Journal of Statistical Physics, Vol. 67, Nos. 5/6, 1992

A Stochastic Model for the Dynamics of a Classical Spin

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Received December 20, 1991

A stochastic model for the dynamics of a macroscopic or classical spin based on a classical generalized Lagrangian formalism is proposed. The model can be used to describe the evolution of the magnetic moment of superparamagnetic particles. In this sense, it is a generalization of the model proposed by Brown, allowing for fluctuations on the magnitudes of the magnetic moments of the particles. The corresponding covariant Fokker–Planck equation is also obtained.

KEY WORDS: Superparamagnetism; stochastic process; classical spin; Brownian motion.

1. INTRODUCTION

It is well known that macroscopic systems undergo irreversible processes which are treated, on the microscopic level, by quantum or classical statistical physics, but on a more phenomenological or thermodynamic level they are treated as dynamical processes of complete sets of macroscopic variables. In this second level of description, the dynamics can be either deterministic or stochastic, depending on the degree of precision adopted. The deterministic description can be viewed as the limit of the stochastic description, when the intensity of the fluctuations becomes negligible. On the other hand, in a stochastic description, the noise can have an external or internal origin.

The system in which we are interested here is a cluster of N ferromagnetically coupled atomic spins $\mathbf{s}_i$ constituting a magnetic monodomain. The coupling among these microspins is assumed to be

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sufficiently strong so that the quantum expectation value of the total spin, $\mathbf{S} = \langle \sum_{i=1}^{N} \mathbf{s}_i \rangle$, can be treated as a macroscopic (or mesoscopic) variable. We will refer to $\mathbf{S}$ as a macrospin or classical spin.

This situation is found, for example, in superparamagnetism. Superparamagnetic particles are very fine particles of a ferromagnetic material containing a single ferromagnetic domain. The study of the dynamics of its magnetic moment $\boldsymbol{\mu}(t)$ is a very interesting problem in nonequilibrium classical statistical mechanics, whose conclusions may be verified by suitable experiments, e.g., magnetic ressonance,[1] Mössbauer effect,[2] etc. Because of their small size, or finite value of N, and the fact that T is different from zero, the magnetic moment, which is proportional to $\mathbf{S}$, shows a random time dependence. Therefore, the origin of the stochastic behavior is internal. When an external magnetic field is applied on a sample of such particles it shows a paramagnetic behavior, with a very big Curie constant, since the individual magnetic moments of the superparamagnetic particles are several orders of magnitude bigger than the Bohr magneton μ_B.

The first stochastic theory proposed for it is due to Brown,[3] who postulated a Langevin type equation obtained from the phenomenological equation of Gilbert[4] by adding to it a noise *field* term, which means treating the noise as being of external origin. The weak point of this approach is that it is not suitable to allow for fluctuations on the magnitudes of $\boldsymbol{\mu}$, which may be very important in case of very fine particles. All subsequent theoretical developments derive from Brown's work[3] and suffer from the same drawback.

This paper is organized as follows. In Section 2 we obtain the deterministic equations of motion of a classical spin from a generalized Lagrangian formalism. The deterministic path obtained, corresponding to the situation of negligible fluctuations, coincides, in its asymptotic limit $t \to \infty$, with that obtained from phenomenological equations, such as the Gilbert equation[4] or the Landau–Lifshitz equation.[5] In Section 3 we introduce the fluctuations in analogy with Langevin's seminal work on ordinary Brownian motion,[6] but the equations of motion so obtained are stochastic differential equations of first order with *multiplicative noise*, which demands the choice of a specific version of stochastic calculus, the Ito or Stratonovich calculus. The corresponding covariant Fokker–Planck equation (FPE) is also obtained. In Section 4 we make some observations about future tasks planned for a future publication.

2. THE DETERMINISTIC MOTION OF THE CLASSICAL SPIN

The basic point in writing down an equation of motion for a magnetic moment is to recognize that $\boldsymbol{\mu}$ is proportional to some angular momentum and that the time derivative of the angular momentum of any system is equal to the torque applied on it. The phenomenological equations of Bloch,[7] Landau and Lifshitz,[5] and Gilbert[4] are well-known. We propose now an alternative way of obtaining an equation of motion for $\boldsymbol{\mu}(t)$. The central idea is to assume that the general form of the equation will not depend on the details of the origin of $\boldsymbol{\mu}(t)$. Therefore we write $\boldsymbol{\mu} = \gamma \mathbf{S}$, where the angular momentum $\mathbf{S}$ will be simulated by that of a rotating symmetric charged body, in the limit of zero moment of inertial and infinite angular velocity $\dot{\psi}$. By this trick we can write down a classical Lagrangian and derive the equations of motion from it.

