

Rotation of Magnetization in Unison and Langevin Equations for a Large Spin

Ivo Klik¹

Received March 1, 1991

A single-domain ferromagnetic particle is represented as a large spin (model of rotation in unison) whose stochastic dynamics is derived from a spin-boson Hamiltonian. It is shown in the Markovian limit that thermal equilibrium exists provided that the fluctuation-dissipation theorem is supplemented by a symmetry constraint which for bilinear anisotropic and nonlinear (magnetoelastic) spin-bath coupling can only be satisfied in the underdamped limit. Only for bilinear isotropic coupling (Gilbert's theory) is it satisfied identically for arbitrary damping strength. Uniaxial and cubic symmetries are considered. For a model uniaxial crystal the thermal decay rate of \mathbf{M} and the thermal enhancement of the macroscopic quantum tunneling rate are calculated for Gilbert and magnetoelastic dissipative couplings and compared. The effects of memory are discussed.

KEY WORDS: Micromagnets; rotation in unison; stochastic dynamics of a large spin; approach to equilibrium; classical and quantum decay rate of magnetization.

The dynamics of the vector of total magnetization $\mathbf{M}(t)$ of a fine single-domain ferromagnetic particle (superparamagnet) is commonly described within the model of rotation in unison. This model assumes that exchange interaction is strong enough to maintain all spins within the particle in parallel at all times and the particle is then represented as a large spin $\mathbf{S} = \gamma_0^{-1} \mathbf{M}$, where γ_0 is the gyromagnetic ratio. Surface effects and nucleation of domain walls on impurities⁽¹⁾ are neglected.

The purpose of this article is to study the stochastic dynamics of a large spin \mathbf{S} with respect to the spatial symmetry of the dissipative coupling; the focus is on the existence of thermal equilibrium. For this reason the

¹ Department of Physics, National Taiwan University, Taipei, Taiwan 10764, R.O.C.

Langevin equations for \mathbf{S} , obtained from a spin-boson Hamiltonian, are treated in the Markovian limit only, where all proofs may rigorously be carried out. One may tentatively assume that the qualitative results of this paper hold at least for near-Markovian systems. A detailed study of non-Markovian systems, for which the Markovian limit does or does not exist, is complex and is deferred to a future publication. First Gilbert's equation for $\mathbf{M} = \gamma_0 \mathbf{S}$ is rederived from an isotropic spin-bath coupling bilinear in both the spin and bath coordinates. Next spin-bath coupling is considered which is bilinear but anisotropic or linear in the bath coordinates only, as corresponds to the magnetoelastic, or dipolar, interaction. It is shown in the Markovian limit that under these circumstances it is in general impossible to write down a Langevin equation describing the evolution of the system toward thermal equilibrium; this observation is the main result of the present article. The time evolution, however, is satisfactory for arbitrary symmetry of the dissipative coupling in the underdamped limit, i.e., in the first order of a small dissipation parameter η , and in this limit for a simple model Hamiltonian the thermal decay rate and the macroscopic quantum tunneling (MQT) rate of magnetization are calculated for both a linear and quadratic spin-bath coupling. The thermal decay rate differs for the two cases only in the prefactor and is unlikely to produce any measurable effects. The MQT rate, however, is enhanced at very low temperatures by an exponential factor which is measurable and its dependence on the crystal parameters is calculated and discussed. All calculations are carried out in the phase space (ϕ, P) introduced by the parametrization

$$\mathbf{M} = \gamma_0 \mathbf{S} = \gamma_0 [(P_0^2 - P^2)^{1/2} \cos \phi, (P_0^2 - P^2)^{1/2} \sin \phi, P] \quad (1)$$

and the saturation magnetization is $M_s = |M(t)| = \gamma_0 P_0 = \text{const}$. In spherical coordinates $P = P_0 \cos \theta$. It is assumed that the magnetic energy H of the particle is known and given in terms of the direction cosines α_i , so that $H(\alpha_i)$ may be written^(2,3) either as $H(S_i)$ or as the Hamiltonian $H(\phi, P)$.

