Fluctuations and dissipation of coherent magnetization

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A quantum mechanical model is used to derive a generalized Landau-Lifshitz equation for a magnetic moment, including fluctuations and dissipation. The magnetic moment is linearly coupled to a reservoir of bosonic degrees of freedom. The model reproduces the Gilbert-Brown form of the equation in the classical limit for a particular choice of the bath parameters. Use of generalized coherent states makes the semiclassical limit more transparent within a path-integral formulation. A general fluctuation-dissipation theorem is derived. The magnitude of the magnetic moment also fluctuates beyond the Gaussian approximation. We discuss how the approximate classical stochastic description of the thermal field follows from our result. We apply these results to the calculation of the correlation functions of the magnetization in a thin film with an easy axis and a hard axis within a linear-response approximation.

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I. INTRODUCTION

The study of thermally induced magnetization reversal was first carried out by Brown.[1] His approach was to introduce a noise term into the Landau-Lifshitz equation of motion, essentially constructing a Langevin-type equation, which we call here the Landau-Lifshitz-Gilbert-Brown equation (LLGB). From the LLGB equation the Fokker-Plank equation can be derived, which describes the time evolution of the probability density distribution of the moment orientations. Solution of this problem was carried out by Brown for the case of an axially symmetric potential and later by Coffey *et al.*[2] for nonaxially symmetric cases. The numerical solution of the Langevin equation was used by Lyberatos *et al.*,[3] and has since been applied to the study of magnetization reversal by a number of authors.[4,5] Recently, Wang *et al.*[6] have developed an approach introducing a tensor form of the damping constant and applied this to the calculation of first mean passage time in the case of an elongated grain represented as a chain of coupled particles. Many of these calculations are motivated by the need to understand high-frequency magnetization processes in magnetic recording. The process of reading information currently involves giant magnetoresistive (GMR) sensors, the size of which is continually reducing as recording densities increase. This led Smith and Arnett[7] to the conjecture that noise due to magnetization fluctuations in the read head would be a limiting factor on the device size. This is clearly an important problem, which has been further developed by Smith[8] and Bertram and co-workers,[9] who have also studied the full micromagnetic description of the problem using an approach in which the thermal noise is distributed among the normal modes.[10]

Clearly the introduction of thermal fluctuations in the micromagnetic formalism is important both from the point of view of the physics of magnetization processes and also in relation to important practical problems of magnetic recording. Central to all models, both analytical and numerical, is the introduction of a magnetization fluctuation or an effective field via the fluctuation-dissipation theorem (FDT).[11] The FDT has a strong physical justification, as discussed in detail by Landau and Lifshitz;[12] however, it should be stressed that it is strictly valid only for small fluctuations about the local minimum. A more serious problem with the use of the Langevin equation in the LLGB form is the dissipative term itself, which has no microscopic justification. It is clearly important to understand the whole problem of fluctuations and dissipation within a first principle of quantum mechanical approach, if the limits of the current models are to be established and more fundamental theoretical approaches are derived. The demand for higher density recording media and faster switching rates requires the use of structures on the nanometer scale or less. Quantum mechanical effects are then bound to become more and more important to consider in these systems. Effects such as magneto-optical interactions may even invalidate the simple damping term that is currently used in the Landau-Lifshitz equation. This prompted us to investigate whether the LLGB equation can be recovered from a more fundamental treatment rather than the *ad hoc* approach presently used. Hence, it seems natural to ask in what limit the LLGB equation can be recovered starting from a quantum model.

In this work, we make first steps towards a more basic understanding of the LLGB equation. To address the above questions, we take a simple quantum model, that of a single particle with large spin interacting with a heat bath and an external magnetic field. The spin is taken to be large since we are primarily interested in a semiclassical representation of the magnetization vector. This simple model is sufficient to allow us to study the effects of thermal fluctuations in many different cases, such as magnetization switching in a single domain magnetic system with uniaxial anisotropy or noise arising from magnetic fluctuation in GMR heads. The bath is taken to be of bosonic nature. Nothing else needs to be assumed to enable us to include various mechanisms of interaction between the magnetic moment and the environment. We calculate the equations of motion of the magnetization and that of an associated fluctuating field in the semiclassical limit. Since our interest is mainly in the semiclassical limit, coherent states (CS's) are the natural choice for the representation of the system. These states, which form an overcomplete basis, have the property of minimizing the Heisenberg uncertainty relations. Bosonic

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CS's were first used by Langer to study dissipation and fluctuations in a superfluid, many-body problem.[13] Starting from the equation of motion of the density matrix of the whole system, ρ,

$$i\frac{\partial\rho}{\partial t}=[\hat{\mathcal{H}},\rho],$$

a Landau-Ginzburg equation was recovered in the equilibrium case and a Fokker-Planck equation in the classical limit. In a CS formulation, only diagonal elements of the reduced density matrix are needed. Instead of starting from the above equation, we can instead start from an integral representation of the diagonal density matrix elements. This method is well known and is based on the Feynman-Vernon formalism.[14,15] This path-integral approach is in real-time as opposed to the imaginary-time approach in equilibrium thermodynamics. Hence, questions like approach to equilibrium can be studied within this approach. This method has seen many different applications since the Caldeira-Leggett (CL) work.[16] The CL model was successful in showing how to recover the Langevin equation by coupling an oscillator to a bath of oscillators. It seems natural then to ask if the LLGB equation can be recovered by coupling a spin to a bath of oscillators. This important question does not seem to have been addressed in the literature. Spin coherent states are the natural language to answer this question. Hence, we formulate the question in terms of CS and use path integral techniques to write the density matrix elements of the system. Use of path-integrals with spin CS is not as straightforward as in the case of bosons.[17] Nevertheless it is the most suitable method by which we can address questions that pertain to the semiclassical limit of the model treated here. Clearly this method allows a consistent treatment of the magnetization and fluctuations from the start. If the thermal field is decoupled from the magnetization, the LLGB equation will be shown to correspond to a given choice of density of states of the reservoir and of its interaction parameters with the magnetic moment.

This work is able to provide a different perspective from which to discuss the LLGB equation and its limitation. We also set a basis against which we can examine the discrepancy in the recent calculations of the noise spectrum in magnetic recording heads.[7,10,18] Therefore, a treatment of the noise problem by a self-consistent method, such as the one presented here, can shed some light on why this difference exists. We stress that our results are very general for the model considered and no linear approximation is assumed.

The paper is organized as follows. In Sec. II, we introduce a simple model Hamiltonian that can describe dissipation and fluctuations. We linearly couple a single domain magnetic particle to an external magnetic field and to a Bosonic bath with infinite number of degrees of freedom. In Sec. III, we show how to calculate the trace of the reduced density matrix of the magnetic moment. The density matrix elements are naturally expressed in terms of path integrals over the phase space of the moment.[15] An appendix supplements this section in which we discuss the topological Wess-Zumino (WZ) term. In Sec. IV, we derive coupled equations for the magnetization and fluctuations. We show that a general fluctuation-dissipation theorem is satisfied. We also demonstrate how to recover the LLGB equation by decoupling the thermal fluctuations, taking the high-temperature limit and constraining the choice of reservoir. In the particular case of LLGB, this corresponds to the Gaussian fluctuations and constant dissipation. Similar results have been obtained for the case when the magnetic moment is replaced by a harmonic oscillator. This is no surprise, since in this case the semiclassical approximation corresponds to a particle with large spin. In Sec. V, we compare the classical stochastic treatment to this quantum treatment. As an example we calculate the correlation functions of the magnetic moment for a single domain particle with an easy axis and a hard axis. The external field is taken to be along the easy axis. Finally, in Sec. VI, we summarize our results.

II. DEFINITION OF THE MODEL

The model we choose is simple but general enough to include many interesting physical situations. It is mainly motivated by the recent work of Safonov and Bertram.[19] They used a two-level impurity system to simulate relaxation effects in a single domain grain. They showed that the damping in their model is of the Gilbert form. No fluctuations are considered in their calculation. If we consider a collection of spins that are independent, then the magnetization vector **M** is a simple sum of these coherent spins,

$$\mathbf{M}=g\mu_B\frac{N\mathbf{S}}{V}, \tag{1}$$

where **S** is the average spin vector of the spin operator $\hat{\mathbf{S}}$ and $g\mu_B/\hbar$ is the gyromagnetic ratio. μ_B is the Bohr magneton, g is the spectroscopic splitting factor, and V is the volume of the system. In the following, we set $\hbar=1$, $g\mu_B=1$, and the density $N/V=1$. In the rest of this paper, we use the words spin and magnetic moment interchangeably.

We take a single spin $\mathbf{S}(\mathbf{S}^2\gg 1)$ and couple it linearly to a set of oscillators and to a constant external field **H**. The former may represent phonons, a time-dependent magnetic field or other Bosonic degrees of freedom. No assumption will be made about the coupling constants or the density of states of the reservoir. The Hamiltonian assumes the following form

$$\hat{\mathcal{H}}=-\mathbf{H}\cdot\hat{\mathbf{S}}+\sum_k\ \omega_k a_k^+ a_k+\sum_k\ \gamma_k a_k^+\hat{S}_-+\sum_k\ \gamma_k^*\hat{S}_+ a_k, \tag{2}$$

where **H** is a static external magnetic field. $\hat{\mathbf{S}}$ is the magnetic moment operator of a single particle. a_k^+ and a_k are creation and annihilation operators of the reservoir. The coupling constants γ_k may be time dependent, but will be taken as independent of time in the final result. A word about notation is that operators are usually represented by a hat unless there is no fear of confusion. The field **H** is taken along the z axis, the axis of spin quantization. Coupling the z component of the vector **S** to the reservoir can be easily added, but it will be omitted in this work. This Hamiltonian is sufficient to

describe all the desired physics. Using the equation of motion for S_z, it is not difficult to show that it is not a constant of the motion, and hence no linearization is implied in this model.

