution:

$$\rho_{\text{eq}}(\mathbf{S}) = \frac{1}{Z} \exp \left(-\frac{H(\mathbf{S})}{k_B T} \right) \quad (6)$$

is a stable solution of this stochastic differential equation. Here k_B is the Boltzmann constant, T is temperature, and Z is the normalization constant. The stochastic Landau-Lifshitz equation is a transverse field equation of motion that maintains the magnitude of spin constant, thus not containing longitudinal field effects. When the stochastic term is not included, or when the system is at zero temperature where the stochastic term vanishes, the stochastic Landau-Lifshitz equation reduces to the deterministic Landau-Lifshitz-Gilbert equation [?, ?].

The main object of study in this paper is the effective Langevin equation used to describe the stochastic motion of spin semiclassical variables. The paper specifically discusses the general form of this effective Langevin equation and the stationary solution of its corresponding Fokker-Planck equation. The results obtained can be regarded as a generalization and supplement to the stochastic Landau-Lifshitz equation. The consideration of the general form of the effective Langevin equation is based on satisfying two requirements: (1) having the classical Boltzmann distribution as the stationary distribution, thereby correctly describing the statistical properties of spin systems in the canonical ensemble; and (2) reducing to the spin semiclassical equation of motion (1) when the damping and stochastic fluctuation terms vanish. Section 2 of this paper derives the general form of the effective Langevin equation in Cartesian coordinates based on these two requirements. Section 3 expresses the results obtained in Section 2 in spherical coordinates, yielding the effective Langevin equation and the corresponding Fokker-Planck equation in spherical coordinates. In spherical coordinates, the longitudinal field effect in the Langevin equation can be discussed and judged more conveniently. Additionally, the paper demonstrates the process of selecting a specific form of the effective Langevin equation and solving it using a concrete simple system as an example. Choosing an appropriate form makes solving the equation and analyzing the system's statistical distribution more straightforward. Finally, Section 4 provides a summary of this work.

2 Spin Semiclassical Langevin Equation and Fokker-Planck Equation

Consider a system described by a Langevin equation, with $\mathbf{S}$ representing the system variable. In the specific example studied here, $\mathbf{S}$ is the spin vector. The Langevin equation generally takes the following form:

$$d\mathbf{S} = \mathbf{a}(\mathbf{S})dt + \mathbf{B}(\mathbf{S}) \cdot \mathbf{h}(t)dt \quad (7)$$

where $\mathbf{a}(\mathbf{S})$ is a vector with the same dimension as $\mathbf{S}$, $\mathbf{B}(\mathbf{S})$ is the coefficient matrix before the stochastic process $\mathbf{h}(t)$, and $\mathbf{h}(t)$ is a Gaussian random vector with the same properties as the stochastic process in (2), satisfying equations (3) and (4). $\mathbf{h}(t)$ can be viewed as the formal derivative of a Wiener process with respect to time. The Langevin equation (7) consists of a deterministic part $\mathbf{a}(\mathbf{S})$ and a stochastic process part $\mathbf{B}(\mathbf{S})\mathbf{h}$. If the coefficient $\mathbf{B}(\mathbf{S})$ depends on the system variable $\mathbf{S}$, the stochastic part is called multiplicative noise; otherwise,

it is called additive noise (for example, when $\mathbf{B}$ is a constant matrix). When the system undergoes stochastic motion following the Langevin equation, the time evolution of its time-dependent probability density distribution $\rho(\mathbf{S}, t)$ is typically described by the famous Fokker-Planck equation. Different stochastic integral interpretations of the Langevin equation lead to different forms of the Fokker-Planck equation, with the most common being the Itô and Stratonovich stochastic integral forms. These two integral forms may produce differences when handling the noise-induced drift term, resulting in different expressions for the Fokker-Planck equation. For stochastic processes with multiplicative noise, this difference is non-zero, whereas for additive noise, this difference does not exist. Since the Stratonovich stochastic integral is generally preferred in physical applications, we adopt the form derived from Stratonovich stochastic integration, which yields the following Fokker-Planck equation [?]:

$$\frac{\partial \rho(\mathbf{S}, t)}{\partial t} = -\frac{\partial}{\partial S_i} [a_i(\mathbf{S})\rho(\mathbf{S}, t)] + \frac{1}{2} \frac{\partial^2}{\partial S_i \partial S_j} [B_{ik}(\mathbf{S})B_{jk}(\mathbf{S})\rho(\mathbf{S}, t)] \quad (8)$$

where S_i refers to the i -th component of $\mathbf{S}$, and $B_{ik}(\mathbf{S})$ refers to the matrix element in the i -th row and k -th column of $\mathbf{B}(\mathbf{S})$. It is easy to see that for stochastic processes with additive noise, the second term on the right-hand side of the equation is zero, and the remaining part is the common result of both Itô and Stratonovich stochastic integrals. Writing the right-hand side of the equation in the form of a time evolution operator $\mathcal{L}$, we have:

$$\frac{\partial \rho(\mathbf{S}, t)}{\partial t} = \mathcal{L}\rho(\mathbf{S}, t) \quad (9)$$

