Statistical equilibrium measures in micromagnetics

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We derive an equilibrium statistical theory for the macroscopic description of a ferromagnetic material at positive finite temperatures. Our formulation describes the most-probable equilibrium macrostates that yield a coherent deterministic large-scale picture varying at the size of the domain, as well as it captures the effect of random spin fluctuations caused by the thermal noise. We discuss connections of the proposed formulation to the Landau-Lifschitz theory and to the studies of domain formation based on Monte Carlo lattice simulations.

I. INTRODUCTION AND SUMMARY OF RESULTS

Based on a lattice model recently used for micromagnetic simulations at positive finite temperatures (see [1]) we derive a statistical equilibrium theory that describes large-scale coherent structures (magnetic domains, domain walls) in the presence of thermal fluctuations. The resulting description of equilibrium states depends only on macroscopic quantities: magnetization m, induced magnetic field h, external magnetic field h_e as well as structural properties of the ferromagnetic material (crystalline anisotropy). Furthermore, our formulation captures thermally induced spatial, as well as spin random fluctuations on the lattice and their effect in the macroscopic model. The Landau-Lifschitz theory (see [2,3]) has been successfully applied to modeling of magnetic microstructures in ferromagnetic materials with crystalline anisotropy. However, the assumptions under which the theory is derived rule out systematic description of thermal noise and the theory is sometimes viewed as a zero-temperature approximation. Recent advances in applications of ultra-thin magnetic films pointed out the importance of thermal fluctuations for studying such effects as spin reversal, nucleation, metastability or hysteresis (see, e.g., [4], [5]).

The approach proposed in this communication provides systematic treatment of the micromagnetic lattice model at a (positive) *finite temperature* It allows for the derivation of, (i) the probability distribution (1.8) of spins at all points of the magnetic specimen by incorporating the entropy, derived from the microscopic model, into the continuum functional (1.12); (ii) a *macroscopic* Ginzburg-Landau type free energy (1.9) for the average

magnetization; (iii) the description of random fluctuations in configuration space given by (1.8) and the derived large deviation principle (2.5) respectively. In the case of a large specimen where one observes well-developed magnetic microstructure with many magnetic domains, our formulation also provides an algorithm to compute spatially averaged magnetization fields. In a follow-up publication we study stochastic dynamics and domain formation and evolution in the context of the statistical framework developed here.

The physics on the regular lattice $\mathcal{L}_N \subset R^d$ $(d = 2, 3)$ with N sites is defined in the standard way by the means of an interaction potential between spins $\sigma(x)$, $\sigma(x')$ with values on the unit sphere S^2 at two different sites x, $x' \in \mathcal{L}_N$. Since we do not pursue an ab initio derivation, we assume that the interaction potential $U(x - x', \sigma(x), \sigma(x'))$ consists of the following terms: $U = U_e + U_a + U_d + U_h$ with particular contributions reflecting different types of interactions between magnetic moments. The underlying crystallographic lattice structure is incorporated through the interaction energy density Ψ rather than by using different lattice geometries. The exchange energy is given by

$$U_e = -\frac{A}{2} \sum_{x,x'} \sum_{i,j} J((x - x')/N^{1/d})\sigma^i(x)\sigma^j(x), \quad (1.1)$$

with the local mean-field interaction described by the positive function J. This term is often approximated by the nearest-neighbor interaction only. The anisotropy energy related to the crystalline structure of the material is defined by the energy density Ψ,

$$U_a = K \sum_x \Psi(\sigma(x)). \quad (1.2)$$

The non-local, long-range interaction between different magnetic moments (spins) is described by the dipole-dipole interaction

$$U_d = \frac{g}{2} \sum_{x,x'} \sum_{i,j} \nabla_{x_i} \nabla_{x_j} \left(\frac{1}{|x - x'|} \right) \sigma^i(x)\sigma^j(x'). \quad (1.3)$$