The operators are in the Heisenberg representation. The spin operator S satisfies the usual commutation relations:[20]

$$[\hat{\mathbf{S}}^2,\hat{S}_\pm]=0, \tag{3}$$

with

$$\hat{\mathbf{S}}^2=\frac{1}{2}\{\hat{S}_+,\hat{S}_-\}+\hat{S}_z^2, \tag{4}$$

where the curly brackets are for anticommutation and

$$\hat{S}_+=\hat{S}_x+i\hat{S}_y, \tag{5}$$

$$\hat{S}_-=\hat{S}_x-i\hat{S}_y, \tag{6}$$

while the operators of the reservoir satisfy Bose commutation relations,

$$[a_k,a_{k'}^+]=\delta_{kk'}. \tag{7}$$

Instead of the usual Fock space representation, we use a CS-space representation for these operators.[21,22]

For a Bosonic harmonic oscillator with position q_k, momentum p_k, and frequency ω_k, the CS $|\Phi_k\rangle$ are defined as eigenfunctions of the annihilation operator $a_k=(\omega_k/2)^{1/2}\{\hat{q}_k+[i/(2\omega_k)^{1/2}]\hat{p}_k\}$:

$$a_k|\Phi_k\rangle=\Phi_k|\Phi_k\rangle, \tag{8}$$

with complex eigenvalues, Φ_k (Ref. 21). These states can also be generated from the ground state $|0_k\rangle$ by applying a displacement operator $D(z_k)$, which defines a one-to-one correspondence between the complex plane and the oscillator states,

$$|z_k\rangle=D(z_k)|0_k\rangle \tag{9}$$

and

$$D(z_k)=\exp(z_k a_k^+-z_k^* a_k). \tag{10}$$

CS's form an overcomplete basis and satisfy the minimum uncertainty relation. Hence, they are the most suitable representation for a semiclassical treatment. We also adopt the normalization in Ref. 22

$$\langle\Phi_k|\Phi_k'\rangle=e^{\Phi_k^*\Phi_k'}. \tag{11}$$

They also satisfy the following relation, the resolution of the identity operator:

$$\int\frac{d\Phi_k^*d\Phi_k}{2\pi i}e^{-\Phi_k^*\Phi_k}|\Phi_k\rangle\langle\Phi_k|=1. \tag{12}$$

The latter relation is essential for a path-integral representation in terms of CS's. It is used repeatedly in the discretization of the path integral when calculating transition rates between various states (Appendix).

Similarly for the spin states, we use a CS representation.[23,24] They are defined by analogy to the harmonic oscillator CS's. The spin components in this state satisfy a minimum uncertainty relation, i.e., two of the three components commute.[25] As in the harmonic oscillator case, a ''ground'' state $|0\rangle$ is required from which to generate all the other states. In this case the state with the largest S_z component is taken as the reference state. If the z axis is taken as the quantization axis and if we take $\mathbf{S}^2=j(j+1)$, then by definition, we have

$$|0\rangle\equiv|j,j\rangle, \tag{13}$$

and

$$\hat{S}_z|0\rangle=j|0\rangle, \tag{14}$$

i.e., the state with the minimum fluctuations.[20] The spin CS's are a generalization of the Holstein-Primakoff construction.[26] They are defined in terms of deviations from the maximum positive z component of the spin $\mathbf{S}$

$$\hat{S}_z|\mathbf{p}\rangle=(j-p)|\mathbf{p}\rangle. \tag{15}$$

The CS's are then constructed by using

$$|\boldsymbol{\mu}\rangle=\frac{1}{(1+|\mu|^2)^j}\exp(\mu\hat{S}_-)|0\rangle$$
$$=\frac{1}{(1+|\mu|^2)^j}\sum_{p=0}^{2j}\left(\frac{(2j)!}{p!(2j-p)!}\right)^{1/2}\mu^p|\mathbf{p}\rangle, \tag{16}$$

where μ is a complex number. Since the configuration space of $\mathbf{S}$ is the surface of a sphere, it will be more clear to have μ parametrize the surface of a sphere through a stereographic projection,

$$\mu=\tan\left(\frac{1}{2}\theta\right)e^{i\varphi}. \tag{17}$$

In this representation, a CS corresponds to a unit vector with a solid angle $\mathbf{\Omega}$:

$$|\mathbf{\Omega}\rangle=|\theta,\varphi\rangle=(\cos\tfrac{1}{2}\theta)^{2j}\exp[\tan(\tfrac{1}{2}\theta)e^{i\varphi}\hat{S}_-]|0\rangle. \tag{18}$$

A useful property for a path integral formulation is that the unit operator has the familiar decomposition in terms of projection operators on all CS's,

$$\frac{2j+1}{4\pi}\int d\mathbf{\Omega}|\mathbf{\Omega}\rangle\langle\mathbf{\Omega}|=1. \tag{19}$$

In this representation, the overlap of two coherent states represents an area on a sphere, the surface of which is the configuration space of the spin $\mathbf{S}$. The overlap is

$$\langle\mathbf{\Omega}'|\mathbf{\Omega}\rangle=[\cos\tfrac{1}{2}\theta\cos\tfrac{1}{2}\theta'+\sin\tfrac{1}{2}\theta\sin\tfrac{1}{2}\theta'e^{i(\varphi-\varphi')}]^{2j} \tag{20}$$

and its magnitude is

$$|\langle \mathbf{\Omega}'|\mathbf{\Omega}\rangle| = \left(\frac{1+\mathbf{n}\cdot\mathbf{n}'}{2}\right)^j. \tag{21}$$

This defines the area of a triangle on a unit sphere with vertices at the points defined by $\mathbf{\Omega},\mathbf{\Omega}'$ and $\theta=0$. This expression is fundamental for the developments below.

Since we plan to use a path-integral technique, we need to write the expectation values of the Hamiltonian in the coherent representation. These expectation values follow, in turn, from those of the operators $\hat{S}_z$, $\hat{S}_+$, and $\hat{S}_-$. The following expectation values are deduced from Eq. (18) and Eq. (20):

$$\langle \mathbf{\Omega}|j-\hat{S}_z|\mathbf{\Omega}\rangle = j(1-\cos\theta), \tag{22}$$

$$\langle \mathbf{\Omega}|\hat{S}_+|\mathbf{\Omega}\rangle = j\sin\theta e^{i\varphi}, \tag{23}$$

$$\langle \mathbf{\Omega}|\hat{S}_-|\mathbf{\Omega}\rangle = j\sin\theta e^{-i\varphi}, \tag{24}$$

$$\langle \mathbf{\Omega}|\hat{\mathbf{S}}|\mathbf{\Omega}\rangle = j\mathbf{n}, \tag{25}$$

where $\mathbf{n}$ is a unit vector with angles (θ,φ). For $j\gg 1$, the off-diagonal terms of the spin operator are smaller than the diagonal ones by a factor of about $\sqrt{j}$. Hence, they are negligible in the classical limit. This limit will be implicit in all subsequent calculations of the reduced density matrix elements.

III. REDUCED DENSITY MATRIX ELEMENTS OF THE SPIN PARTICLE

In the following, we make use of CS for both the bath degrees of freedom and the magnetic moment. The procedure we follow is by now mostly standard. Reference 27 (and references therein) provides a general overview of these methods and hence we omit most of the intermediate steps in our calculation.

The calculation we present below takes into account the correct boundary conditions as emphasized in Ref. 17. However, we avoid using the abstract but more appropriate holomorphic representation in favor of a more geometric one, i.e., in terms of unit vectors. The physical space for the Hamiltonian , Eq. (2), is the product of the Hilbert space of the spin particle and that of the harmonic oscillators,

$$\prod_k |\mathbf{S}\rangle\otimes|\Phi_k\rangle. \tag{26}$$

Using the expectation values of the different operators in the Hamiltonian, Eq. (22)–(25), we get the expectation value of the Hamiltonian in the coherent representation,

$$\begin{aligned}\mathcal{H}[\Phi^*,\Phi,\mathbf{S}] = &-H_z j\cos\theta(t)+\sum_k \omega_k\Phi_k^*(t)\Phi_k(t)\\ &+j\sum_k \gamma_k\Phi_k^*(t)\sin\theta(t)e^{-i\varphi(t)}\\ &+j\sum_k \gamma_k^*\Phi_k(t)\sin\theta(t)e^{i\varphi(t)}.\end{aligned} \tag{27}$$

From now on, we normalize the magnitude of all spin vectors by j. Since all classical physical properties of the system involve a tracing operation, it is enough to consider only diagonal elements of the density matrix. The reduced diagonal density matrix element of the spin particle, ρ_{ff}, is by definition the density matrix element of the whole system averaged over the states, $|\Phi_k\rangle$, of the bath,

$$\rho_{ff}(t)=\langle \mathbf{S}_f|\rho(t)|\mathbf{S}_f\rangle = \int\prod_k \mathfrak{D}\Phi_k^*\mathfrak{D}\Phi_k\langle \mathbf{S}_f;\mathbf{\Phi}|\rho(t)|\mathbf{S}_f;\mathbf{\Phi}\rangle, \tag{28}$$

where $|\mathbf{S}_f\rangle$ and $|\mathbf{\Phi}\rangle$ are two arbitrary CS of the spin and the bath, respectively. Here the state $\mathbf{\Phi}$ is a k vector, $\mathbf{\Phi}=(\Phi_1,\Phi_2,\Phi_3,\ldots)$.