The spin-boson phenomenological Hamiltonian H_{tot} is constructed in such a way as to be invariant under both time and space inversion⁽⁴⁾; the derivation of a stochastic equation from this model follows ref. 5. Gilbert's equation of motion⁽⁶⁾ is obtained if we interpret the boson heat bath as an electromagnetic field given by the Hamiltonian

$$H_f = \frac{1}{2} \sum_{\mathbf{k}} (\mathbf{p}_{\mathbf{k}}^2 + \omega_{\mathbf{k}}^2 \mathbf{q}_{\mathbf{k}}^2) \quad (2)$$

where \mathbf{k} is the wave vector, $k = |\mathbf{k}|$, and $\mathbf{q}_{\mathbf{k}}$ and $\mathbf{p}_{\mathbf{k}}$ are the position and momentum coordinates of the field normal modes. The spin couples to

individual modes \mathbf{B}_k of the magnetic field⁽⁷⁾ and the interaction Hamiltonian is the bilinear form

$$H_{\text{int}} = \sum_k c_k \mathbf{B}_k \cdot \mathbf{S} = \sum_k (\mathbf{S} \times \mathbf{k}) \cdot (a_k \omega_k \mathbf{q}_k + b_k \mathbf{p}_k) \quad (3)$$

The coupling constants a_k, b_k are independent of each other. They are chosen to be scalars, which corresponds to isotropic dissipative coupling. The spin-boson Hamiltonian must yet be supplemented⁽⁴⁾ by the counter-term $H_c = 1/2 \sum_k (\mathbf{S} \times \mathbf{k})^2 (a_k^2 + b_k^2)$, which ensures that the bath oscillates around its current equilibrium position given by $H_f + H_{\text{int}}$. From the full Hamiltonian $H_{\text{tot}} = H + H_f + H_{\text{int}} + H_c$ we obtain for the bath coordinates

$$\begin{aligned} \mathbf{q}_k(t) &= \frac{1}{\omega_k} \int_0^t dt' \sin \omega_k(t-t') [b_k \dot{\mathbf{S}}(t') - a_k \omega_k \mathbf{S}(t')] \times \mathbf{k} + \mathbf{q}_k^{(0)}(t) \\ \mathbf{p}_k(t) &= - \int_0^t dt' \sin \omega_k(t-t') [a_k \dot{\mathbf{S}}(t') + b_k \omega_k \mathbf{S}(t')] \times \mathbf{k} + \mathbf{p}_k^{(0)}(t) \end{aligned} \quad (4)$$

where $\mathbf{q}_k^{(0)}(t)$ and $\mathbf{p}_k^{(0)}(t)$ are the proper oscillations of the bath.

In order to find the effective magnetic field \mathbf{B}_{eff} acting on the spin \mathbf{S} , we take the derivative $\partial H_{\text{tot}}/\partial \mathbf{S}$ and substitute in here from Eq. (4). We shall further assume that at the time $t=0$ the heat bath was in thermal equilibrium,⁽⁵⁾ so that $\langle q_{i,\mathbf{k}}(0) q_{j,\mathbf{k}'}(0) \rangle = \omega_k^{-2} T \delta_{i,j} \delta_{\mathbf{k},\mathbf{k}'}$ and $\langle p_{i,\mathbf{k}}(0) p_{j,\mathbf{k}'}(0) \rangle = T \delta_{i,j} \delta_{\mathbf{k},\mathbf{k}'}$, where T is the bath temperature. Then, on taking the averages,

$$-\mathbf{B}_{\text{eff}} = \langle (H_{\text{tot}})_{\mathbf{S}} \rangle = H_{\mathbf{S}} + \int_0^t dt' \gamma(t-t') \dot{\mathbf{S}}(t') + \tilde{\mathbf{b}}(t) \quad (5)$$

with $H_{\mathbf{S}} = \partial H/\partial \mathbf{S}$. The two-time correlation function of the noise field $\tilde{\mathbf{b}}$ is given in terms of the memory kernel $\gamma(t-t')$ as

$$\langle \tilde{b}_i(t) \tilde{b}_j(t') \rangle = T \gamma(t-t') \delta_{i,j} \quad \text{with} \quad \langle \tilde{\mathbf{b}}(t) \rangle = \mathbf{0} \quad (6)$$

and the Laplace transform of the memory kernel $\gamma(t)$ is

$$\hat{\gamma}(z) = 2 \sum_{\mathbf{k}} (a_k^2 + b_k^2) \frac{z}{z^2 + \omega_k^2} k_i^2$$

where $i = 1$ or 2 or 3 . Isotropy of space has been made use of in deriving $\hat{\gamma}$ and all odd powers of k_i in the sum were omitted. In the memoryless case $\gamma(t) = 2\eta\delta(t)$ and $\tilde{b}_i \rightarrow b_i = (2\eta T)^{1/2} w_i(t)$, where $w_i(t)$ are three independent Wiener processes. Gilbert's equation for the magnetization $\mathbf{M}(t)$ is

obtained if the Markovian equation of motion $\dot{\mathbf{S}} = \mathbf{S} \times \mathbf{B}_{\text{eff}}$ is multiplied by the gyromagnetic ratio γ_0 . One has $\mathbf{S} \cdot \mathbf{S} = P_0^2$ for any \mathbf{B}_{eff} . Equations (5) and (6) hold for arbitrary choice of $\{a_k, b_k\}$. Thus, Gilbert's equation follows from an isotropic spin-bath coupling bilinear in the spin and bath coordinates; any other information is contained in the kernel $\hat{\gamma}$.