With a slight abuse of notation we write $\sigma(x)\sigma(x') \equiv \sum_{i,j} \sigma^i(x)\sigma^j(x')$ for the scalar product of two unit vectors at sites x and x' and points on S^2 are represented by unit vectors with the components σ^i, $i = 1, 2, 3$. We define the interaction Hamiltonian of the system

$$H_N(\sigma) = -\frac{1}{N^2} \sum_{x,x' \in \mathcal{L}_N} U(x - x', \sigma(x), \sigma(x')) \,. \quad (1.4)$$

The particular scaling guarantees that for the interaction potentials considered in the sequel the Hamiltonian remains finite as $N \to \infty$. To simplify notation we absorb the physical interaction parameters A, g, K into definitions of corresponding interaction potentials. In the derivation of the statistical model we omit the external field to keep the notation simple and focused to the averaging procedure only. However, in the presence of an external magnetic field h_e the Hamiltonian also involves the interaction energy

$$U_h = -\frac{1}{N} \sum_x \sum_i h_e^i(x) \sigma^i(x) \,. \quad (1.5)$$

The central object describing the statistical ensemble on the lattice is the *canonical* Gibbs measure at the inverse temperature $\beta = \frac{1}{kT}$, defined on the configuration space $\Sigma = \{\sigma \,|\, \sigma(x) \in S^2, x \in \mathcal{L}_N\}$,

$$P_{N,\beta}(d\sigma) = \frac{1}{Z_{N,\beta}} e^{-\beta H_N(\sigma)} \, \Pi_N(d\sigma) \,, \quad (1.6)$$

where

$$Z_{N,\beta} = \int_\Sigma e^{-\beta H_N(\sigma)} \Pi_N(d\sigma) \quad (1.7)$$

denotes the partition function. The *prior distribution* $\Pi_N(d\sigma)$ models the small scale fluctuations of the spins; we assume it is a product measure on the lattice $\mathcal{L}_N$ of uniform distributions on S^2, i.e., that spins at different lattice sites are independent, uniformly distributed random variables on S^2. Note that we can alternatively incorporate the anisotropy energy in the prior distribution. Here we study the most probable configuration on $\mathcal{L}_N$ according to the Gibbs measure $P_{N,\beta}$ as $N \to \infty$. In this limit, we assume the lattice $\mathcal{L}_N$ approximates a physical domain $\Omega \subset R^d$. We show that the energetically most favorable configuration describing the large-scale features on $\mathcal{L}_N \approx \Omega$ is given by the Maxwellian distribution,

$$\mathrm{M}(x,v) = \frac{1}{Z_\beta(x)} e^{-\beta[\Psi(v) + v(\nabla\bar{u}(x) - J*\bar{m}(x) - h_e)]} \,, \quad (1.8)$$

yielding the probability of having a spin $v \in S^2$ at the location $x \in \Omega$. Here $Z_\beta(x)$ denotes the partition function. The corresponding average magnetization is $\bar{m}(x) = \int_{S^2} v\,\mathrm{M}(x,v)\,dv$ with magnetization potential $\bar{u}$ given by $\Delta\bar{u} = \mathrm{div}(\chi_\Omega \bar{m})$. Furthermore $(\bar{u}, \bar{m})$ minimizes a newly derived *free energy* of Ginzburg-Landau type, at a finite temperature:

$$F_\beta[m] = \int_{R^d} \frac{1}{2}|\nabla u|^2 \, dx - \int_\Omega \frac{1}{2}(J*m)\,m\,dx +$$
$$+ \int_\Omega a_\beta^*(m)\,dx - \int_\Omega h_e m\,dx \,, \quad (1.9)$$

subject to the constraint

$$\Delta u = \mathrm{div}(\chi_\Omega m), \ \ \text{in } R^d \,. \quad (1.10)$$

The equation (1.10), involving the characteristic function χ_Ω of the domain Ω, is understood in the weak sense (see [6]). Furthermore $J*m(x) = \int_\Omega J(x-y)m(y)dy$ and

$$a_\beta^*(m) = \sup_{p \in R^d} \{mp - a_\beta(p)\}$$

is the Legendre-Fenchel transform of the function

$$a_\beta(p) = \frac{1}{\beta} \log \int_{S^2} e^{-\beta(\Psi(v) + vp)} \, dv \,. \quad (1.11)$$

As in the case of the Boltzmann theory of dilute gases the equilibrium measure is defined by the macroscopic quantities: the magnetic potential $\bar{u}$ which defines the induced magnetic field $h(x) = -\nabla\bar{u}(x)$ and the magnetization $\bar{m}(x) = \int_{S^2} v\,\mathrm{M}(x,v)\,dv$. A related approach is also adopted in the statistical description of coherent structures in 2D turbulence (see [7]).