For simplicity, from now on we use the following notation for the functional measure of the Bosonic degrees of freedom,

$$\int \mathfrak{D}(\mathbf{\Phi}^*,\mathbf{\Phi}) \equiv \int\prod_k \mathfrak{D}\Phi_k^*\mathfrak{D}\Phi_k. \tag{29}$$

The calculation of density matrix elements is easily carried out using a path integral representation. The propagator of the Bosonic part can be written in terms of a path integral,[22]

$$\begin{aligned}&\langle \mathbf{\Phi}_f|\mathcal{T}e^{-i\int_0^t d\tau\hat{\mathcal{H}}(\tau)}|\mathbf{\Phi}_i\rangle\\ &\quad=\int_{\mathbf{\Phi}(0)=\Phi_i}^{\mathbf{\Phi}^*(t)=\Phi_f^*}\mathfrak{D}(\mathbf{\Phi}^*,\mathbf{\Phi})\exp\left\{\sum_k \Phi_k^*(t)\Phi_k(t)\right.\\ &\qquad\left.+i\int_0^t d\tau\left[\sum_k i\Phi_k^*(\tau)\partial_\tau\Phi_k(\tau)-\mathcal{H}(\mathbf{\Phi}^*,\mathbf{\Phi},\hat{\mathbf{S}})\right]\right\}.\end{aligned} \tag{30}$$

$\mathcal{T}$ is the time-ordering operator. Running from an initial time $\tau=0$ to time $\tau=t$, we use a real-time path integral to average over all intermediate states. The trace of the density matrix is then expressed as an integral in terms of the initial density matrix element of the system,

$$\begin{aligned}\mathrm{Tr}\rho_{ff}(t)=&\int\mathfrak{D}(\mathbf{\Phi}^*,\mathbf{\Phi})\int\mathfrak{D}\mu(\mathbf{\Omega}_1)\int\mathfrak{D}\mu(\mathbf{\Omega}_2)\\ &\times\int\mathfrak{D}(\mathbf{\Phi}_1^*,\mathbf{\Phi}_1)\int\mathfrak{D}(\mathbf{\Phi}_2^*,\mathbf{\Phi}_2)\\ &\times\langle \mathbf{S}_f,\mathbf{\Phi};t|\mathbf{\Omega}_1,\Phi_1;0\rangle\langle\mathbf{\Omega}_1,\mathbf{\Phi}_1;0|\rho|\mathbf{\Omega}_2,\mathbf{\Phi}_2;0\rangle\\ &\times\langle\mathbf{\Omega}_2,\mathbf{\Phi}_2;0|\mathbf{S}_f,\Phi,t\rangle.\end{aligned} \tag{31}$$

The integrand is now expressed in terms of c numbers only.

We make no assumption about the initial state of the spin particle. Hence, we have to calculate a forward propagator, a backward propagator, and the density matrix element at the initial time. The system is assumed to be at finite temperature. Since the Hamiltonian is quadratic, the integrations are easily carried out in the stationary-phase approximation. We show a few steps in the calculation of the forward propagator. Similar calculations are also done for the other two fac-

tors in Eq. (31). Some of the steps in these calculations are, however, valid only within a trace calculation and not for the seperate propagators (see Appendix for further details). The forward propagator is first written as a path integral,

$$\begin{aligned}\langle \mathbf{S}_f,\mathbf{\Phi};t|\mathbf{\Omega}_1,\mathbf{\Phi}_1;0\rangle &= \langle \mathbf{S}_f,\mathbf{\Phi}|\mathcal{T}e^{-i\int_0^t\hat{\mathcal{H}}d\tau}|\mathbf{\Omega}_1,\mathbf{\Phi}_1\rangle \\ &= \int_{\mathbf{\Omega}_1}^{\mathbf{S}_f}\mathfrak{D}\mu(\mathbf{S}_1)\int_{\mathbf{\Phi}_1}^{\mathbf{\Phi}}\mathfrak{D}(\mathbf{\Phi}_1^*,\mathbf{\Phi}_1) \\ &\times\exp\Bigg\{\sum_k \Phi_{1,k}^*(t)\Phi_{1,k}(t) \\ &+ i\int_0^t d\tau\Bigg[i\sum_k \Phi_{1,k}^*(\tau)\partial_\tau\Phi_{1,k}(\tau) \\ &- \mathcal{H}(\mathbf{\Phi}_1^*,\mathbf{\Phi}_1,\mathbf{S}_1)\Bigg]\Bigg\}\exp\{i\mathbb{S}_{WZ}[\mathbf{S}_1]\},\end{aligned} \tag{32}$$

The measure of the integration over the spin variables is the measure of the $SU(2)$ Lie group over a sphere S^2. If $\mathbf{S}$ is a three-vector, then the $SU(2)$-invariant measure is given by

$$\int \mathfrak{D}\mu(\mathbf{S})\equiv\frac{2j+1}{4\pi}\int \mathfrak{D}\mathbf{S}\delta(S^2-1). \tag{33}$$

The last factor in Eq. (32) is a geometrical term, the Wess-Zumino term[28] (and references therein), which for our purposes will be enough to be taken of this form, but with the correct boundary conditions (see Appendix for details)

$$\mathbb{S}_{WZ}[\mathbf{S}_1]=\int_0^1 ds\int_0^t d\tau\mathcal{S}(s,\tau)\cdot\left(\frac{\partial\mathcal{S}(s,\tau)}{\partial s}\times\frac{\partial\mathcal{S}(s,\tau)}{\partial\tau}\right), \tag{34}$$

where $\mathcal{S}(s,\tau)$ is a homotopy map between the side $(\mathbf{z},\mathbf{\Omega}_1)$ and the side $(\mathbf{z},\mathbf{S}_f)$.[29] This term therefore represents the area enclosed by the trajectory of the spin vector.[24] This formula will be only used as part of a trace calculation such as in Sec. V below. The bath degrees of freedom are eliminated by a stationary-phase evaluation of the integral. The phase is an extremum for states that satisfy

$$i\partial_\tau\Phi_{1,k}(\tau)=\frac{\delta\mathcal{H}}{\delta\Phi_{1,k}^*(\tau)} \tag{35}$$

and similar equations for $\Phi_{1,k}^*$. We have, for all k,

$$i\partial_\tau\Phi_{1,k}(\tau)=\omega_k\Phi_{1,k}(\tau)-\gamma_k(\tau)S_-, \tag{36}$$

$$i\partial_\tau\Phi_{1,k}^*(\tau)=\omega_k\Phi_{1,k}^*(\tau)-\gamma_k^*(\tau)S_+. \tag{37}$$

The solutions with the correct boundary conditions are

$$\Phi_{1,k}(\tau)=\Phi_{1,k}e^{-i\omega_k\tau}+ie^{-i\omega_k\tau}\int_0^\tau dt'e^{i\omega_kt'}\gamma_k(t')S_-(t'), \tag{38}$$

$$\Phi_{1,k}^*(\tau)=\Phi_k^*e^{i\omega_k(\tau-t)}+ie^{i\omega_k\tau}\int_\tau^t dt'e^{-i\omega_kt'}\gamma_k^*(t')S_+(t'),$$

$$0\leqslant\tau\leqslant t.$$

At the endpoints, we then have

$$\begin{aligned}\Phi_{1,k}(t)&=\Phi_{1,k}e^{-i\omega_kt}+ie^{-i\omega_kt}\int_0^t dt'e^{i\omega_kt'}\gamma_k(t')S_-(t'), \\ \Phi_{1,k}^*(0)&=\Phi_k^*e^{-i\omega_kt}+i\int_0^t dt'e^{-i\omega_kt'}\gamma_k^*(t')S_+(t').\end{aligned} \tag{39}$$

These solutions are then put back in Eq. (31). Similar expressions follow from the calculations of the backward propagator. The density matrix element at the initial time is calculated with the assumption that the bath is initially at equilibrium with the spin. The bath relaxes much faster than the spin, a reasonable approximation in many problems in magnetics. In this case the density matrix is separable at the initial time, i.e., $\rho(0)=\rho_S(0)\rho_B(0)$. The bath density matrix, ρ_B, is then known and its matrix elements can be written explicitly in terms of the Hamiltonian, $\hat{\mathcal{H}}_B$, of the bath only,

$$\begin{aligned}\langle\mathbf{\Phi}_1|\rho_B(0)|\mathbf{\Phi}_2\rangle&=\frac{1}{Z_B}\langle\mathbf{\Phi}_1|\mathcal{T}e^{-\beta\hat{\mathcal{H}}_B}|\mathbf{\Phi}_2\rangle \\ &=\frac{1}{Z_B}\int_{\mathbf{\Phi}_2}^{\mathbf{\Phi}_1}\mathfrak{D}(\mathbf{\Phi}^*,\mathbf{\Phi})\exp\Bigg\{\Phi_k^*(\beta)\Phi_k(\beta) \\ &+i\int_0^\beta d\tau[i\Phi_k^*(\tau)\partial_\tau\Phi_k(\tau)-\mathcal{H}(\tau)]\Bigg\},\end{aligned} \tag{40}$$

with the boundary conditions

$$\begin{aligned}\mathbf{\Phi}(0)&=\mathbf{\Phi}_2, \\ \mathbf{\Phi}^*(\beta)&=\mathbf{\Phi}_2^*.\end{aligned} \tag{41}$$

Here Z_B is the partition function of the bath only and summation over k is implicit above. The constant β is equal to the inverse temperature T with the Boltzmann constant k_B set to 1.