For the intended discussion of the (Stratonovich) Fokker-Planck equation we require the Langevin equation in the (ϕ, P) phase space; only the memoryless case is considered here. Proceeding as before, we obtain

$$\begin{aligned} \dot{\phi} &= \langle (H_{\text{tot}})_P \rangle = H_P + \mathbf{S}_P \cdot [\eta \dot{\mathbf{S}} + \mathbf{b}] \\ \dot{P} &= -\langle (H_{\text{tot}})_\phi \rangle = -H_\phi - \mathbf{S}_\phi \cdot [\eta \dot{\mathbf{S}} + \mathbf{b}] \end{aligned} \quad (7)$$

with $H_P = \partial H / \partial P$, etc. The vector \mathbf{S} is a function of (ϕ, P) and these equations constitute a linear system for the pair $(\dot{\phi}, \dot{P})$. The corresponding Fokker-Planck equation in the (ϕ, θ) parametrization was given first by Brown⁽⁶⁾ and in the (ϕ, p) parametrization ($P = P_0 p$) by Klik and Gunther.⁽²⁾ Here it will be only observed that the discriminant of the system (7) is $\Delta = 1 + \eta^2 P_0^2$; this factor represents an overall time scaling parameter.

Looking back at the construction of the Hamiltonian H_{tot} , we see that it is of an oddly hybrid form: On one hand, \mathbf{S} is treated as a *bona fide* spin interacting with magnetic field, yet we also treat it as a vector representing the particle magnetization and we allow it to interact "with itself," i.e., with the effective crystal field of magnetic anisotropy given by the Hamiltonian $H(S_i)$. This suggests that within the model of rotation in unison we consider next to the $\mathbf{B} \cdot \mathbf{S}$ spin-bath coupling also interactions of the magnetoelastic type $H_{\text{int}} \sim a_{ijkl} u_{ij} S_k S_l + \dots$, where \mathbf{u} is the elastic displacement.^(8,9) Let first $\mathbf{S}(t) = \mathbf{S}_0 + \delta \mathbf{S}(t)$ and let the deviation $\delta \mathbf{S}(t)$ from the initial state \mathbf{S}_0 be so small that H_{int} can be linearized in $\delta \mathbf{S}$. Then for isotropic a_{ijkl} the theory of Gilbert follows. What happens to the anisotropic linearized theory shall be explained presently.

The point symmetry of the magnetic energy H , of the bath (elastic oscillations) H_f , and of the magnetoelastic coupling H_{int} is given by the crystal symmetry of the particle. In order to avoid complicated expressions, we shall assume that a canonical transformation diagonalizing the field Hamiltonian H_f has already been performed so that it has the form (2). Let a model coupling Hamiltonian be written as

$$H_{\text{int}} = \sum_{\mathbf{k}} c_{\mathbf{k}} \mathbf{q}_{\mathbf{k}} \cdot \mathbf{f}[S_i(\phi, P)] \quad (8)$$

where the functions f_i are polynomials in the three spin components S_i . Again we choose the special case of scalar coupling constants $c_{\mathbf{k}}$ to arrive

at a scalar rather than a tensorial dissipation constant. If f_i are homogeneous, quadratic in S_i , then this *ansatz* corresponds, e.g., to the leading order of magnetoelastic coupling in cubic crystals.⁽⁸⁾ The memoryless stochastic equations generalizing the system (7) are

$$\begin{aligned} \dot{\phi} &= \langle (H_{\text{tot}})_P \rangle = H_P + \mathbf{f}_P \cdot [\eta \dot{\mathbf{f}} + \mathbf{b}] \\ \dot{P} &= -\langle (H_{\text{tot}})_\phi \rangle = -H_\phi - \mathbf{f}_\phi \cdot [\eta \dot{\mathbf{f}} + \mathbf{b}] \end{aligned} \tag{9}$$

and the equivalent effective magnetic field generalizing (5) is given by

$$-(\mathbf{B}_{\text{eff}})_i = \langle (H_{\text{tot}})_{S_i} \rangle = H_{S_i} + \mathbf{f}_{S_i} \cdot (\eta \dot{\mathbf{f}} + \mathbf{b}) \tag{10}$$

Memory is included in a straightforward manner since the relation (6) holds. Its effects are briefly addressed in the discussion of the MQT rate of magnetization.