The probability density distribution function $\rho(\mathbf{S}, t)$ evolves from an initial distribution at time $t = 0$ (for example, $\rho(\mathbf{S}, 0) = \delta(\mathbf{S} - \mathbf{S}_0)$) according to the Fokker-Planck equation (8), eventually reaching the long-time limit stationary state $\rho(\infty, \mathbf{S})$, which is the stable solution of the Fokker-Planck equation. This stationary solution is commonly referred to as the stationary or invariant distribution, and in this paper we denote it as $\rho_{\text{st}}(\mathbf{S})$, where the subscript “st” indicates stationary. Obviously, the time derivative of $\rho_{\text{st}}(\mathbf{S})$ is zero, so substituting $\rho_{\text{st}}(\mathbf{S})$ into the right-hand side of the Fokker-Planck equation (8) yields zero, that is:

$$\mathcal{L}\rho_{\text{st}}(\mathbf{S}) = 0 \quad (10)$$

The system studied in this paper is a spin semiclassical system. Our research framework explores Langevin equations suitable for spin semiclassical systems such that they have the classical Boltzmann distribution as a stable solution and reduce to the spin semiclassical equation of motion (1) when the damping and stochastic terms vanish. Starting from this premise and focusing on the specific example of spin systems, the form of the Langevin equation is:

$$d\mathbf{S} = [-\gamma\mathbf{S} \times \mathbf{H}_{\text{eff}} + \mathbf{b}(\mathbf{S})] dt + \mathbf{B}(\mathbf{S}) \cdot \mathbf{h}(t)dt \quad (11)$$

The semiclassical equation of motion and the damping term together constitute the deterministic part of the equation, where $\mathbf{b}(\mathbf{S})$ is the damping coefficient. The stochastic part is still written as the product of the coefficient matrix $\mathbf{B}(\mathbf{S})$ and the Gaussian white noise random vector $\mathbf{h}(t)$. For convenience, we include a constant $S\mu$, similar to the stochastic Landau-Lifshitz equation (2). Adopting this form for the Langevin equation obviously satisfies the requirement of reducing to the semiclassical equation of motion (1) when both damping and stochastic parts disappear.

Let us now analyze the corresponding Fokker-Planck equation. According to equation (8), we can directly write:

$$\frac{\partial \rho(\mathbf{S}, t)}{\partial t} = -\frac{\partial}{\partial S_i} [(-\gamma(\mathbf{S} \times \mathbf{H}_{\text{eff}})_i + b_i(\mathbf{S})) \rho(\mathbf{S}, t)] + \frac{1}{2} \frac{\partial^2}{\partial S_i \partial S_j} [B_{ik}(\mathbf{S}) B_{jk}(\mathbf{S}) \rho(\mathbf{S}, t)] \quad (12)$$

The third term on the right-hand side of equation (9) obviously satisfies:

$$\frac{\partial}{\partial S_i} (\mathbf{S} \times \mathbf{H}_{\text{eff}})_i = 0 \quad (13)$$

Thus, equation (9) can be written in a more compact form:

$$\frac{\partial \rho(\mathbf{S}, t)}{\partial t} = -\frac{\partial}{\partial S_i} [b_i(\mathbf{S}) \rho(\mathbf{S}, t)] + \frac{1}{2} \frac{\partial^2}{\partial S_i \partial S_j} [B_{ik}(\mathbf{S}) B_{jk}(\mathbf{S}) \rho(\mathbf{S}, t)] \quad (14)$$

The time-dependent probability density function $\rho(\mathbf{S}, t)$ of the system satisfies this evolution equation. We require that its stationary solution in the long-time limit, $\rho_{\text{st}}(\mathbf{S})$, be the Boltzmann distribution:

$$\rho_{\text{st}}(\mathbf{S}) = \frac{1}{Z} \exp \left(-\frac{H(\mathbf{S})}{k_B T} \right) \quad (15)$$

Substituting the specific form of the Boltzmann distribution into the right-hand side should yield zero. The first term, through vector algebra analysis, is easily found to be zero. To ensure the second term is zero, a natural choice is:

$$b_i(\mathbf{S}) = \lambda B_{ik}(\mathbf{S}) B_{jk}(\mathbf{S}) \frac{\partial H}{\partial S_j} \quad (16)$$

Equation (15) represents the fluctuation-dissipation relation. With this choice, the Boltzmann distribution satisfies the Fokker-Planck equation as a stable solution. The Langevin equation (11) can then be written explicitly as:

$$d\mathbf{S} = \left[-\gamma \mathbf{S} \times \mathbf{H}_{\text{eff}} + \lambda \mathbf{B}(\mathbf{S}) \mathbf{B}^T(\mathbf{S}) \cdot \frac{\partial H}{\partial \mathbf{S}} \right] dt + \mathbf{B}(\mathbf{S}) \cdot \mathbf{h}(t) dt \quad (17)$$

Equations (16) and (17) constitute an effective unified framework, where the matrix $\mathbf{B}(\mathbf{S})$ remains to be determined. By appropriately selecting the matrix $\mathbf{B}(\mathbf{S})$, one can obtain effective Langevin equations describing the statistical behavior of spin semiclassical systems in the canonical ensemble. This is the main result obtained in Cartesian coordinates in this paper.