The equilibrium measure with the density $\mathrm{M}(x,v)$ is identified as the minimizer of the energy functional

$$E_\beta[f] = \int_{R^d} \frac{1}{2}|\nabla u|^2 \, dx - \int_\Omega \frac{1}{2}(J*m)\,m\,dx +$$
$$+ \int_\Omega \int_{S^2} \Psi(v)\,f(x,v)\,dv\,dx +$$
$$+ \frac{1}{\beta} \int_\Omega \int_{S^2} f(x,v) \log f(x,v)\,dv\,dx \,. \quad (1.12)$$

Since the minimization is over the space of probability densities f the following constraints must be satisfied

$$f: \Omega \times S^2 \to R^+ \,, \quad \int_\Omega \int_{S^2} f(x,v)dvdx = 1 \,,$$
$$\int_{S^2} f(x,v)dv = \frac{1}{|\Omega|} \,, \quad (1.13)$$

together with (1.10) that relates u and m, where

$$m(x) = \int_{S^2} v\,f(x,v)dv \,. \quad (1.14)$$

The last constraint in (1.13) is due to the fact that at every lattice site there is one and only one spin. The quantity (1.14) evaluated at the minimizing density $f = \mathrm{M}$, represents the average (macroscopic) magnetization. The last term of the energy functional is interpreted as the thermodynamic entropy and mathematically it is the *relative entropy* with respect to the prior distribution of the Gibbs measure (1.6).

We conclude the discussion of our main results with two brief comments on the random, thermally induced fluctuations. First, (1.8) is the probability density of the spin v at each spatial location x, and upon averaging over the spin space yields $\bar{m}$. Furthermore, the large deviation

principle derived below with the rate $E_\beta[f]$, describes the equilibrium random fluctuations around the most probable macro-state (1.8) as a function of the specimen size N. In the following sections we outline the main steps leading from the microscopic Hamiltonian to the macroscopic variational principle involving energies E_β and F_β. The detailed mathematical derivation is described in [8].

II. THERMODYNAMIC LIMIT AND LARGE DEVIATION PRINCIPLE

We employ the theory of large deviations (see [9]) to obtain the functional E_β from the spin Hamiltonian (1.4). We define the empirical measure on $\mathcal{N} := \Omega \times S^2$ corresponding to the spin configurations σ,

$$\mu^N(dy, dv) = \frac{1}{N} \sum_{x \in \mathcal{L}_N} \delta_x(dy) \delta_{\sigma(x)}(dv). \qquad (2.1)$$

Integrating over the domain $A \times \{v\} \subset \mathcal{N}$, we readily see that $\mu^N(A \times \{v\})$ is a coarse-grained random variable counting the number of spins v contained in the region A. In the $N \to \infty$ limit it will give rise to the probability distribution of spins in A. The empirical measure allows us to show that, (i) the corresponding Gibbs states yield a coherent deterministic large scale picture, referred to as a "macrostate" and varying at the size of the domain $\Omega \times S^2$, and (ii) the microscopic random fluctuations at the lattice cell size around the macrostates can be described explicitly in terms of E_β.