We find, after applying a stationary-phase approximation to the integral, the expression

$$\langle\mathbf{\Phi}_1|\rho_B(0)|\mathbf{\Phi}_2\rangle=\exp\Bigg\{\sum_k \Phi_{1,k}^*\Phi_{2,k}e^{-\beta\omega_k}\Bigg\}. \tag{42}$$

After integrating out the degrees of freedom of the bath, we are left with only integrals over paths in the spin space. The effective action of the spin is now complex, as is common with dissipative systems. The trace of the reduced density matrix is now given by

$$\sum_f \rho_{ff}(t)=\sum_f \int \mathcal{D}\mu(\mathbf{\Omega}_1)\int \mathcal{D}\mu(\mathbf{\Omega}_2)\langle\mathbf{\Omega}_1|\rho_s(0)|\mathbf{\Omega}_2\rangle\int_{\mathbf{\Omega}_1}^{\mathbf{S}_f}\mathcal{D}\mu(\mathbf{S}_1)\int_{\mathbf{S}_f}^{\mathbf{\Omega}_2}\mathcal{D}\mu(\mathbf{S}_2)$$
$$\times\exp\left\{iH_z\int_0^t dt'(S_{1,z}(t')-S_{2,z}(t'))+i\mathbb{S}_{WZ}[\mathbf{S}_1]-i\mathbb{S}_{WZ}[\mathbf{S}_2]\right\}\mathcal{W}(\mathbf{S}_1,\mathbf{S}_2), \tag{43}$$

where the last factor is entirely due to the coupling between the bath and the spin particle and often called the Feynman-Vernon functional.[16] It is given by

$$\ln\mathcal{W}(\mathbf{S}_1,\mathbf{S}_2)=-\int_0^t dt'\int_0^t dt''\exp[-i\omega_k(t'-t'')]\gamma_k^*(t')\gamma_k(t'')\{\Theta(t''-t')S_{2,+}(t')S_{2,-}(t'')$$
$$+[1-\Theta(t''-t')]S_{1,+}(t')S_{1,-}(t'')\}+\int_0^t dt'\int_0^t dt''\exp[-i\omega_k(t'-t'')]\gamma_k^*(t')\gamma_k(t'')S_{2,+}(t')S_{1,-}(t'')$$
$$+\frac{1}{e^{\beta\omega_k}-1}\int_0^t dt'\int_0^t dt''\exp[-i\omega_k(t'-t'')]\gamma_k^*(t')\gamma_k(t'')\{S_{1,+}(t')S_{2,-}(t'')+S_{2,+}(t')S_{1,-}(t'')\}$$
$$-\frac{1}{e^{\beta\omega_k}-1}\int_0^t dt'\int_0^t dt''\exp[-i\omega_k(t'-t'')]\gamma_k(t'')\gamma_k^*(t')[S_{1,+}(t')S_{1,-}(t'')+S_{2,+}(t')S_{2,-}(t'')], \tag{44}$$

where Θ is the unit step function. The variables $\mathbf{S}_1$ and $\mathbf{S}_2$ are associated with forward and backward propagation in time, respectively.

By taking the limit of an infinite number of oscillators, this latter term becomes responsible for the appearance of dissipation in this model. After calculating the elements of the reduced density matrix, we can now calculate its time evolution and find a Fokker-Plank-type equation, as was done in the original work of CL.[16] We choose rather to take the semiclassical limit of this expression and see under what conditions, if any, a LLGB equation can be recovered.

IV. THE SEMI-CLASSICAL APPROXIMATION

In this section, we find the equation of motion of the magnetization by calculating the most probable configurational paths. This is done by calculating the path in the reduced density matrix element for the spin field that has the largest weight. Then we show that these paths are really the semiclassical limit of the classical paths averaged over the thermal fluctuations in the LLGB equation. We also show that the fluctuation-dissipation theorem is naturally satisfied. It reduces to the Brown form only in the high-temperature limit and only in the linear-response approximation. It is claimed that this approximation fails when the system is highly anisotropic,[10] but as we will show in the following section we see no evidence that this is the case (but see Ref. 18).

To facilitate the taking of the classical limit we make the change of variables,

$$\mathbf{S}(\tau)=\tfrac{1}{2}[\mathbf{S}_1(\tau)+\mathbf{S}_2(\tau)], \tag{45}$$

$$\mathbf{D}(\tau)=\mathbf{S}_1(\tau)-\mathbf{S}_2(\tau).$$

The variable $\mathbf{D}$, we will see, represents the fluctuating field that is coupled to the classical spin and is due to the inherent irreversibility in the system. In terms of these new variables, the trace of the reduced density matrix becomes

$$\mathrm{Tr}\rho=\sum_f \int \mathcal{D}\mu(\mathbf{\Omega}_1)\int \mathcal{D}\mu(\mathbf{\Omega}_2)\langle\mathbf{\Omega}_1|\rho_s(0)|\mathbf{\Omega}_2\rangle$$
$$\times\int \mathcal{D}\mu(\mathbf{S})\int \mathcal{D}\mu(\mathbf{D})\exp\left\{i\int_0^t dt'\mathbf{H}\cdot\mathbf{D}(t')\right.$$
$$\left.+i\mathbb{S}_{WZ}^{eff}[\mathbf{S},\mathbf{D}]\right\}\mathcal{W}(\mathbf{S},\mathbf{D}), \tag{46}$$

where

$$\mathbb{S}_{WZ}^{eff}[\mathbf{S},\mathbf{D}]=\mathbb{S}_{WZ}[\mathbf{S}_1]-\mathbb{S}_{WZ}[\mathbf{S}_2]. \tag{47}$$

The Feynman-Vernon functional $\mathcal{W}(\mathbf{S}_1,\mathbf{S}_2)$ now becomes

$$\mathcal{W}[\mathbf{S},\mathbf{D}]=\exp\left\{\int_0^t dt'\int_0^t dt''J(t',t'')\left[-\frac{1}{2}D_+(t')D_-(t'')\right.\right.$$
$$+\Theta(t''-t')S_+(t')D_-(t'')$$
$$\left.-[1-\Theta(t''-t')]D_+(t')S_-(t'')\right]$$
$$\left.-\int_0^t dt'\int_0^t dt''F_\beta(t',t'')D_+(t')D_-(t'')\right\}, \tag{48}$$

with $D_\pm=D_x\pm iD_y$. The functions $J(t',t'')$ and $F_\beta(t',t'')$ are dependent solely on the bath parameters,

$$J(t',t'')=\sum_k e^{-i\omega_k t'}e^{i\omega_k t''}\gamma_k^*(t')\gamma_k(t''), \tag{49}$$

$$F_\beta(t',t'')=\sum_k \frac{e^{-i\omega_k t'}e^{i\omega_k t''}\gamma_k^*(t')\gamma_k(t'')}{e^{\beta\omega_k}-1}. \tag{50}$$

In these new variables, the phase of $\ln \mathcal{W}$ clearly shows that the action of the reservoir results in an extra linear coupling in **S** and **D**. Moreover, we now have a quadratic term involving the variable **D**. This quadratic term is easily seen to be real and negative, assuring convergence of the sum over all configurations of **D**. The linear term describing interaction of the fields **S** and **D** is imaginary, however. In fact, it is such a term that gives rise to dissipation in the energy of the spin **S**. As we will show below, **D** is the field that is associated with the classical random field in the LLGB equation. If this is the case than averaging out **D** should give us a Langevin-type equation for the spin variable **S**. This Feynman-Vernon factor does *not* depend on the nature of the variable **S**. The same factor would have been obtained if we replace **S** by another oscillator.[27] The difference between an oscillator and a spin lies in $\mathbb{S}_{WZ}^{eff}$. It is this latter term, which is responsible for not having only additive noise, but also multiplicative one, as will be seen below.