We begin by writing the Lagrangian of a rotating charged symmetric body,[8]

$$L = \tfrac{1}{2} I_1 \dot{\phi}^2 \sin^2 \theta + \tfrac{1}{2} I_1 \dot{\theta}^2 + \tfrac{1}{2} I_3 (\dot{\psi} + \dot{\phi} \cos \theta)^2 - V(\theta, \phi) \tag{1}$$

where I_1 and I_3 are the moments of inertia and θ, ϕ, and ψ the usual Euler angles, and $V(\theta, \phi)$ represents the total potential energy, corresponding to all interactions of the system with its neighborhood. The generalized Lagrangian equations of motion read[8]

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = Q_i(t) \tag{2}$$

where the generalized coordinates q_i are in the present case the Euler angles θ, ϕ, and ψ, and the generalized forces Q_i contain the dissipative contribution to the total torque, which cannot be included in the Lagrangian. The total angular momentum is given by[9]

$$\mathbf{J} = -I_1 \dot{\phi} \sin \hat{e}_1' + I_1 \dot{\theta} \hat{e}_2' + I_3 (\dot{\psi} + \dot{\phi} \cos \theta)\, \hat{e}_3 \tag{3}$$

where $\hat{e}_3$ is the unit vector along the symmetry axis of the rotating body, and $\hat{e}_1'$ and $\hat{e}_2'$ are the unit vectors, perpendiculars to $\hat{e}_3$, used in the definition of Euler angles.[8,9]

We assume for Q_i the form[9]

$$Q_i(t) = -\frac{\partial \mathscr{F}}{\partial \dot{q}_i} \tag{4}$$

derived from a Rayleigh dissipative function[8]

$$\mathscr{F} = \tfrac{1}{2} \alpha (\dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta) + \mathscr{F}_0(\dot{\psi}) \tag{5}$$

where α is a dissipative constant and $\mathscr{F}_0(\dot{\psi})$ is a function to be defined below. In order to simulate the behavior of a classical spin, we take, for these equations, the limit $I_1 \to 0$, $I_3 \to 0$, and $\dot{\psi} \to \infty$, but maintaining $I_3\dot{\psi} = S(t) = \text{finite}$. In this limit we have $\mathbf{J} \to \mathbf{S} = S(t)\,\hat{e}_r(t)$, where $\hat{e}_r = \hat{e}_3$, and the equations of motion obtained by substituting Eqs. (1), (4), and (5) into Eq. (2) can be written as

$$\dot{S} = -\beta(S - S_0) \equiv f_r \tag{6a}$$

$$\dot{\theta} = -a(S)\,V_\theta + \frac{b(S)}{\sin\theta}\,V_\phi - \beta b(S)(S - S_0)\,\mathrm{ctg}\,\theta \equiv f_\theta \tag{6b}$$

$$\dot{\phi} = -\frac{b(S)}{\sin\theta}\,V_\theta - \frac{a(S)}{\sin^2\theta}\,V_\phi + \beta a(S)(S - S_0)\,\frac{\mathrm{ctg}\,\theta}{\sin\theta} \equiv f_\phi \tag{6c}$$

where $V_\theta \equiv \partial V/\partial\theta$, $V_\phi \equiv \partial V/\partial\phi$, $a(S) \equiv \alpha/(\alpha^2 + S^2)$, and $b(S) \equiv S/(\alpha^2 + S^2)$. In the derivation of these equations, we have assumed that

$$\mathscr{F}_0 = \frac{\beta}{2}\,(S - S_0)^2 \tag{7}$$

which may be justified whenever $S(t)$ does not deviate too much from the equilibrium value S_0. The model therefore has two relaxation constants, one, α, for relaxation in direction (θ, ϕ) of $\mathbf{S}(t)$ and the other, β, for relaxation in the magnitude of $\mathbf{S}(t)$.