The discriminant of the linear system (9) may be written as

$$\Delta[\mathbf{f}] = 1 + \eta^2 (\mathbf{f}_P \times \mathbf{f}_\phi)^2 \tag{11}$$

and it was already noted in conjunction with the system (7) that $\Delta[\mathbf{S}] = 1 + \eta^2 P_0^2$ is an overall scaling factor of time occurring both in the Langevin and the Fokker–Planck equations. The expression (11) is, however, in general not independent of (ϕ, P) and there exists then a *local*, (ϕ, P) -dependent time scale. It is not difficult, albeit laborious, to show that the stationary solution of the corresponding Fokker–Planck equation is not $e^{-H/T}$, but rather $e^{-H/T + O(\eta^2)}$ ($k_B = 1$ throughout). Thus, in the case of several independent noise fields coupling to both momentum and position, the state of thermal equilibrium is a stationary solution of the Fokker–Planck equation only if the fluctuation-dissipation theorem (6) is supplemented by the condition that $\Delta[\mathbf{f}]$ be constant on the phase space (ϕ, P) :

$$\Delta_\phi[\mathbf{f}] = \Delta_P[\mathbf{f}] = 0 \quad \forall \phi, P \Leftrightarrow \dot{\Delta}[\mathbf{f}] = 0 \quad \forall t \tag{12}$$

This condition severely curtails the range of applicability of the model of rotation in unison. It is satisfied for the $\mathbf{S} \cdot \mathbf{B}$ isotropic coupling (3), but an extensive search failed to produce a satisfactory \mathbf{f} quadratic in S_i and by the same token it is not possible to generalize the bilinear Gilbert theory to anisotropic noise (tensorial dissipation): the corresponding discriminant Δ fails to satisfy (12). The trivial case $\Delta[\mathbf{f}] = 1$ occurs if $f_1 = f_2 = f_3$ or if all but one of the components f_i are zero, but these two cases do not correspond to any physical situation. The isotropic bilinear coupling of Gilbert thus occupies a truly unique position.

Despite these constraints, Eqs. (9) need not be rejected out of hand: the key observation is the fact that the general stationary state deviates from thermal equilibrium by a factor which is $O(\eta^2)$, corresponding to the η^2 deviation of the local time scale Δ from unity. This suggests that Langevin equations for (ϕ, P) be considered in the first order of η only, i.e., in the underdamped limit where $\Delta[\mathbf{f}] = 1 \forall \mathbf{f}$. Two symmetries of the dissipative coupling are of particular interest: uniaxial and cubic. In order to avoid^(2,3) the singular points $\pm P_0$ in the $[0, 0, 1]$ direction [compare the parametrization (1)], the easy axis of the uniaxial crystal will be placed into the $[1, 0, 0]$ direction (minima at $P=0, \phi=0, \pi$) and we shall assume that there are four equivalent saddles in the directions $[0, 1, 0]$ and $[0, 0, 1]$. The trivial coupling along the easy axis, $\mathbf{f} = [S_1^2, 0, 0]$, offers a chance to write down a Fokker–Planck equation valid for all η , but it cannot drive decay from one minimum along $[1, 0, 0]$ to the other. Hence we choose $\mathbf{f} = [0, S_2^2, S_3^2]$. For a cubic crystal with easy axes in the $[1, 0, 0]$, $[0, 1, 0]$, and $[0, 0, 1]$ directions there is in the first approximation⁽⁸⁾ $f_i = S_i^2$. The noiseless equations of motion in the *first order* of *small* η have the form ($x_1 = \phi, x_2 = P$)

$$\dot{x}_i = h_i - \eta A_{i,j} H_{x_j} \quad (13)$$

where $\mathbf{h} = [H_{x_2}, -H_{x_1}] = [H_P, -H_\phi]$, $A_{i,j} = A_{j,i}$, and η has been scaled by a factor of 2: $\eta \rightarrow \eta/2$. The full Langevin equations are too complicated to be given here *in extenso*; moreover, they are easily derived from Eqs. (9), and only the corresponding Fokker–Planck equation is given here:

$$\begin{aligned} \frac{\partial W}{\partial t} = LW \equiv & - \frac{\partial}{\partial x_i} \left\{ \left[h_i - \eta A_{i,j} H_{x_j} + \eta T \frac{\partial A_{i,j}}{\partial x_j} \right] W \right\} \\ & + \eta T \frac{\partial^2}{\partial x_i \partial x_j} [A_{i,j} W] \end{aligned} \quad (14)$$