To find the semiclassical result for the reduced density matrix, we again resort to a stationary-phase approximation to the phase of the path integrals in Eq. (46). First, we impose constraints on the spin magnitude by introducing two Lagrangian multiplier fields, $\eta_1(t)$ and $\eta_2(t)$. These are then coupled to the spin fields $\mathbf{S}_1$ and $\mathbf{S}_2$, respectively, as follows,

$$\delta(\mathbf{S}_1^2(\tau)-1)=\int \mathfrak{D}\eta_1(\tau)e^{i\int d\tau\eta_1(\tau)(\mathbf{S}_1^2(\tau)-1)}. \tag{51}$$

A similar expression holds for the other spin vector variable $\mathbf{S}_2$ and η_2. These constraints are then put back in the expression for the reduced density matrix element. The phase of the path integral is now a function of four independent fields η_1, η_2, **S**, and **D**. Extremizing the phase of these paths gives the semiclassical solution in the large spin limit. After solving for the constrained fields in terms of the spin fields $\mathbf{S}_1$ and $\mathbf{S}_2$, we write the remaining two equations in **S** and **D** only, obtaining a generalized form of the LLGB equation

$$\frac{d\mathbf{S}(t')}{dt'}=\mathbf{S}\times(\mathbf{H}+\mathbf{T}^{(S)}+\mathbf{T}^{(D)})+\frac{1}{4}\mathbf{D}\times\mathbf{W}, \tag{52}$$

and

$$\frac{d\mathbf{D}(t')}{dt'}=\mathbf{D}\times(\mathbf{H}+\mathbf{T}^{(S)}+\mathbf{T}^{(D)})+\mathbf{S}\times\mathbf{W}. \tag{53}$$

The vectors $\mathbf{T}^{(S)}$, $\mathbf{T}^{(D)}$, and **W** are associated with dissipation, thermal fluctuations and magnitude fluctuations, respectively. In the Cartesian form, they are, respectively, given in terms of the functions J and F_β by

$$\mathbf{T}^{(S)}(u)=\begin{bmatrix} i\int_0^u dt'\Theta(u-t')[J(u-t')S_-(t')-J^*(u-t')S_+(t')] \\ -\int_0^u dt'\Theta(u-t')[J(u-t')S_-(t')+J^*(u-t')S_+(t')] \\ 0 \end{bmatrix}, \tag{54}$$

$$\mathbf{T}^{(D)}(u)=\begin{bmatrix} i\int_0^t dt'\left\{\left[\frac{1}{2}J(u-t')+F_\beta(u-t')\right]D_-(t')+\left[J^*(u-t')+F_\beta^*(u-t')\right]D_+(t')\right\} \\ -\int_0^t dt'\left\{\left[\frac{1}{2}J(u-t')+F_\beta(u-t')\right]D_-(t')-\left[J^*(u-t')+F_\beta^*(u-t')\right]D_+(t')\right\} \\ 0 \end{bmatrix}, \tag{55}$$

and

$$\mathbf{W}(u)=\begin{bmatrix} -i\int_0^t dt'\Theta(t'-u)[J(u-t')D_-(t')-J^*(u-t')D_+(t')] \\ \int_0^t dt'\Theta(t'-u)[J(u-t')D_-(t')+J^*(u-t')D_+(t')] \\ 0 \end{bmatrix}. \tag{56}$$

These vectors are, in general, nonlocal in time and hence include memory effects in the equations of motion for **S** and **D**. This type of behavior is clearly needed when the relaxation time of the reservoir is of the same order as that of the spin particle. We will not discuss such a situation here. We are mainly interested to recover the constant dissipation case. Even though we called Eqs. (52) and (53) generalized LLGB equations, it is *not* yet clear how a Gilbert damping term can arise in these equations. However, through a careful choice of the density of states of the bath, the coupling constants, and the initial conditions, such damping form can be recovered as shown below.

To describe dissipation, we take the continuum limit for the bath states,

$$\sum_k \rightarrow \int d\omega \frac{dk}{d\omega}. \tag{57}$$

Then the spectral functions J and F_β are given by

$$J(\tau-\tau') = \int_0^\infty d\omega \lambda(\omega) |\gamma(\omega)|^2 \exp[-i\omega(\tau-\tau')] \tag{58}$$

and

$$F_\beta(\tau-\tau') = \int_0^\infty d\omega \frac{\lambda(\omega)}{\exp[\beta\omega]-1} |\gamma(\omega)|^2 \exp[-i\omega(\tau-\tau')]. \tag{59}$$

F_β is simply the nonzero temperature counterpart of J. $\lambda(\omega)$ is the density of states of the bath. In fact, the function

$$\mathcal{G}(\tau-\tau') = \frac{1}{2} J(\tau-\tau') + F_\beta(\tau-\tau') \tag{60}$$

is the inverse of the free propagator of the field **D**.

The vectors **S** and **D** are orthogonal as follows from the constraint equations, Eq. (51). Note that when **D** is set to zero, the density matrix becomes diagonal but the equation of motion for **S** will still have an extra term besides the precessional term that is due to the external field **H**. This extra term $\mathbf{T}^{(S)}(u)$ clearly always has a damping effect. We conclude that it is the vector **S** that must be identified with the classical magnetization and that **D** is the part that gives rise to the thermal fluctuations in **S**. Finally, we observe that the last term in Eq. (52) cannot be recovered in the classical limit. This quantum mechanical term is not present in the LLGB equation and is beyond a classical linear-response treatment of the problem of fluctuations. It is of higher order in **D** and temperature independent. It is easy to see that this term gives rise to fluctuations in the magnitude of the spin. These fluctuations cannot be accounted for classically since the magnitude of the magnetization is assumed to be constant.

One important thing to note from Eq. (52) is that the vector $\mathbf{T}^{(D)}$ is complex and hence, if fluctuations are present, the equation of motion for **S** becomes complex. The physical interpretation of this equation then becomes obscure at this level and may not be used as it stands to get the effective magnetization of the particle. Having a complex equation for the extremum path of the spin is, however, expected, given the dissipation present in the spin subsystem. The same result happens in the case of the harmonic oscillator.[16] A solution for the fluctuating magnetization is then sought through a direct calculation of the propagators in Eq. (31).

Now we show that a generalized fluctuation-dissipation theorem is satisfied as expected for this system since we started from a closed system and integrated out a large part of its degrees of freedom. We will also show that it is indeed the vector **D** that should be regarded as the quantum source of the thermal fluctuations in the spin system as treated in LLGB. The average of **S** is then the physically measurable magnetization. To better understand the physical meaning of the field **D** and to recover the standard stochastic description of the thermal fluctuations, we introduce yet another field, $\boldsymbol{\xi}(t)$. In Eq. (46), we replace the quadratic term in **D** in the Feynman-Vernon functional by an average over a Gaussian field, i.e., the left hand side of the following expression with its right-hand side:

$$\begin{aligned}
&\exp\left(-\int_0^t dt' \int_0^t dt'' D_+(t') \mathcal{G}(t'-t'') D_-(t'') \right) \\
&= \mathcal{N} \int \mathcal{D}\boldsymbol{\xi} \exp\left(-\frac{1}{2} \int_0^t dt' \int_0^t dt'' \xi_l(t') \frac{1}{2} \mathcal{G}_{ll}^{-1}(t'-t'') \xi_l(t'') \right. \\
&\left. -i \int_0^t dt' \xi_l(t') D_l(t') \right),
\end{aligned} \tag{61}$$

where $\mathcal{N}$ is a normalization constant. The quadratic term in **D** is then assumed to be a result of an averaging over all configurations of the field $\boldsymbol{\xi}$. Hence the path integral for the reduced density, Eq. (46), is now in terms of three fields. The field $\boldsymbol{\xi}$ will now result in a third equation of motion. However, to recover a thermal field similar to that introduced by Brown,[1] we proceed by assuming that the field $\boldsymbol{\xi}$ is classical, i.e., we ignore its equation of motion. At this point the field $\boldsymbol{\xi}$ is treated as a nondynamical field similar to the external field **H**. Next we solve for the magnetization **S** for a given $\boldsymbol{\xi}$ and only then do we average over all configurations of $\boldsymbol{\xi}$ with the quadratic weight that we originally ignored in the solution. In fact, $\boldsymbol{\xi}$ becomes the Brown stochastic field if we take the classical limit, that of high temperature and set $\mathbf{D}=0$. This is easily seen from the fact that $\boldsymbol{\xi}$ and **H** enter the same way in the exponent and hence in the equation of motion of **S**. From this, we clearly see that the LLGB equation is essentially correct *only* for small fluctuations, i.e., small **D**, so higher-order terms in **D** in the geometrical term $\mathbb{S}_{WZ}^{eff}$ can be neglected. Given these observations, we can now assume that the effective thermal field with which the spin is interacting is really nothing more than the abstract **D** field that has been introduced in this calculation of the reduced density matrix element. In fact $\boldsymbol{\xi}$ has the following correlation functions

$$\langle \xi_l(\tau)\xi_{l'}(\tau')\rangle = 2\delta_{ll'}\mathcal{G}(\tau-\tau')$$
$$= \frac{1}{\pi}\delta_{ll'}\int_0^\infty d\omega\,\omega\coth\left(\frac{\beta\omega}{2}\right)\frac{\pi\lambda(\omega)|\gamma(\omega)|^2}{\omega}$$
$$\times\exp[-i\omega(\tau-\tau')]. \tag{62}$$

To recover the correlations of the thermal field assumed in the LLGB equation, we simply take the high-temperature limit and require that the bath satisfies the condition,

$$\frac{\pi\lambda(\omega)|\gamma(\omega)|^2}{\omega} = \alpha, \tag{63}$$

where α is a constant. This condition provides the simplest relation between fluctuations and dissipation. In this case, the real part of the correlation functions for the random field become simply that of white noise,

$$\mathrm{Re}\langle \xi_l(\tau)\xi_{l'}(\tau')\rangle = 2\delta_{ll'}\alpha k_B T\delta(\tau-\tau'). \tag{64}$$

A similar condition arises if we replace the spin degrees of freedom by those of a harmonic oscillator.[16] However, at high temperature, as we mentioned earlier, a large spin can be approximated well by an oscillator. This condition is, however, still true even if the bosonic degrees of freedom of the bath are replaced by fermionic degrees of freedom.