It is easy to verify that if we choose the matrix $\mathbf{B}(\mathbf{S})$ as:

$$\mathbf{B}_{\text{LL}}(\mathbf{S}) = \begin{pmatrix} 0 & -S_z & S_y \\ S_z & 0 & -S_x \\ -S_y & S_x & 0 \end{pmatrix} \quad (18)$$

then for any vector $\mathbf{y}$ we have $\mathbf{B}_{\text{LL}}(\mathbf{S})\mathbf{y} = -\mathbf{S} \times \mathbf{y}$, and $\mathbf{B}_{\text{LL}}(\mathbf{S})\mathbf{B}_{\text{LL}}^T(\mathbf{S}) = S^2 \mathbf{1} - \mathbf{S}\mathbf{S}^T$. The Langevin equation (17) then becomes:

$$d\mathbf{S} = -\gamma \mathbf{S} \times \mathbf{H}_{\text{eff}} dt + \lambda \mathbf{S} \times (\mathbf{S} \times \mathbf{H}_{\text{eff}}) dt + \mathbf{S} \times \mathbf{h}_{\text{th}} dt \quad (19)$$

This is precisely the stochastic Landau-Lifshitz equation (2). Thus, the stochastic Landau-Lifshitz equation can be regarded as a specific form of the effective Langevin equation obtained here. We denote the choice of $\mathbf{B}(\mathbf{S})$ in (18) as $\mathbf{B}_{\text{LL}}(\mathbf{S})$. Substituting $\mathbf{B}_{\text{LL}}(\mathbf{S})$ into (17), we can directly write the explicit expression for its Fokker-Planck equation:

$$\frac{\partial \rho(\mathbf{S}, t)}{\partial t} = -\frac{\partial}{\partial \mathbf{S}} \cdot \left[-\gamma \mathbf{S} \times \mathbf{H}_{\text{eff}} \rho + \lambda k_B T \mathbf{S} \times \left(\mathbf{S} \times \frac{\partial \rho}{\partial \mathbf{S}} \right) \right] \quad (20)$$

Many previous studies have conducted detailed derivations and analyses of this expression [?, ?], which can be viewed here as a specific form of a unified framework.

3 Spherical Coordinate Form and Longitudinal Field Effects

Analyzing the stochastic Landau-Lifshitz equation (20), it is evident that the magnitude S of the spin variable remains constant in the equation, because the time derivative of S is perpendicular to $\mathbf{S}$, and S does not change during time evolution. Solving the stochastic Landau-Lifshitz equation thus yields a probability distribution of $\mathbf{S}$ on a sphere of fixed radius. This indicates that the stochastic Landau-Lifshitz equation includes only transverse field effects and no

longitudinal field effects. For probability distributions on a sphere, a natural approach is to transform the system to spherical coordinates and analyze the form of the stochastic differential equation and its corresponding probability density function. This section derives the general form of the effective Langevin equation in spherical coordinates, obtains its corresponding Fokker-Planck equation, and determines whether longitudinal field effects are present in the Langevin equation.

3.1 Effective Langevin Equation and Fokker-Planck Equation in Spherical Coordinates

For the spin vector $\mathbf{S}$, its spherical coordinate representation is $\mathbf{S}_{\text{sph}} = (S, \theta, \phi)$, where S is the magnitude of $\mathbf{S}$, θ is the angle between $\mathbf{S}$ and the z -axis in Cartesian coordinates ($0 \leq \theta \leq \pi$), and ϕ is the angle between the projection of $\mathbf{S}$ onto the xy -plane and the x -axis ($0 \leq \phi < 2\pi$). For convenience, we denote $\mathbf{S}_{\text{sph}} = (S_1, S_2, S_3)$, where the subscript “sph” indicates spherical. The relationship between spherical and Cartesian coordinate variables is:

$$S_x = S \sin \theta \cos \phi, \quad S_y = S \sin \theta \sin \phi, \quad S_z = S \cos \theta \quad (21)$$

The Jacobian matrix of the coordinate transformation and its inverse matrix are respectively:

$$\mathbf{C} = \frac{\partial \mathbf{S}}{\partial \mathbf{S}_{\text{sph}}^T} = \begin{pmatrix} \sin \theta \cos \phi & S \cos \theta \cos \phi & -S \sin \theta \sin \phi \\ \sin \theta \sin \phi & S \cos \theta \sin \phi & S \sin \theta \cos \phi \\ \cos \theta & -S \sin \theta & 0 \end{pmatrix} \quad (22)$$

$$\mathbf{D} = \mathbf{C}^{-1} = \begin{pmatrix} \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \\ \frac{\cos \theta \cos \phi}{S} & \frac{\cos \theta \sin \phi}{S} & -\frac{\sin \theta}{S} \\ -\frac{\sin \phi}{S \sin \theta} & \frac{\cos \phi}{S \sin \theta} & 0 \end{pmatrix} \quad (23)$$

The Jacobian determinant of the coordinate transformation is $J = S^2 \sin \theta$.