for which $Le^{-H/T} = 0$. The functions $A_{i,j}(\phi, P)$ are given for uniaxial symmetry by

$$\begin{aligned} A_{1,1} &= (1 + \sin^4 \phi) P^2, & A_{2,2} &= \cos^2 \phi \sin^2 \phi (P_0^2 - P^2)^2 \\ A_{1,2} &= A_{2,1} = \cos \phi \sin^3 \phi P (P_0^2 - P^2) \end{aligned} \quad (15)$$

whereas for the cubic case one obtains

$$\begin{aligned} A_{1,1} &= (1 + \sin^4 \phi + \cos^4 \phi) P^2, & A_{2,2} &= 2 \cos^2 \phi \sin^2 \phi (P_0^2 - P^2)^2 \\ A_{1,2} &= A_{2,1} = \cos \phi \sin \phi (\sin^2 \phi - \cos^2 \phi) P (P_0^2 - P^2) \end{aligned} \quad (16)$$

The isotropic Gilbert system assumes for small η the form (14) as well⁽²⁾:

$$A_{1,1} = P_0^2(P_0^2 - P^2)^{-1}, \quad A_{2,2} = P_0^2 - P^2, \quad A_{1,2} = A_{2,1} = 0 \quad (17)$$

Contrary to the previous two cases, the crystal orientation in space is here arbitrary, i.e., not specified by the chosen dissipative coupling. $(\mathbf{f}_p \times \mathbf{f}_\phi)^2 \sim \cos^2 \phi \sin^2 \phi P^2(P_0^2 - P^2)^2$ for both the uniaxial and cubic crystals, so that it vanishes with its first derivatives in the planes (1, 0, 0), (0, 1, 0), and (0, 0, 1). Its second derivatives are, however, nonvanishing and the linearized full Fokker-Planck equation about $P = 0$ does not have the stationary solution $e^{-H/T}$.

From Eq. (14) it is easy to find for small η the mean first passage time τ out of the domain of attraction of a metastable minimum. The Dynkin equation $L^* \tau = -1$ is to be solved in the underdamped limit with the boundary condition⁽¹⁰⁾ $\tau|_{E_1} = 0$ at the saddle point energy E_1 . It is then an easy exercise^(2,10) to show that, neglecting backscattering, the corresponding decay rate through one saddle for $T \ll Q$ is

$$\kappa = \frac{\omega_0}{2\pi} \frac{\Delta E}{T} e^{-Q/T} \quad \text{with} \quad \Delta E = \eta \oint_{E_1} (-1)^{j+1} dx_j A_{i,j} H_{x_i} \quad (18)$$

Here ω_0 is the well frequency, $\omega_0^2 = H_{PP}^{(0)} H_{\phi\phi}^{(0)} - (H_{P\phi}^{(0)})^2$, Q is the barrier height, and ΔE is the energy loss per cycle at the energy E_1 in the first order of η . This result, with suitably calculated ΔE , holds for non-Markovian processes as well.⁽¹⁰⁾

For realistic systems the integral in (18) can only be evaluated numerically.⁽³⁾ A simple uniaxial Hamiltonian for which ΔE can be calculated analytically is

$$H = K'_3 \alpha_3^2 + K'_2 \alpha_2^2 = K_3 P^2 + K_2 (P_0^2 - P^2) \sin \phi \quad (19)$$

Here $K'_i = P_0^2 K_i = M_s^2 \gamma_0^{-2} K_i$ and $0 < K_2 < K_3$. The easy axis lies along the [1, 0, 0] direction, with the minima $E_0 = 0$ at (0, 0) and (π , 0), and there are but two equivalent saddles, $E_1 = K_2 P_0^2$, in the [0, 1, 0] direction, at ($\pm \pi/2$, 0). This model affords a good approximation of the vicinity of a single saddle point, but in the underdamped limit the dynamics in a larger part of the phase space, along the contour of E_1 , contributes to the prefactor and results derived from (19) must be regarded as qualitative only, since all real uniaxial systems have at least quartic symmetry in the basis plane. One has $\omega_0^2 = 4K_2 K_3 P_0^2$ and

$$\Delta E = \begin{cases} 8\eta P_0^3 K_3 [a(1-a)]^{1/2} & \text{for } \mathbf{f} = \mathbf{S} \\ 8\eta P_0^5 (K_2^2 + K_3^2) K_3^{-1} [a(1-a)]^{1/2} & \text{for } \mathbf{f} = [0, S_2^2, S_3^2] \end{cases} \quad (20)$$