Finally, we consider recovering the LLG equation with the Gilbert form of damping. Equations (52) and (53) are very general as they stand and it is not clear if the dissipation has the Gilbert form. To deduce the very special case of constant damping with the Gilbert form, we set the fluctuations to zero and take the following form for the spectral function J:

$$J(\tau'-\tau) = i\alpha\frac{d}{dt}\delta(\tau'-\tau). \tag{65}$$

After an integration by parts of the term containing $\mathbf{T}^{(S)}$ in the reduced density matrix element, Eq. (31), the equation of motion for $\mathbf{S}$, the magnetization, becomes simply

$$\frac{d\mathbf{S}(\tau)}{d\tau} = \mathbf{S}(\tau)\left[\mathbf{H}+\alpha\left(\frac{d\mathbf{S}(\tau)}{d\tau}-\frac{d(\mathbf{S}(\tau)\cdot\hat{\mathbf{z}})}{d\tau}\hat{\mathbf{z}}\right)\right]. \tag{66}$$

The boundary terms in the integration by parts are easily dealt with by a renormalization of the measure of the path integral. Keeping in mind the model used to derive this result, this equation reduces to the LLG form only in the limit of small deviations from local equilibrium. It is also important to note that the choice we made for J, Eq. (65), is compatible with the Gaussian white noise approximation for the thermal field. Hence the stochastic LLG equation, i.e., LLGB, is compatible with the FDT at high temperature and small fluctuations. Therefore, as far as the model considered here, we do not see any breakdown of LLGB within the above stated approximations. However, since the bath is very general, this does not preclude other equations that describe the dynamics of a spin in contact with a reservoir. The LLGB equation is just the simplest equation with white noise and small fluctuations. The condition on the bath, Eq. (65), to get LLG is clearly an artificial one. Moreover, the integration by parts alluded to above give rise to boundary terms. These terms are basically ignored. This means that LLG cannot capture the true transient behavior of the system. In fact, this is observed in experiments on small magnetic particles with fast switching rates.[30] In the following section we study a concrete example where we show how to recover classical results, which are consistent with LLGB, from our simple model.

Before we end this section, we make a final comment about the condition, Eq. (63), by which we recovered the LLG limit. If we assume constant coupling constants for the interaction between the spin and the bath, we find that the density of states must be linear. For phonons, the density of states is quadratic and hence, based on this assumption, cannot be the major source of the damping constant α. In fact, dissipation due to currents is believed to be much larger.[31] Ferromagnetic compounds, such as FeNi, show a complex density of states for the nonlocalized electrons; hence a condition such as that given in Eq. (63) is representative of many competing mechanisms. It is only the lower part of the spectrum that is important for a constant approximation to dissipation. In fact, in Eq. (58), the limit of integration cannot be taken to be infinite for a real bath. This, in turn, will introduce a new cutoff parameter in condition (63), which will be system dependent.

V. CORRELATION FUNCTIONS OF THE MAGNETIZATION IN THIN FILMS

In this last section, we study the magnetic noise in a thin anisotropic film. The magnetization is taken to be uniform and near equilibrium, that is, along an easy axis ($\mathbf{z}$) in the plane of the film. Here we are simply interested in the case that reproduces the classical LLG results for this problem. The general case includes other possible solutions and is treated elsewhere.[18]

Clearly the bath influence on the magnetic moment with and without anisotropy is the same as before, but now there is coupling between the fluctuating field and the spin field that is anisotropy dependent.

The Hamiltonian of the spin-bath system is taken in this case to be

$$\hat{\mathcal{H}} = -H\hat{S}_z - K\hat{S}_z^2 + K_p\hat{S}_x^2 - \sum_k \gamma_k a_k^\dagger \hat{S}_-$$
$$-\sum_k \gamma_k^* \hat{S}_+ a_k + \sum_k \omega_k a_k^\dagger a_k, \tag{67}$$

where H is a large positive external in-plane magnetic field along the z axis and the hard axis is along the x axis. K and K_p are positive constants. The remaining terms describe the interaction of the heat bath with the transverse components of the magnetization. We are only interested in the regime where the equilibrium position is along the z axis and the coupling between the spin and the bath is small. After writing $\hat{S}_x^2$ in terms of $\hat{S}_\pm$, dropping a term proportional to $\hat{S}^2$, a constant, the Hamiltonian of the spin subsystem becomes

$$\hat{\mathcal{H}}_0 = \tfrac{1}{2}A\hat{S}_x^2 + \tfrac{1}{2}B\hat{S}_y^2, \tag{68}$$

where the coefficients A and B are given in terms of the initial physical constants,

$$A = H + 2K + 2K_p, \tag{69}$$

and

$$B = H + 2K. \tag{70}$$

After integrating out the bath degrees of freedom, we find that the sum of the diagonal reduced density matrix elements in the presence of anisotropy becomes

$$\begin{aligned}\sum_f \rho_{ff}(t) = \sum_f \int \mathcal{D}\mathbf{S}_i \int \mathcal{D}\mathbf{S}_i' \langle \mathbf{S}_i|\rho_s(t_0)|\mathbf{S}_i'\rangle \\ \times \int_{\mathbf{S}_i}^{\mathbf{S}_f} \mathcal{D}\mathbf{S}_1 \int_{\mathbf{S}_f}^{\mathbf{S}_i'} \mathcal{D}\mathbf{S}_2 \exp\Bigg[i(S_{WZ}[\mathbf{S}_1] - S_{WZ}[\mathbf{S}_2]) \\ + iH_z \int_{t_0}^{t} dt' [S_{1,z}(t') - S_{2,z}(t')] \\ - i\int_{t_0}^{t} dt' \Bigg(\frac{1}{2}A[S_{1,x}^2(t') - S_{2,x}^2(t')] \\ + \frac{1}{2}B[S_{1,y}^2(t') - S_{2,y}^2(t')] \Bigg) \Bigg] \mathcal{W}(\mathbf{S}_1, \mathbf{S}_2).\end{aligned} \tag{71}$$

In the following we are interested only in calculating the fluctuations in the magnetization around equilibrium. Hence nonlinear terms in **D** will be neglected. Moreover, we shall not study the short time behavior of the system, hence initial conditions are irrelevant. It will therefore be assumed that the initial density matrix element is nonzero only for one state, the initial equilibrium state. We also take the limit $t_0 \to -\infty$ and $t \to \infty$. Since, we will be calculating correlation functions, we define the following effective action functional $\Gamma[\mathbf{S_1}, \mathbf{S_2}]$ which is needed in finding averages,

$$\begin{aligned} i\Gamma[\mathbf{S_1}, \mathbf{S_2}] = -(\mathbb{S}_{WZ}[\mathbf{S}_1] - \mathbb{S}_{WZ}[\mathbf{S}_2]) - H_z \int_{t_0}^{t} dt' [S_{1,z}(t') \\ - S_{2,z}(t')] + \int_{t_0}^{t} dt' \Bigg(\frac{1}{2}A[S_{1,x}^2(t') - S_{2,x}^2(t')] \\ + \frac{1}{2}B[S_{1,y}^2(t') - S_{2,y}^2(t')] \Bigg) + i \ln \mathcal{W}(\mathbf{S}_1, \mathbf{S}_2). \end{aligned} \tag{72}$$

The minimization of this action gives the equations of motion for the magnetization **S** and the corresponding fluctuations **D**,

$$\frac{d\mathbf{S}}{dt} = \mathbf{S} \times (\mathbf{H} + \mathbf{T}^{(S)} + \mathbf{T}^{(D)} - \overline{\mathbf{S}}), \tag{73}$$

$$\frac{d\mathbf{D}}{dt} = \mathbf{D} \times (\mathbf{H} + \mathbf{T}^{(S)} + \mathbf{T}^{(D)} - \overline{\mathbf{D}}). \tag{74}$$

The vectors $\mathbf{T}^{(S)}$ and $\mathbf{T}^{(D)}$ have the same definitions as above, Eqs. (52) and (53), and account for the dissipation and the fluctuations, respectively. The remaining vectors $\overline{\mathbf{S}}$ and $\overline{\mathbf{D}}$ are due to the specific coupling considered in this section among the spin components due to anisotropy. They have the following definitions:

$$\overline{\mathbf{S}} = (AS_x,\ BS_y,\ 0), \tag{75}$$

$$\overline{\mathbf{D}} = (AD_x,\ BD_y,\ 0). \tag{76}$$

Note that for small fluctuations, the magnetization is constant in magnitude within this approximation.