For $\beta t \gg 1$ these equations may be approximated by

$$S = S_0 \tag{8a}$$

$$\dot{\theta} = -a_0\,V_\theta + \frac{b_0}{\sin\theta}\,V_\phi \tag{8b}$$

$$\dot{\phi} = -\frac{b_0}{\sin\theta}\,V_\theta - \frac{a_0}{\sin^2\theta}\,V_\phi \tag{8c}$$

where $a_0 = a(S_0)$ and $b_0 = b(S_0)$; these equations are equivalent to the Gilbert equation

$$\frac{d\boldsymbol{\mu}}{dt} = \gamma\boldsymbol{\mu} \times \left(\mathbf{H}_{\text{eff}} - \frac{\alpha}{\mu^2}\frac{d\boldsymbol{\mu}}{dt}\right) \tag{9}$$

with $\boldsymbol{\mu} = \gamma\mathbf{S}$ and the effective magnetic field given by $\mathbf{H}_{\text{eff}} = -\partial V/\partial\boldsymbol{\mu}$. In the $\mathbf{S}$ space spanned by $\{S_x, S_y, S_z\}$ the evolution of the macrostate of the system can be associated with the trajectory of a *representative point* $\mathbf{S}(t) = S(t)\,\hat{e}_r(t)$. The velocity of a representative point in the $\mathbf{S}$ space,

$$\frac{d\mathbf{S}}{dt} = \dot{S}(t)\,\hat{e}_r(t) + S(t)[\dot{\theta}\hat{e}_\theta(t) + \dot{\phi}\sin\theta\hat{e}_\phi(t)] \tag{10}$$

is also proportional to the total torque on the macrospin.

3. THE STOCHASTIC EQUATIONS

The complete motion of the macrospin $\mathbf{S}(t)$ in $\mathbf{S}$ space is the combination of the deterministic motion described in the last section with a random motion produced by the stochastic torque $\mathbf{N}(t) = N_x(t)\,\hat{e}_x + N_y(t)\,\hat{e}_y + N_z(t)\,\hat{e}_z$, whose Cartesian components will be assumed to be Gaussian, isotropic, orthogonal white noise, with intensity $2D$,

$$\langle N_i(t) \rangle = 0, \qquad \langle N_i(t)\, N_j(t') \rangle = 2D\delta_{ij}\delta(t - t') \tag{11}$$

where $\langle \cdots \rangle$ denotes an average over the realizations of the noise.

It is convenient to write the stochastic equations of motion for $\mathbf{S}(t)$ in terms of the spherical coordinates (S, θ, ϕ),

$$\dot{S} = f_r + N_r(t) \tag{12a}$$

$$S\dot{\theta} = Sf_\theta + N_\theta(t) \tag{12b}$$

$$S\dot{\phi}\sin\theta = Sf_\phi \sin\theta + N_\phi(t) \tag{12c}$$

where f_r, f_θ, and f_ϕ are defined in Eqs. (6). Since the spherical components of the noise N_r, N_θ, and N_ϕ depend not only on the Cartesian components N_x, N_y, and N_z, but also on $\mathbf{S}(t)$, Eqs. (12) are stochastic differential equations with *multiplicative* noise. As usual in physics, we will interpret them in the *Stratonovich* sense,[10] because this approach has a physical motivation: it is equivalent to starting all the calculations with each Cartesian component $N_i(t)$ being *colored* noise, with finite correlation time τ_c, and taking, at the end, the limit $\tau_c \to 0$. Using

$$\hat{e}_x = \hat{e}_r \sin\theta\cos\phi + \hat{e}_\theta \cos\theta\cos\phi - \hat{e}_\varphi \sin\phi \tag{13a}$$

$$\hat{e}_y = \hat{e}_r \sin\theta\sin\phi + \hat{e}_\theta \cos\theta\sin\phi + \hat{e}_\varphi \cos\phi \tag{13b}$$

$$\hat{e}_z = \hat{e}_r \cos\theta - \hat{e}_\theta \sin\theta \tag{13c}$$

one can write the set of equations (12) in the general form

$$dq_\nu(t) = f_\nu(q)\,dt + \sum_j g_{\nu j}(q)\,dW_j(t) \tag{14}$$

where Greek subscripts (ν) run over spherical components, $q_1 = S$, $q_2 = \theta$, $q_3 = \phi$, and Latin subscripts (j) run over Cartesian components, x, y, z. The differential $dW_j(t)$ is the infinitesimal increment of a Cartesian component of the Wiener process,

$$W_j(t) = \int_0^t N_j(t')\,dt' \tag{15}$$

and the matrix of $g_{\nu j}$ coefficient is

$$g = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ S^{-1}\cos\theta\cos\phi & S^{-1}\cos\theta\sin\phi & -S^{-1}\sin\theta \\ -S^{-1}\sin\phi/\sin\theta & S^{-1}\cos\phi/\sin\theta & 0 \end{pmatrix} \tag{16}$$