In either case $a = K_2 K_3^{-1} < 1$; also note that for the Gilbert-type coupling (17), $\eta \sim P_0^{-1}$, whereas for (15), $\eta \sim P_0^{-3}$. Numerical calculations show that if an external magnetic field B in the $[1, 0, 0]$ direction is present, ΔE decreases approximately linearly with B as the contour E_1 contracts toward the metastable minimum. For $a = 1$ the Hamiltonian (19) is strictly axially symmetric, the saddles vanish, and the calculation leading to (18) becomes meaningless. It is interesting to observe that none of the currently available methods of decay rate calculation is applicable to this two-dimensional saddleless system embedded in three-dimensional space.⁽²⁾

According to the formulas (20), it is, in principle, possible to distinguish between the linear and nonlinear coupling in measurements of the thermal decay rate; the prefactor, however, can only be observed with difficulty. For this reason we now turn our attention to macroscopic quantum tunneling of magnetization,^(9,11,12) where the symmetry of dissipative coupling influences also the more easily observable exponential factor. We wish to determine the dependence of thermal enhancement of the MQT decay rate on the anisotropy coefficients K_i . A model calculation for weak dissipation will be carried out for the Hamiltonian (19) within the phase-space path integral formalism of Enz and Schilling.^{(12),2} Here Wick rotation is achieved by the analytic continuation $t \rightarrow -i\hbar\beta$, $\beta = T^{-1}$, and by introducing the imaginary momentum $\psi = iP$ so that Hamilton's equations remain real and $S^2[\phi, -i\psi] = P_0^2$. The phase space $\langle 0, 2\pi \rangle \times (-P_0, P_0)$ is mapped onto the strip $\langle 0, 2\pi \rangle \times R^1$ with the poles $\pm P_0$ removed to infinity. The quasiclassical ($P_0 \gg \hbar$) tunneling rate is given by⁽⁴⁾

$$\kappa = Ae^{-S_E/\hbar} \tag{21}$$

where $S_E = S_E[\phi_B, \psi_B]$ is the Euclidean action of the bounce trajectory in the Wick rotated phase space and A is a prefactor. It is easy to show^(4,12) that the interaction Hamiltonian (8) together with H_f of (2) and the corresponding counterterm leads to

$$\begin{aligned} S_E[\phi, \psi] &= \int_0^{\hbar\beta} d\tau (H - \psi\dot{\phi}) + \int_0^{\hbar\beta} \int_0^{\hbar\beta} d\tau d\tau' k(\tau - \tau') \mathbf{f}(\tau) \cdot \mathbf{f}(\tau') \\ &= \int_0^{\hbar\beta} d\tau (H - \psi\dot{\phi}) + \hbar\beta \sum_{n=-\infty}^{\infty} \alpha(n) \mathbf{f}_n \cdot \mathbf{f}_{-n} \end{aligned} \tag{22}$$

where $k(\tau) = 1/\hbar\beta \sum_n \alpha(n) e^{iv_n\tau}$, $v_n = 2\pi n/\hbar\beta$, $\alpha(n) = |v_n| \hat{\gamma}(|v_n|)$, and $\mathbf{f} = \sum_n \mathbf{f}_n e^{iv_n\tau}$. For $k(\tau) = \eta(2\pi)^{-1} \tau^{-2}$ the first variation $\delta S_E[\phi, \psi] = 0$

² According to R. Schilling (personal communication), there is a misprint in Eqs. (15) of ref. 12: \tanh^{-1} should be \coth^{-1} in the first equation and $[(1 - a^2)^{1/2} - \cos q]$ should read $[(1 - a^2)^{1/2} \pm \cos q]$ in the second one.

yields upon inverse Wick rotation the system (9) in its noiseless form. The reader is referred to the work of Enz and Schilling⁽¹²⁾ for a discussion of the difficult ordering problem in the phase-space path integral.

A Euclidean action of form similar to (22) was studied previously⁽¹¹⁾ in the parametrization (ϕ, θ) . Note that while $S_3 = -i\psi$ is imaginary, the sum in (22) is positive definite. This follows from the fact that for every sufficiently large N the sequence $\{\alpha(n)\}$ has a lower bound $\bar{\alpha} > 0$ so that $\sum_{n=-N}^N \alpha(n) \mathbf{S}_n \cdot \mathbf{S}_{-n} > \bar{\alpha} \sum_{n=-N}^N \mathbf{S}_n \cdot \mathbf{S}_{-n} > 0$, since $\mathbf{S} \cdot \mathbf{S} = P_0^2 > 0$. In the limit of high temperature it is not difficult⁽¹³⁾ to derive from (22) the Grote-Hynes result for the classical decay rate at moderate dissipation strength:

$$\kappa = \frac{1}{2\pi} \frac{\omega_0}{\omega_1} v_c e^{-Q/T} \tag{23}$$

where ω_0 and ω_1 are the well and saddle frequencies. The frequency v_c of the unstable mode is given by the largest positive root⁽¹³⁾ of the equation

$$v_c^2 + [H_{\phi\phi}^{(1)} + P_0^2 v_c \hat{\gamma}(|v_c|)] [H_{PP}^{(1)} + v_c \hat{\gamma}(|v_c|)] = 0$$