For spherical coordinates $\mathbf{S}_{\text{sph}}$, the Boltzmann distribution takes the form:

$$\rho_{\text{eq}}(\mathbf{S}_{\text{sph}}) = \frac{1}{Z} \exp \left(-\frac{H_{\text{sph}}(\mathbf{S}_{\text{sph}})}{k_B T} \right) \quad (24)$$

where we define the effective spherical coordinate Hamiltonian:

$$H_{\text{sph}}(\mathbf{S}_{\text{sph}}) = H(\mathbf{S}(\mathbf{S}_{\text{sph}})) \quad (25)$$

Using the transformation matrix, we can conveniently convert the Langevin equation (16) obtained in the previous section to spherical coordinates:

$$d\mathbf{S}_{\text{sph}} = \mathbf{D} \cdot \left[-\gamma \mathbf{S} \times \mathbf{H}_{\text{eff}} + \lambda \mathbf{B}(\mathbf{S}) \mathbf{B}^T(\mathbf{S}) \cdot \frac{\partial H}{\partial \mathbf{S}} \right] dt + \mathbf{D} \cdot \mathbf{B}(\mathbf{S}) \cdot \mathbf{h}(t) dt \quad (26)$$

Let us analyze each term on the right-hand side. First, corresponding to $\mathbf{B}_{\text{LL}}(\mathbf{S})$ in the stochastic Landau-Lifshitz equation [see (18)], we have:

$$\mathbf{D} \cdot \mathbf{B}_{\text{LL}}(\mathbf{S}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\frac{\cos \theta}{S} & -\frac{\sin \phi}{\sin \theta} \\ 0 & \frac{\cos \phi}{\sin \theta} & -\cot \theta \sin \phi \end{pmatrix} \quad (27)$$

Thus, the first term on the right-hand side of (26) becomes:

$$\mathbf{D} \cdot [-\gamma \mathbf{S} \times \mathbf{H}_{\text{eff}}] = -\gamma \begin{pmatrix} 0 \\ \frac{1}{S} \frac{\partial H_{\text{sph}}}{\partial \theta} \\ -\frac{1}{S \sin \theta} \frac{\partial H_{\text{sph}}}{\partial \phi} \end{pmatrix} \quad (28)$$

For the second term, we first have:

$$\frac{\partial H}{\partial \mathbf{S}} = \mathbf{C}^{-T} \cdot \frac{\partial H_{\text{sph}}}{\partial \mathbf{S}_{\text{sph}}} = \mathbf{D}^T \cdot \frac{\partial H_{\text{sph}}}{\partial \mathbf{S}_{\text{sph}}} \quad (29)$$

Next, we analyze the vector $\mathbf{b}(\mathbf{S})$. The components of $\mathbf{b}(\mathbf{S})$ were defined in (10), and here we express them using spherical coordinate variables:

$$b_i(\mathbf{S}) = \lambda B_{ik}(\mathbf{S}) B_{jk}(\mathbf{S}) \frac{\partial H}{\partial S_j} = \lambda B_{ik}(\mathbf{S}) B_{jk}(\mathbf{S}) D_{mj} \frac{\partial H_{\text{sph}}}{\partial S_{\text{sph},m}} \quad (30)$$

The last step uses $\mathbf{D}^T$ to denote the transpose of $\mathbf{D}$ and utilizes results derived from (23). From (30), we can clearly express the vector $\mathbf{b}(\mathbf{S})$ in a more compact form:

$$\mathbf{b}(\mathbf{S}) = \lambda \mathbf{B}(\mathbf{S}) \mathbf{B}^T(\mathbf{S}) \mathbf{D}^T \cdot \frac{\partial H_{\text{sph}}}{\partial \mathbf{S}_{\text{sph}}} = \lambda \mathbf{C}^T \mathbf{d}(\mathbf{S}_{\text{sph}}) \quad (31)$$

where the vector $\mathbf{d}(\mathbf{S}_{\text{sph}})$ is defined as:

$$d_m(\mathbf{S}_{\text{sph}}) = B_{ik}(\mathbf{S}) B_{jk}(\mathbf{S}) D_{mj} D_{nj} \frac{\partial H_{\text{sph}}}{\partial S_{\text{sph},n}} \quad (32)$$

This definition is similar in form to $\mathbf{b}(\mathbf{S})$ in Cartesian coordinates. Now substituting (28), (29), and (31) into (26), we obtain:

$$d\mathbf{S}_{\text{sph}} = \left[-\gamma \begin{pmatrix} 0 \\ \frac{1}{S} \frac{\partial H_{\text{sph}}}{\partial \theta} \\ -\frac{1}{S \sin \theta} \frac{\partial H_{\text{sph}}}{\partial \phi} \end{pmatrix} + \lambda \mathbf{d}(\mathbf{S}_{\text{sph}}) \right] dt + \mathbf{D} \cdot \mathbf{B}(\mathbf{S}) \cdot \mathbf{h}(t) dt \quad (33)$$

This is the spherical coordinate form of the effective Langevin equation (16). The selection of matrix $\mathbf{B}$ now transforms into the selection of matrix $\mathbf{D}$. The choice corresponding to the stochastic Landau-Lifshitz equation is $\mathbf{D}_{\text{LL}}$ shown in (28), where the first row is a zero vector.