The associated FPE is given by[10]

$$\frac{\partial P}{\partial t} = -\sum_{\nu} \frac{\partial}{\partial q_\nu} [A_\nu(q)\, P(q, t)] + \frac{1}{2} \sum_{\nu\mu} \frac{\partial^2}{\partial q_\nu\, \partial q_\mu} [B_{\nu\mu}(q)\, P(q, t)] \tag{17}$$

where the drift and diffusion coefficients are, respectively, given by[10]

$$A_\nu(q) = \lim_{\Delta t \to 0} \frac{\langle \Delta q_\nu \rangle}{\Delta t} = f_\nu(q) + D \sum_{\mu j} \frac{\partial q_{\nu j}}{\partial q_\mu}\, g_{\mu j} \tag{18a}$$

$$B_{\nu\mu}(q) = \frac{\langle \Delta q_\nu\, \Delta q_\mu \rangle}{\Delta t} = 2D \sum_j g_{\nu j}(q)\, g_{\mu j}(q) \tag{18b}$$

and $\Delta q_\nu \equiv q_\nu(t + \Delta t) - q_\nu(t)$. Substituting Eq. (16) obtained above into (18a) and (18b), we get

$$A_\theta = f_\theta + \frac{D}{S^2} \operatorname{ctg}\theta \tag{19a}$$

$$A_\phi = f_\phi \tag{19b}$$

$$A_r = f_r + \frac{2D}{S} \tag{19c}$$

for the drift coefficients, and

$$B = \begin{pmatrix} 2D & 0 & 0 \\ 0 & 2D/S^2 & 0 \\ 0 & 0 & 2D/S^2 \sin^2\theta \end{pmatrix} \tag{20}$$

for the diffusion matrix.

The probability density $P(q, t) = P(S, \theta, \phi, t)$ is normalized as

$$\int P(S, \theta, \phi, t)\, dS\, d\theta\, d\phi = 1 \tag{21}$$

We can put this FPE in a form manifestly covariant by introducing another probability density, $\bar{P}(S, \theta, \phi, t)$, so that $P(\mathbf{S}, t) = S^2 \sin\theta \bar{P}(\mathbf{S}, t)$, whose normalization condition is, evidently,

$$\int \bar{P}(\mathbf{S}, t)\, S^2 \sin\theta\, d\theta\, d\phi\, dS = 1 \tag{22}$$

This probability density, $\bar{P}(\mathbf{S}, t)$, becomes independent of θ and ϕ for the special case $V = \text{const}$. In terms of $\bar{P}$, the FPE can be written as a continuity equation,

$$\frac{\partial \bar{P}}{\partial t} = -\nabla \cdot \mathbf{J}^{P}(\mathbf{S}, t) \tag{23}$$

where $\nabla\cdot$ is the divergence in $\mathbf{S}$ space, and the probability current is given by

$$\mathbf{J}^{P}(\mathbf{S}, t) = \mathbf{K}(\mathbf{S})\, \bar{P}(\mathbf{S}, t) - D\, \nabla \bar{P}(\mathbf{S}, t) \tag{24}$$

The covariant drift vector,

$$\mathbf{K} = f_r \hat{e}_r + S f_\theta \hat{e}_\theta + S \sin\theta f_\phi \hat{e}_\phi \tag{25}$$

is the velocity of a representative point in $\mathbf{S}$ space when the noise is absent, $\mathbf{K}\bar{P}$ is the *drift current*, and $-D\,\nabla\bar{P}$ is the *diffusion current*.

4. CONCLUDING REMARKS

Using a generalized Lagrangian formalism for a symmetric charged rotating body, we have obtained, in a convenient limit, a set of stochastic equations of motion for a classical spin, which performs "Brownian motion" in $\mathbf{S}$ space. These equations reduce to the stochastic equations of Brown,[3] or to the deterministic equations of Gilbert[4] or of Landau and Lifshitz,[5] when the appropriate limits are taken. In the general case these equations form a set of nonlinear, coupled, stochastic differential equations which are too difficult to be formally integrated. Even the associated Fokker–Planck equation is too difficult, in the general case, for a formal analytical solution in terms of the potential $V(\theta, \phi)$ to be obtained. Two alternative numerical procedures may be followed: (i) to integrate the FPE for special potentials, obtaining the time evolution of the probability distribution in $\mathbf{S}$ space; (ii) to integrate the stochastic equations for randomly selected realizations, a kind of Monte Carlo simulation. Results obtained along these lines will be presented in a future paper, when it will also be shown that *detailed balance* conditions[10] are not satisfied by the stationary form of the FPE.

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