$H_{x_1, x_2}^{(1)}$ are the partial derivatives at the saddle and it was assumed that $H_{\phi P}^{(1)} = 0$, which is true for all crystal symmetries of interest apart from the case of a uniaxial crystal with rhombohedral anisotropy in the basis plane.⁽³⁾ This equation generalizes the memoryless result,^(2,3) where $\hat{\gamma} = \eta$, but a rigorous proof that the non-Markovian system (5) goes to thermal equilibrium is outstanding.

The dissipationless decay rate (21), including the prefactor A , has been calculated by path integral methods at $T = 0$ for the Hamiltonian (19) by several authors.^(9,12) To find the thermal enhancement of the decay rate for small T and η , we first determine the dissipationless dynamics⁽¹⁴⁾ in the Wick rotated phase space (ϕ, ψ) . For

$$H = -K_3 \psi^2 + K_2 (P_0^2 + \psi^2) \sin^2 \phi = K_2 P_0^2 (1 - \varepsilon)$$

where $1 \geq \varepsilon > 0$ and $\varepsilon = 1$ at $T = 0$; there follows for $S_i[\phi(\tau), -i\psi(\tau)]$

$$\begin{aligned} S_1^2(\tau) &= 16P_0^2(1+q)^{-1} (\hbar\beta\omega_0)^{-2} K^2(k) k^2 \operatorname{sn}^2(\tilde{\omega}\tau|k) \\ S_2^2(\tau) &= 16P_0^2(\hbar\beta\omega_0)^{-2} K^2(k) \operatorname{dn}^2(\tilde{\omega}\tau|k) \\ S_3^2(\tau) &= -16qP_0^2(1+q)^{-1} (\hbar\beta\omega_0)^{-2} K^2(k) k^2 \operatorname{cn}^2(\tilde{\omega}\tau|k) \end{aligned} \tag{24}$$

Here $k^2 = \varepsilon(1+q)(1+q\varepsilon)^{-1}$ for the modulus and $q = K_2(K_3 - K_2)^{-1} > 0$. The $K(k)$ is an elliptic integral of the first and $\operatorname{sn}(u|k)$, etc., are Jacobi

elliptic functions (ref. 15, §10.3). The oscillation energy $K_2 P_0^2(1 - \varepsilon)$ is linked to temperature by the periodicity condition⁽¹⁶⁾

$$\hbar\beta\tilde{\omega} = 4K(k), \quad \text{where } \tilde{\omega} = \omega_0(1 + q\varepsilon)^{1/2}$$

The physical picture corresponding to Eqs. (24) is the following: The saddle point at $(\phi, P) = (\pi/2, 0)$ is mapped onto a local maximum at $(\phi, \psi) = (\pi/2, 0)$ and the absolute maximum at the pole $P = P_0$ has been removed to infinity, where $H \sim -\psi^2$. The minima at $(\phi, P) = (0, 0)$ and $(\pi, 0)$ become saddles at these points. Equations (24) describe periodic clockwise motion with period $\hbar\beta$ around the maximum at $(\pi/2, 0)$ at the energy $H = K_2 P_0^2(1 - \varepsilon) > 0$. With the phase chosen here one has $(\phi(0), \psi(0)) = (\pi/2, \psi_{\max})$, where $\psi_{\max}^2 = q\varepsilon P_0^2$. In order to calculate S_E within the first order of small η , it is sufficient to substitute the Fourier components of the nondissipative solution (24) into the sum (22). The Fourier transform of $\text{cn}^2(u|k)$ is known⁽¹⁴⁾ and for Ohmic damping one has^(4,13,14) $\alpha(n) = \eta |v_n|$. Using the Euler–McLaurin summation formula, we obtain for the dissipative contribution to the Euclidean action for $\mathbf{f}(\tau) = [0, S_2^2(\tau), S_2^2(\tau)]$ the expression

$$\pi\eta \sum_{n=-\infty}^{\infty} |n| \mathbf{f}_n \cdot \mathbf{f}_{-n} = \frac{8}{3} \eta P_0^4 \frac{K_2^2 + K_3^2}{K_3^2} \left\{ \frac{9}{2\pi^3} \zeta(3) - \frac{1}{\pi} \vartheta^2 - \frac{\pi}{20} \vartheta^4 + \dots \right\} \quad (25)$$