For the time evolution of the probability density function $\rho(\mathbf{S}_{\text{sph}}, t)$, it satisfies the Fokker-Planck equation in spherical coordinates. Similar to the analysis in Section 2, we can obtain the spherical coordinate Fokker-Planck equation corresponding to (33):

$$\frac{\partial \rho(\mathbf{S}_{\text{sph}}, t)}{\partial t} = -\frac{\partial}{\partial S_{\text{sph},i}} \left[(-\gamma(\mathbf{S} \times \mathbf{H}_{\text{eff}})_{\text{sph},i} + \lambda d_i(\mathbf{S}_{\text{sph}})) \rho(\mathbf{S}_{\text{sph}}, t) \right] + \frac{1}{2} \frac{\partial^2}{\partial S_{\text{sph},i} \partial S_{\text{sph},j}} \left[(\mathbf{D}\mathbf{B}(\mathbf{S})\mathbf{B}^T(\mathbf{S})\mathbf{D}^T)_{ij} \rho(\mathbf{S}_{\text{sph}}, t) \right] \quad (34)$$

It is straightforward to verify that the Boltzmann distribution in spherical coordinates (24) is a stable solution of this Fokker-Planck equation. Substituting (24) into the right-hand side of (34) yields zero, demonstrating the validity of this Langevin equation in spherical coordinates. Equations (33) and (34) represent the spherical coordinate manifestation of the general forms of the effective Langevin equation and its corresponding Fokker-Planck equation (16) and (17). This is the main result obtained in spherical coordinates in this paper.

3.2 Discussion of Longitudinal Field Effects

From the spherical coordinate form of the effective Langevin equation (33), we can directly see that if only transverse field effects are present, conserving the magnitude S , the first row of matrix $\mathbf{D}$ must be a zero vector. The $\mathbf{D}_{\text{LL}}$ for the stochastic Landau-Lifshitz equation [see (28)] is an example satisfying this condition. Writing out the explicit spherical coordinate form of the stochastic Landau-Lifshitz equation:

$$d\mathbf{S}_{\text{sph}} = \begin{pmatrix} 0 \\ -\gamma \frac{1}{S} \frac{\partial H_{\text{sph}}}{\partial \theta} + \lambda \frac{1}{S^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial H_{\text{sph}}}{\partial \theta}) + \lambda \frac{1}{S^2 \sin^2 \theta} \frac{\partial^2 H_{\text{sph}}}{\partial \phi^2} \\ \gamma \frac{1}{S \sin \theta} \frac{\partial H_{\text{sph}}}{\partial \phi} + \lambda \frac{1}{S^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial H_{\text{sph}}}{\partial \phi}) - \lambda \frac{\cot \theta}{S^2} \frac{\partial H_{\text{sph}}}{\partial \phi} \end{pmatrix} dt + \begin{pmatrix} 0 \\ \frac{\sqrt{2\lambda k_B T}}{S} \eta_\theta(t) \\ \frac{\sqrt{2\lambda k_B T}}{S \sin \theta} \eta_\phi(t) \end{pmatrix} dt \quad (35)$$

where S is constant, and the equation reduces to two stochastic differential equations for the angular variables:

$$\begin{aligned}
d\theta &= \left(-\gamma \frac{1}{S} \frac{\partial H_{\text{sph}}}{\partial \theta} + \lambda \frac{1}{S^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial H_{\text{sph}}}{\partial \theta} \right) + \lambda \frac{1}{S^2 \sin^2 \theta} \frac{\partial^2 H_{\text{sph}}}{\partial \phi^2} \right) dt + \frac{\sqrt{2\lambda k_B T}}{S} \eta_\theta(t) dt \\
d\phi &= \left(\gamma \frac{1}{S \sin \theta} \frac{\partial H_{\text{sph}}}{\partial \phi} + \lambda \frac{1}{S^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial H_{\text{sph}}}{\partial \phi} \right) - \lambda \frac{\cot \theta}{S^2} \frac{\partial H_{\text{sph}}}{\partial \phi} \right) dt + \frac{\sqrt{2\lambda k_B T}}{S \sin \theta} \eta_\phi(t) dt
\end{aligned} \tag{36}$$

Correspondingly, the probability density function $\rho(\theta, \phi, t)$ contains only the two angular variables and time variable, and the Fokker-Planck equation can be written as:

$$\frac{\partial \rho}{\partial t} = -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \left(-\gamma \frac{1}{S} \frac{\partial H_{\text{sph}}}{\partial \theta} + \lambda \frac{k_B T}{S^2} \frac{\partial}{\partial \theta} \right) \rho \right] - \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \left[\left(\gamma \frac{1}{S \sin \theta} \frac{\partial H_{\text{sph}}}{\partial \phi} + \lambda \frac{k_B T}{S^2 \sin^2 \theta} \frac{\partial}{\partial \phi} \right) \rho \right] \tag{37}$$