Next we calculate the correlation functions of the magnetization vector **S**. This is done more effectively through the method of virtual external sources.[32,33] This functional method is an extension of similar methods applied to the equilibrium case.[34] First, we observe that the correlation function

$$\langle S_x(t) S_x(0) \rangle = Tr(S_x(t) S_x(0) \rho) \tag{77}$$

can be derived by first coupling the transverse components of **S** and **D** to time-dependent external sources **P** and **Q**. The effective action of the system becomes

$$\Gamma^{eff}[\mathbf{S}, \mathbf{D}; \mathbf{P}, \mathbf{Q}] = \Gamma[\mathbf{S}, \mathbf{D}] + \int dt [\mathbf{P} \cdot \mathbf{S} + \mathbf{Q} \cdot \mathbf{D}]. \tag{78}$$

Γ is the action of the spin system and the bath with the external sources set to zero. Next, we define the generating functional

$$\mathbb{Z}[\mathbf{P}, \mathbf{Q}] = \int \mathcal{D}\mathbf{S} \mathcal{D}\mathbf{D}\, e^{i\Gamma^{eff}[\mathbf{S}, \mathbf{D}; \mathbf{P}, \mathbf{Q}]}. \tag{79}$$

The correlation functions are then found by differentiating this latter functional with respect to the external sources,

$$\begin{aligned} \left[\frac{\delta^2 \ln \mathbb{Z}}{\delta P_i(t)\, \delta P_j(t')} \right]_{\mathbf{P}=\mathbf{Q}=0} = \langle S_i(t) S_j(t') \rangle, \\ t > t',\ \ i,j = x,y. \end{aligned} \tag{80}$$

Since we are looking for small deviations from equilibrium, we have for the transverse components

$$\langle S_i(t) \rangle = 0, \tag{81}$$

$$\langle D_i(t) \rangle = 0, \tag{82}$$

$$\langle D_i(t) D_j(0) \rangle = 0,\ \ t > 0 \tag{83}$$

in the absence of any external forces.

To calculate two-point correlation functions, we average the previous equations of motion for **S** and **D** in the presence of the external sources and then differentiate with respect to **P** or **Q**, e.g.,

$$\frac{\delta\langle S_i(t)\rangle}{\delta P_j(t')} = i\langle S_i(t)S_j(t')\rangle, \quad t>t'. \tag{84}$$

To recover the correlation functions of the original system, we set the fields **P** and **Q** to zero at the end of the calculations. Hence these fields are assumed small but arbitrary in the rest of this calculation. This is equivalent to a linear-response calculation in this particular system.

In the following we will be interested in studying the case where the bath is chosen such that

$$J(t-t') = i\alpha\frac{d}{dt}\delta(t-t'). \tag{85}$$

This corresponds to the LLG case, which is equivalent to assuming the following form for the bath parameters:

$$\lambda(\omega)|\gamma(\omega)|^2 = \frac{\alpha\omega}{\pi}, \tag{86}$$

where, as before, $\lambda(\omega)$ is the density of states of the bath and α is a constant that we will consider to be small here.

The damping term $\mathbf{T}^{(S)}$ becomes after an integration by parts,

$$T_i^S(t) = -\alpha\frac{d}{dt}S_i(t), \quad i=x,y. \tag{87}$$

The fluctuation term is simply

$$T_i^D(t) = i\int_0^\infty dt'\mathcal{G}(t-t')D_i(t'), \quad i=x,y, \tag{88}$$

where $\mathcal{G}(t-t')$ is in the high-temperature limit,

$$\mathcal{G}(t-t') = \alpha k_B T\delta(t-t') + i\frac{\alpha k_B T}{\pi}\mathcal{P}\left(\frac{1}{t-t'}\right). \tag{89}$$

The imaginary part of $\mathcal{G}$ is absorbed in the definition of the coefficients A and B. The equations of motion for the **S** field in the presence of the external sources then take the form of those of a damped harmonic oscillator with source terms that are functions of the external source **Q** and the fluctuations **D**,

$$\int dt' G_S^{-1}(t,t')S_x(t') = A[T_x^D(t)+Q_x(t)] + \frac{d}{dt}[T_y^D(t)+Q_y(t)], \tag{90}$$

$$\int dt' G_S^{-1}(t,t')S_y(t') = B[T_y^D(t)+Q_y(t)] - \frac{d}{dt}[T_x^D(t)+Q_x(t)], \tag{91}$$

where G_S is the "free" propagator of the **S** field

$$G_S^{-1}(t,t') = \left(\frac{d^2}{dt^2}+\omega_0^2+\alpha(A+B)\frac{d}{dt}\right)\delta(t-t'), \tag{92}$$

and $\omega_0^2 = AB$ is the renormalized ferromagnetic resonance frequency. Similarly, the **D** field has the equations of motion

$$\int dt' G_D^{-1}(t,t')S_x(t') = AP_x(t) + \frac{d}{dt}P_y(t), \tag{93}$$

$$\int dt' G_D^{-1}(t,t')S_y(t') = BP_y(t) - \frac{d}{dt}P_x(t), \tag{94}$$

where G_D^{-1} is the propagator associated with the **D** field and is equal to G_S^{-1}.

It is interesting to note that within this approximation the external source **P** does not appear in the equations of motion of **S** and hence accounts only for nonlinear terms in the equation of motion. For the **S** field equations, the **D** field appears on the right-hand side of Eqs. (90) and (91) as a source term, while the **D** field equations are sourceless, which is consistent with having random forces acting on the magnetization with no back reaction. Even though these equations are similar to those of a damped harmonic oscillator, the equation of motion for **S** has additional terms on the right-hand side that depend on the derivative of the fluctuations.

To get the two-point correlation functions of the magnetization, we average the equations of motion for **S** and **D** with respect to the reduced density matrix of the spin system. Since these equations are linear, the average values have similar equations of motion. To get the equation of motion for $\langle S_x(t)S_x(t')\rangle$, we differentiate $\langle S_x(t)\rangle$ with respect to $\mathbf{P}(t')$. The other equations of motion are obtained in the same way. These equations are easily solved in the Fourier space. However, in this particular linear case, these correlation functions can also be derived by a simpler method by first deriving the classical equation of motion for the average magnetization and then applying the FDT to get the average of any anticommutator of two operators.[27] In the equation of motion for **S**, Eq. (73), quantum effects are included through the fluctuations **D**, and hence the classical equation of motion is found by setting the field **D** to zero and invoke the Ehrenfest theorem to write the equations of motion for the average magnetization:

$$\int dt' G_S^{-1}(t,t')\langle S_x(t')\rangle = AQ_x(t) + \frac{d}{dt}Q_y(t), \tag{95}$$

$$\int dt' G_S^{-1}(t,t')\langle S_y(t')\rangle = BQ_y(t) - \frac{d}{dt}Q_x(t). \tag{96}$$

We observe that in this case the derivative of the magnetization **S** with respect to **Q** is the response function:

$$\frac{\delta\langle S_i(t)\rangle}{\delta\langle Q_j(0)\rangle} = \chi_{ij}(t), \quad t>0. \tag{97}$$

Now a straightforward application of the FDT gives the magnetization correlation functions

$$S_{ij}(t)=\tfrac{1}{2}\langle S_i(t)S_j(0)+S_j(0)S_i(t)\rangle. \tag{98}$$

In the Fourier space they are related to the dissipative part of the response function χ,

$$S_{ij}(\omega)=\coth(\beta\omega/2)\chi''_{ij}(\omega), \tag{99}$$

where χ'' is the imaginary part of the susceptibility tensor.[35] It is not difficult now to show that the different two-point correlation functions of the magnetization vector **S** are

$$S_{xx}(\omega)=2\alpha k_B T\left[\frac{\omega^2+B^2}{(\omega_0^2-\omega^2)^2+(\alpha_{LLG}\omega)^2}\right], \tag{100}$$

$$S_{yy}(\omega)=2\alpha k_B T\left[\frac{\omega^2+A^2}{(\omega_0^2-\omega^2)^2+(\alpha_{LLG}\omega)^2}\right], \tag{101}$$

$$S_{xy}(\omega)=S_{yx}(-\omega)=2i\alpha_{LLG}k_B T\left[\frac{\omega}{(\omega_0^2-\omega^2)^2+(\alpha_{LLG}\omega)^2}\right], \tag{102}$$

where

$$\alpha_{LLG}=\alpha(A+B). \tag{103}$$

Similar correlation functions have been derived from classical LLG by Smith.[8] These results can also be derived from the Heisenberg equations of motion by assuming from the start that the commutation relations of $\hat{S}_+$ and $\hat{S}_-$ are similar to those of a harmonic oscillator.[36,18] This shows again that LLGB is very reasonable within the assumptions stated in the last section. Finally, we would like to mention that had we not set **D** to zero, then differentiation of the average of **D** with respect to **P** will give the average of the two-point correlation functions of the fluctuations or the average of the commutator of the magnetization due to quantum effects.

VI. CONCLUSION

Using coherent states and a simple quantum mechanical model for a single large spin particle, we have shown that a generalized form of the Landau-Lifshitz equation can be recovered in the semiclassical limit. We have also shown how fluctuations give rise to two different contributions to the magnetization. One contribution is magnitude conserving and the other is not. We derived generalized equations for the magnetization that include nonlocal effects in the dissipation term and go beyond the simple linear-response approach. An immediate result of this work is the dependence of fluctuations on the anisotropy of the system, especially if the fluctuations are large. In this latter case, the fluctuations cannot be treated by a simple isotropic thermal field. The LLGB equation, i.e., Gaussian white noise thermal field, is clearly inadequate in this respect. However, these deficiencies can be corrected by using the right correlation functions for the fluctuations. Changing the damping to a tensor quantity in the LLG equation[10] to account for noise is then not necessary; however, it cannot be ruled out either based on the work presented here.[18] Only experiment can decide which model is best suited to explain its results. The LLGB equation is clearly a consistent theory within the assumptions stated in the text. But the assumption, Eq. (65), on the bath to reproduce it is highly idealized and cannot be taken seriously. In the last section, we have shown how the classical results of LLGB can be recovered from this quantum model. More complicated couplings, other than the linear coupling considered here, naturally induce a tensor character for the relaxation. Most of these conclusions are true even in the purely classical treatment. Garcia-Palacios treated similar questions at the classical level and our results agree with his results in that limit.[37] Future work will address questions beyond which LLGB is not valid.