where $\zeta(z)$ is the Riemann zeta function (ref. 15, §1.3), and $\vartheta = 2\pi T/\hbar\omega_0$ for brevity. Unfortunately, this procedure fails for the Gilbert coupling $\mathbf{f}(\tau) = \mathbf{S}(\tau)$. The reason is that $S_{1,n} S_{1,-n} \sim n \sinh^{-2}(\pi n \vartheta)$, n odd, and the Euler–McLaurin formula becomes inapplicable for small n . The sum is an even function of ϑ and examination of the formulas (24) suggests that

$$\pi\eta \sum_{n=-\infty}^{\infty} |n| \mathbf{S}_n \cdot \mathbf{S}_{-n} \sim \eta P_0^2 \frac{c_2 K_2 + c_3 K_3}{K_3} \quad (26)$$

where c_i are numerical factors independent of K_i and T .

The polynomial decrease in Euclidean action with temperature for small damping leads to an exponential increase in the MQT rate κ . The preceding formulas give the dependence of the exponential thermal enhancement of κ on the anisotropy coefficients for the simple Hamiltonian (19), which is a rather poor representation of a realistic system, so that these results are qualitative only. Nonetheless, if for small η , $S_E \approx S_E^0 + \eta S_E^1$, then for $f_i \sim S_i$ the thermal enhancement $S_E^1 = S_E^1 [K_i/K_j, \vartheta^2]$, whereas in the nonlinear coupling $f_i \sim S_i^2$ one has $S_E^1 [(K_i/K_j)^2, \vartheta^2]$ also for more realistic crystal symmetries. These results are independent of the specific choice of

the coefficients $\alpha(n)$. Garg and Kim⁽¹¹⁾ analyze magnetoelastic dissipative coupling in superparamagnets and conclude that the dynamics of \mathbf{M} is underdamped, so that the above analysis applies, and that $\alpha(n) = \eta |v_n^3|$, for which the Markovian limit does not exist. It is at the moment altogether unclear whether for this choice of memory thermal equilibrium exists even in the underdamped limit. Further study of the non-Markovian equations of motion is clearly required, both in the case where the Markovian limit exists and where it does not, as in the above case.

ACKNOWLEDGMENTS

I acknowledge with gratitude the many fruitful discussions I had with L. Gunther of Tufts University, Massachusetts, on the physics of micromagnets and his helpful comments during the preparation of this manuscript.

REFERENCES

1. A. Aharoni, *J. Appl. Phys.* **61**:3302 (1987), **62**:2576 (1987); W. F. Brown, *Micromagnets* (R. E. Krieger, 1978), §5.2.
2. I. Klik and L. Gunther, *J. Stat. Phys.* **60**:473 (1990).
3. I. Klik and L. Gunther, *J. Appl. Phys.* **67**:4505 (1990).
4. A. O. Caldeira and A. J. Leggett, *Ann. Phys.* **149**:374 (1983).
5. H. Dekker, *Physica* **144A**:453 (1987).
6. T. L. Gilbert, *Phys. Rev.* **100**:1243 (1955); W. F. Brown, *Phys. Rev.* **130**:1677 (1963).
7. L. Landau and E. Lifshitz, *The Classical Theory of Fields* (Addison-Wesley, 1951), §6.9.
8. E. A. Turov, *Physical Properties of Magnetically Ordered Systems* (Academic Press, 1965), Appendix C.
9. E. M. Chudnovsky and L. Gunther, *Phys. Rev. Lett.* **60**:661 (1988); *Phys. Rev. B* **37**:9455 (1988).
10. B. J. Matkowsky, Z. Schuss, and C. Tier, *J. Stat. Phys.* **35**:443 (1984); M. M. Dygas, B. J. Matkowsky, and Z. Schuss, *SIAM J. Appl. Math.* **46**:265 (1986).
11. A. Garg and G.-H. Kim, *Phys. Rev. Lett.* **63**:2512 (1989); *Phys. Rev. B* **43**:712 (1991).
12. M.ENZ and R. Schilling, *J. Phys. C: Solid State Phys.* **19**:1765 (1986); L711.
13. P. Hänggi, *Z. Phys. B Condensed Matter* **68**:181 (1987).
14. E. Freidkin, P. S. Riseborough, and P. Hänggi, *Z. Phys. B Condensed Matter* **64**:237 (1986).
15. W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics* (Springer-Verlag, 1966).
16. E. M. Cudnovsky, *JETP* **50**:1035 (1979).