This result has been analyzed and discussed in many works [?, ?]. If the first row of matrix $\mathbf{D}$ is not a zero vector, the Langevin equation includes longitudinal field effects, and the magnitude S cannot remain constant. In reference [?], the authors proposed a Langevin equation that includes longitudinal field fluctuations and showed that the stochastic Landau-Lifshitz equation is a projection of this equation onto a sphere of radius S . In our framework, this equation is obtained by simply choosing $\mathbf{B} = \mathbf{1}$ in (16), or equivalently choosing $\mathbf{D} = \mathbf{C}^{-1}$ in spherical coordinates. The first row of matrix $\mathbf{D}$ chosen this way is obviously not a zero vector, so the equation includes longitudinal field effects. In addition to Langevin equations, studies of longitudinal field effects can also be found in Monte Carlo simulations [?].

If only transverse field effects are considered, the effective Langevin equation can also take forms other than the stochastic Landau-Lifshitz equation. In reference [?], the authors adopted:

$$\mathbf{D} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{S} & 0 \\ 0 & 0 & \frac{1}{S \sin \theta} \end{pmatrix} \tag{38}$$

It can be seen that, compared with the stochastic Landau-Lifshitz equation (40), the Langevin equation in this form has coupled dynamics in both angular variables during evolution, meaning the equations of motion are not independent. The main difference lies in the stochastic part: this equation requires only a 2-dimensional Gaussian random vector field, whereas the stochastic Landau-Lifshitz equation requires a full 3-dimensional Gaussian stochastic process. Detailed analysis and numerical calculations of this equation are not discussed here.

3.3 Simple Application

This paper has obtained the general form of the effective Langevin equation applicable to spin semiclassical systems, presenting expressions for the effective Langevin equation and its corresponding Fokker-Planck equation in both Cartesian and spherical coordinates. For specific systems with specific Hamiltonians, selecting a particular form may simplify the solution of the equations. This section discusses a relatively simple system, selecting one form of the effective Langevin equation and solving it.

Consider a system of a single spin in a constant external magnetic field $\mathbf{H}$. The Hamiltonian of the system is the Zeeman energy of the spin in the magnetic field:

$$H = -\mathbf{m} \cdot \mathbf{H} = -\gamma \mathbf{S} \cdot \mathbf{H} \quad (39)$$

Since $\mathbf{H}$ is a constant vector, for convenience we can set the direction of $\mathbf{H}$ as the positive z -axis direction, so the Hamiltonian becomes $H = -\gamma S H \cos \theta$, which does not contain ϕ . The spherical coordinate Hamiltonian has the simple form:

$$H_{\text{sph}}(S, \theta) = -\gamma S H \cos \theta \quad (40)$$

Substituting this into the general form of the effective Langevin equation (33) yields:

$$d\mathbf{S}_{\text{sph}} = \begin{pmatrix} 0 \\ \gamma H \sin \theta + \lambda d_2 \\ \lambda d_3 \end{pmatrix} dt + \mathbf{D} \cdot \mathbf{B}(\mathbf{S}) \cdot \mathbf{h}(t) dt \quad (41)$$

To ensure a legitimate Boltzmann distribution, we do not introduce longitudinal field effects, so S is constant, and the system's Boltzmann distribution does not explicitly depend on ϕ . For matrix $\mathbf{D}$, we choose the very simple form:

$$\mathbf{D} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{S} & 0 \\ 0 & 0 & \frac{1}{S} \end{pmatrix} \quad (42)$$

The resulting explicit expression for the Langevin equation is:

$$\begin{aligned} d\theta &= \left(\gamma H \sin \theta - \lambda \frac{k_B T}{S} \cot \theta \right) dt + \frac{\sqrt{2\lambda k_B T}}{S} \eta_\theta(t) dt \\ d\phi &= \frac{\sqrt{2\lambda k_B T}}{S \sin \theta} \eta_\phi(t) dt \end{aligned} \quad (43)$$

It can be seen that the equations of motion for the two angular variables are independent Langevin equations. Solving these two equations separately yields the probability distributions for θ and ϕ .

First, we analyze the equation for θ :

$$d\theta = \left(\gamma H \sin \theta - \lambda \frac{k_B T}{S} \cot \theta \right) dt + \frac{\sqrt{2\lambda k_B T}}{S} \eta_\theta(t) dt \quad (44)$$

This is an overdamped form of the Langevin equation. Clearly, this equation has an additive noise stochastic process, with the coefficient before the stochastic term and the damping factor satisfying the fluctuation-dissipation relation. Using the analysis method from Section 2, it is easy to see that the stationary distribution obtained from this Langevin equation is the Boltzmann distribution for θ :

$$\rho_{\text{st}}(\theta) = \frac{1}{Z_\theta} \exp \left(\frac{\gamma S H \cos \theta}{k_B T} \right) \sin \theta \quad (45)$$