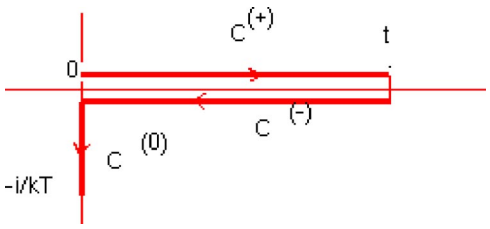

FIG. 1. Complex time path for the trace of the density matrix, Eq. (31).

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APPENDIX

Here we briefly address some questions related to the boundary conditions on the path integrals in the density matrix representation. The path integrals in Eq. (31) are time-ordered expressions along the path $C=C^{(-)}\cup C^{(0)}\cup C^{(+)}$, Fig. 1. For the trace only diagonal elements of the density matrix are needed; hence we apply periodic boundary conditions at the end points of the path similar to the equilibrium case.

The density matrix element at time t of a state **S** can be expressed as an integral along a single path in the complex time plane,

$$\rho(\mathbf{S},t)=\langle\mathbf{S},t|\rho|\mathbf{S},t\rangle \tag{A1}$$

$$=\langle\mathbf{S}|\rho(t)|\mathbf{S}\rangle=\langle\mathbf{S}|\mathcal{T}e^{-i\hat{\mathcal{H}}t}\rho(0)\mathcal{T}^{-1}e^{i\hat{\mathcal{H}}t}|\mathbf{S}\rangle, \tag{A2}$$

where $\mathcal{T}$ is the time-ordering operator. Assuming the system is initially at equilibrium, we have

$$\rho(0)=e^{-\beta\hat{\mathcal{H}}}. \tag{A3}$$

Hence, if we make use of the trace property, $\mathrm{Tr}\hat{A}\hat{B}=\mathrm{Tr}\hat{B}\hat{A}$, the trace of the density matrix can be written in the following form:

$$\mathrm{Tr}\rho = \int \mathcal{D}\mathbf{S}\langle \mathbf{S}|\mathcal{T}_C e^{-i\int_C \hat{\mathcal{H}}dt'}|\mathbf{S}\rangle. \tag{A4}$$

$\mathcal{T}_C$ is now a time-ordering operator along the path C, Fig. 1. It can be shown that if time t is taken to be very large or the initial time is taken to be $-\infty$, the initial conditions will be irrelevant and the contribution of the path $C^{(0)}$ is factored out.[18] This is the case of interest in the main text. The discretization of the path integral in the general case of arbitrary t is carried out exactly as in the equilibrium case,[29] except that here we have three branches for the complex time path rather than one as in the equilibrium case. First, we divide the path into $3N$ subintervals each of length $\Delta t=(2t+\beta)/3N$, $t_0=0$, $t_1=\Delta t, \ldots,$ $t_N=t, t_{N+1}=t-\Delta t, \ldots,$ $t_{2N}=0$, $t_{2N+1}=-i\beta/N, \ldots, t_{3N+1}=-i\beta$. Hence, the integral operators can be written in the following discrete form:

$$e^{-i\int dt'\hat{\mathcal{H}}} = e^{-i\sum_{i=1}^{3N}\hat{\mathcal{H}}(t_i)\Delta t}. \tag{A5}$$

At each point t_i, we insert a resolution of the identity operator, Eq. (19),

$$\langle \mathbf{S}_{3N}|e^{-i\int\hat{\mathcal{H}}dt}|\mathbf{S}_0\rangle = \prod_{i=1}^{3N-1}\int_C d\mu(\mathbf{S}_i)\langle \mathbf{S}_i|e^{-i\hat{\mathcal{H}}(t_i)\Delta t}|\mathbf{S}_{i-1}\rangle. \tag{A6}$$

From Eq. (20), we have

$$\langle \mathbf{S}_i|\mathbf{S}_{i-1}\rangle = e^{ij\,\mathrm{Area}(\mathbf{S}_i,\mathbf{S}_{i-1},\mathbf{z})}\left(\frac{1+\mathbf{S}_i\cdot\mathbf{S}_{i-1}}{2}\right)^j, \tag{A7}$$

where $\mathrm{Area}(\mathbf{S}_i,\mathbf{S}_{i-1},\mathbf{z})$ is the area on the sphere of the triangle with vertices $\mathbf{S}_i,\mathbf{S}_{i-1}$, and $\mathbf{z}$. The path-integral representation of a diagonal element of the density matrix along the path C is then given by

$$\rho = \int_C \prod_{i=1}^{3N-1} d\mu(\mathbf{S}_i)\exp\left\{ i\,j\mathbb{S}_{WZ}[\mathbf{S}] + \frac{j\Delta t}{4}\int_C dt'(\partial_{t'}\mathbf{S}(t'))^2 - i\int_C dt'\mathcal{H}[\mathbf{S}]\right\}, \tag{A8}$$

where the Wess-Zumino term $\mathbb{S}_{WZ}[\mathbf{S}]$ is given as in the equilibrium case by the following integral formula:

$$\mathbb{S}_{WZ}[\mathbf{S}] = \int_0^1 d\tau\int_C dt\mathcal{S}(t,\tau)\cdot(\partial_t\mathcal{S}(t,\tau)\times\partial_\tau\mathcal{S}(t,\tau)) \tag{A9}$$

with the boundary conditions

$$\mathcal{S}(t,0)=\mathbf{S}(t),$$

$$\mathcal{S}(t,1)=\mathbf{z},$$

$$\mathbf{S}_0=\mathcal{S}(t_0,\tau)=\mathcal{S}(t_{3N},\tau)=\mathbf{S}_{3N}. \tag{A10}$$

The expressions used in the propagators in the main text, Eq. (34), follow by writing $\mathbb{S}_{WZ}[\mathbf{S}]$ as a sum of three contributions from the different branches of the complex time path,

$$\mathbb{S}_{WZ}[\mathbf{S}] = \mathbb{S}^{(+)}_{WZ}[\mathbf{S}] + \mathbb{S}^{(-)}_{WZ}[\mathbf{S}] + \mathbb{S}^{(0)}_{WZ}[\mathbf{S}], \tag{A11}$$

where $\mathbb{S}^{(+)}_{WZ}[\mathbf{S}]$ is the contribution coming from $\mathbf{S}\in\mathbf{C}^{(+)}$ and so on. Hence, it is permissible to use the Wess-Zumino formula for a segment of a closed path, as long as we are calculating properties that depend solely on closed paths, such as the trace of the density matrix and the correlation functions of the magnetization. An alternate expression for the WZ term in terms of the components of the vector $\mathbf{S}$ is also possible. We first observe that the overlap of two nearest unit vectors $\mathbf{s}_n(\theta_n,\phi_n)$ and $\mathbf{s}_{n+1}(\theta_{n+1},\phi_{n+1})$ on the path C,

$$\langle \mathbf{s}_{n+1}|\mathbf{s}_n.\rangle = \left(\cos\frac{\theta_{n+1}}{2}\cos\frac{\theta_n}{2} + \sin\frac{\theta_{n+1}}{2}\sin\frac{\theta_n}{2}e^{-i(\phi_{n+1}-\phi_n)}\right)^{2j}, \tag{A12}$$

can be written, to first order in $\Delta\theta_n=\theta_{n+1}-\theta_n$ and $\Delta\phi_n=\phi_{n+1}-\phi_n$, as a phase

$$\langle \mathbf{s}_{n+1}|\mathbf{s}_n\rangle = \exp[-ij(1-\cos\theta_n)\Delta\phi_n]. \tag{A13}$$

Recalling that on a unit sphere with tangent vectors $(\mathbf{e}_\theta,\mathbf{e}_\phi)$, we have

$$\Delta\mathbf{s}_n\cdot\mathbf{e}_\phi = \sin\theta_n\Delta\phi_n. \tag{A14}$$

Then we can define a vector potential $\mathbf{A}(\mathbf{s})$ as

$$\mathbf{A}(\mathbf{s}) = \frac{1-\cos\theta}{\sin\theta}\mathbf{e}_\phi \tag{A15}$$

and write the overlap between the two nearest neighbors

$$\langle \mathbf{s}_{n+1}|\mathbf{s}_n\rangle = \exp\{-ij\mathbf{A}(\mathbf{s}_n)\cdot\Delta\mathbf{s}_n\}. \tag{A16}$$

Hence, the Wess-Zumino term for the whole path C becomes

$$\prod_{n=1}^{3N}\langle \mathbf{s}_{n+1}|\mathbf{s}_n\rangle = \exp\left[-ij\sum_n \mathbf{A}(\mathbf{s}_n)\cdot\Delta\mathbf{s}_n\right] = \exp\left[ij\int_C dt(\cos\theta-1)\dot{\phi}\right]. \tag{A17}$$

Finally, it can be shown that the WZ term can be written, within a constant, in terms of the components of the spin vector $\mathbf{S}$,

$$\mathbb{S}_{WZ}[\mathbf{S}] = \int_C dt\frac{S_z}{S_x^2+S_y^2}(S_x\dot{S}_y-\dot{S}_xS_y). \tag{A18}$$

Such an expression for the WZ term could have been used from the start; however, it is very cumbersome due to the first term in the integrand and hence the holomorphic representation does seem to be the natural representation for the spin systems, especially in the problems where the calculation of transition rates is needed.[18]

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