The formal solution of this equation can be written directly. Next, consider ϕ :

$$d\phi = \frac{\sqrt{2\lambda k_B T}}{S \sin \theta} \eta_\phi(t) dt \quad (46)$$

The formal solution is:

$$\phi(t) = \phi_0 + \int_0^t \frac{\sqrt{2\lambda k_B T}}{S \sin \theta(s)} dW_\phi(s) \quad (47)$$

where ϕ_0 is the initial condition. From the formal solution, we see that $\phi(t)$ follows a Gaussian distribution with mean ϕ_0 and variance:

$$\text{Var}[\phi(t)] = \int_0^t \frac{2\lambda k_B T}{S^2 \sin^2 \theta(s)} ds \quad (48)$$

If ϕ were an unbounded variable on the real line, the time-dependent probability density in the long-time limit would have only the trivial solution 0, and no stationary distribution would exist. However, in spherical coordinates, ϕ is confined to the interval $[0, 2\pi)$, and the formal solution (47) of the Langevin equation should include periodic boundary conditions. Clearly, under periodic boundary conditions, the mean of the random variable $\phi(t)$ also lies in the interval $[0, 2\pi)$. In this case, the Gaussian probability density (48) in the long-time limit should approach a uniform probability density over the interval of the random variable. Consequently, the stationary distribution for ϕ is uniform on $[0, 2\pi)$:

$$\rho_{\text{st}}(\phi) = \frac{1}{2\pi} \quad (49)$$

Thus, the total stationary distribution of the system in spherical coordinates can be obtained:

$$\rho_{\text{st}}(\theta, \phi) = \rho_{\text{st}}(\theta)\rho_{\text{st}}(\phi) = \frac{1}{2\pi Z_\theta} \exp\left(\frac{\gamma SH \cos \theta}{k_B T}\right) \sin \theta \quad (50)$$

This is precisely the Boltzmann distribution in spherical coordinates.

This section analyzes a specific system, selects a particular form of the effective Langevin equation, and solves it relatively easily to obtain the stationary Boltzmann distribution. This represents a simple application of the general form of the effective Langevin equation derived in this paper. Additionally, the transverse field spin semiclassical Langevin equation can take many forms beyond the stochastic Landau-Lifshitz equation, and this section provides a concrete example.

4 Conclusion

This paper, targeting the classical Boltzmann distribution in the canonical ensemble and starting from Langevin stochastic differential equations, derives the general form of an effective Langevin equation for spin semiclassical systems and the corresponding Fokker-Planck equation. This effective Langevin equation has the Boltzmann distribution as its stationary distribution, thus correctly describing the statistical physical properties of spin systems in the canonical ensemble. Moreover, when the damping and stochastic terms vanish, the equation reduces to the spin semiclassical equation of motion, thereby also encompassing the semiclassical motion modes of spin systems. This result represents a generalization and supplement to the stochastic Landau-Lifshitz equation. In spherical coordinates, the form of the equation allows for convenient determination of whether longitudinal field effects are included. In a specific system of a single spin in a constant external magnetic field, the effective Langevin equation was successfully applied to analyze the statistical distribution, verifying the accuracy of the equation. Simultaneously, this provides a concrete example of the many possible forms of transverse field spin Langevin equations beyond the stochastic Landau-Lifshitz equation. This work can broaden the application scope of Langevin stochastic differential equations as a theoretical and computational tool, while also providing a reference at the theoretical tool level for the study of dynamics and statistical mechanics of spin semiclassical systems.

References

- [1] Gilbert T L 2004 *IEEE Trans. Magn.* **40** 3443 <https://doi.org/10.1109/TMAG.2004.836740>
- [2] Antropov V P, Katsnelson M I, van Schilfgaarde M, Harmon B N 1995

- Phys. Rev. Lett.* **75** 729 <https://doi.org/10.1103/PhysRevLett.75.729>
- [3] Antropov V P, Katsnelson M I, Harmon B N, van Schilfgaarde M, Kusnezov D 1996 *Phys. Rev. B* **54** 1019 <https://doi.org/10.1103/PhysRevB.54.1019>
- [4] Ma P-W, Woo C H, Dudarev S L 2008 *Phys. Rev. B* **78** 024434 <https://doi.org/10.1103/PhysRevB.78.024434>
- [5] Guo B, Ding S 2008 *Landau-Lifshitz Equations* (Singapore: World Scientific)
- [6] Brown W F 1963 *Phys. Rev.* **130** 1677 <https://doi.org/10.1103/PhysRev.130.1677>
- [7] Kubo R, Hashitsume N 1970 *Prog. Theor. Phys. Suppl.* **46** 210 <https://doi.org/10.1143/ptps.46.210>
- [8] García-Palacios J L, Lázaro F J 1998 *Phys. Rev. B* **58** 14937 <https://doi.org/10.1103/PhysRevB.58.14937>
- [9] Ma P-W, Dudarev S L 2011 *Phys. Rev. B* **83** 134418 <https://doi.org/10.1103/PhysRevB.83.134418>
- [10] Coffey W T, Kalmykov Y P 2012 *J. Appl. Phys.* **112** 121301 <https://doi.org/10.1063/1.4754272>
- [11] Atxitia U, Hinzke D, Nowak U 2017 *J. Phys. D: Appl. Phys.* **50** 033003 <https://doi.org/10.1088/1361-6463/50/3/033003>
- [12] Landau L, Lifshitz E 1992 in *Perspectives in Theoretical Physics*, edited by L. P. Pitaevski (Amsterdam: Pergamon) p51
- [13] Saslow W M 2009 *J. Appl. Phys.* **105** 07D315 <https://doi.org/10.1063/1.3077204>
- [14] Lakshmanan M 2011 *Phil. Trans. R. Soc. A* **369** 1280 <https://doi.org/10.1098/rsta.2010.0319>
- [15] Eriksson O, Bergman A, Bergqvist L, Hellsvik J 2017 *Atomistic Spin Dynamics: Foundations and Applications* (New York: Oxford University Press)
- [16] Risken H 1989 *The Fokker-Planck Equation: Methods of Solution and Applications* (Berlin: Springer-Verlag)
- [17] Zwanzig R 2001 *Nonequilibrium Statistical Mechanics* (New York: Oxford University Press)
- [18] Kampen N G v 2009 *Stochastic Processes in Physics and Chemistry* 3rd ed (Amsterdam: Elsevier)
- [19] Klyatskin V I 2015 *Stochastic Equations: Theory and Applications in Acoustics, Hydrodynamics, Magnetohydrodynamics, and Radiophysics, Volume 1, Understanding Complex Systems* (Switzerland: Springer)
- [20] Garanin D A, Ishchenko V V, Panina L V 1990 *Theor. Math. Phys.* **82** 169 <https://doi.org/10.1007/BF01079045>
- [21] Garanin D A 1997 *Phys. Rev. B* **55** 3050 <https://doi.org/10.1103/PhysRevB.55.3050>
- [22] Martínez E, López-Díaz L, Torres L, Alejos O 2004 *Physica B* **343** 252 <https://doi.org/10.1016/j.physb.2003.08.103>
- [23] Mayergoyz I D, Bertotti G, Serpico C 2009 *Nonlinear Magnetization Dynamics in Nanosystems* (Amsterdam: Elsevier)
- [24] Ma P-W, Dudarev S L, Semenov A A, Woo C H 2010 *Phys. Rev. E* **82** 031111 <https://doi.org/10.1103/PhysRevE.82.031111>
- [25] Evans R F L, Hinzke D, Atxitia U, Nowak U, Chantrell R W, Chubykalo-Fesenko O 2012 *Phys. Rev. B* **85** 014433 <https://doi.org/10.1103/PhysRevB.85.014433>
- [26] Coffey W T, Geoghegan D 1996 *J. Mol. Liq.* **69** 1 [https://doi.org/10.1016/S0167-7322\(96\)90006-9](https://doi.org/10.1016/S0167-7322(96)90006-9)
- [27] Fredkin D R 2001 *Physica B* **306** 26 [https://doi.org/10.1016/S0921-4526\(01\)00958-9](https://doi.org/10.1016/S0921-4526(01)00958-9)

- [28] Cheng X Z, Jalil M B A, Lee H K, Okabe Y 2006 *Phys. Rev. Lett.* **96** 067208 <https://doi.org/10.1103/PhysRevLett.96.067208>
- [29] Denisov S I, Sakmann K, Talkner P, Hänggi P 2007 *Phys. Rev. B* **75** 184432 <https://doi.org/10.1103/PhysRevB.75.184432>
- [30] Serpico C, Bertotti G, d' Aquino M, Ragusa C, Ansalone P, Mayergoyz I D 2008 *IEEE Trans. Magn.* **44** 3157 <https://doi.org/10.1109/TMAG.2008.2001793>
- [31] Denisov S I, Polyakov A Y, Lyutyy T V 2011 *Phys. Rev. B* **84** 174410 <https://doi.org/10.1103/PhysRevB.84.174410>
- [32] Giordano S, Dusch Y, Tiercelin N, Pernod P, Preobrazhensky V 2013 *Eur. Phys. J. B* **86** 249 <https://doi.org/10.1140/epjb/e2013-40128-x>
- [33] Aron C, Barci D G, Cugliandolo L F, Arenas Z G, Lozano G S 2014 *J. Stat. Mech.* **2014** P09008 <https://doi.org/10.1088/1742-5468/2014/09/P09008>
- [34] Titov S V, Coffey W T, Zarifakis M, Kalmykov Y P, Titov A S 2021 *J. Magn. Mater.* **539** 168365 <https://doi.org/10.1016/j.jmmm.2021.168365>
- [35] Ma P-W, Dudarev S L 2012 *Phys. Rev. B* **86** 054416 <https://doi.org/10.1103/PhysRevB.86.054416>
- [36] Pan F, Chico J, Delin A, Bergman A, Bergqvist L 2017 *Phys. Rev. B* **95** 184432 <https://doi.org/10.1103/PhysRevB.95.184432>

Note: Figure translations are in progress. See original paper for figures.

Source: ChinaXiv –Machine translation. Verify with original.