A crucial step of the derivation is to compute a suitable limit of the lattice Hamiltonian and of the Gibbs measure (1.6) as $N \to \infty$. Using the empirical measure we can write the lattice Hamiltonian as

$$\tilde{H}(\mu^N) = -\int_{\mathcal{N}} \int_{\mathcal{N}} U(x - x', v, v') \, \mu^N(dx, dv) \mu^N(dx', dv').$$

The partition function corresponding to the re-scaled Gibbs measure $P_{N,N\beta}$ is

$$Z_{N,N\beta} = \int_\Sigma e^{-N\beta H_N(\sigma)} \Pi_N(d\sigma), \qquad (2.2)$$

and using the Hamiltonian $\tilde{H}$ we write

$$\frac{1}{N} \log Z_{N,N\beta} = \frac{1}{N} \log \int_\mathcal{P} e^{-N\beta\tilde{H}(\mu)} \Pi_N(\mu^N = \mu) d\mu,$$

where $\mathcal{P}$ is the set of all probability measures μ on $\mathcal{N}$ that satisfy (1.13) (observe that if μ^N converge in the sense of measures as $N \to \infty$ to a probability measure on $\mathcal{N}$ with density f then f satisfies the constraints (1.13)). Using Sanov's Theorem and an auxiliary coarse grained process (see [10]) we can show the large deviation principle for the prior distribution with the *rate functional* $S(\mu)$:

$$\Pi_N(\mu^N = \mu) \approx e^{-NS(\mu)}, \qquad (2.3)$$

as $N \to \infty$. Here

$$S(\mu) = \int f(x, v) \log f(x, v) \, dxdv \quad \text{if } d\mu = f dxdv,$$

and $S(\mu) = \infty$ otherwise, which is known in probability theory as the *relative entropy* with respect to the uniform measure $dxdv$ [9]. For the rigorous meaning of the approximation sign above in the framework of the theory of large deviations, we refer to [9]. By employing the asymptotics of $\Pi_N(\mu^N = \mu)$, as well as the Laplace principle, [9], we compute the limit as $N \to \infty$

$$\lim_{N \to \infty} \frac{1}{N} \log Z_{N,N\beta} = \lim_{N \to \infty} \frac{1}{N} \log \int_\mathcal{P} e^{-N(\beta\tilde{H}(\mu) + S(\mu))} d\mu$$
$$= -\inf_{\mu \in \mathcal{P}} \{\beta\tilde{H}(\mu) + S(\mu)\}. \qquad (2.4)$$

Similarly we obtain the large deviation principle for the Gibbs measure, as $N \to \infty$,

$$P_{N,N\beta}(\mu^N = \mu) \approx e^{-N[\beta\tilde{H}(\mu) + S(\mu) - \inf_\mu\{\beta\tilde{H}(\mu) + S(\mu)\}]}. \qquad (2.5)$$

The rigorous derivation is technically involved due to the nature of the singularity in the dipole-dipole interaction (see also [11]). We address rigorously this issue in [8].

The expression (2.5) is interpreted as follows: the most probable configuration μ of the Gibbs measure is the *minimizer* of $\beta\tilde{H}(\mu) + S(\mu)$, yielding the large scale structure (at the size of the domain $\mathcal{N}$) at equilibrium. As we show below, this minimizer turns out to be the probability density (1.8). Note here that $\beta\tilde{H}(\mu) + S(\mu)$ is finite if and only if the measure μ has a density f, in which case we define the energy functional

$$E_\beta[f] = \tilde{H}(\mu) + \frac{1}{\beta} S(\mu).$$

Substituting for expressions on the right hand side and using (1.10) we immediately obtain (1.12).

Finally, (2.5) captures the microscopic *spatial* random fluctuations of the empirical measure μ^N as a function of N (i.e., the total number of spins in the specimen), around the most probable macrostate given by the minimizer (1.8) of (1.12).

III. VARIATIONAL PRINCIPLE

We show that the Maxwellian $M(x, v)$ which represents the equilibrium macrostate of the microscopic system is the minimizer of the energy functional E_β. Using (1.10) we define an auxiliary functional,

$$\mathcal{E}_\beta[f, u] = -\int_{R^d} \frac{1}{2} |\nabla u|^2 dx - \int_\Omega \frac{1}{2} (J * m) \, m \, dx +$$
$$+ \int_\Omega \int_{S^2} (\Psi(v) + v\nabla u) \, f(x, v) dvdx +$$
$$+ \frac{1}{\beta} \int_\Omega \int_{S^2} f(x, v) \log f(x, v) dxdv. \qquad (3.1)$$

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We observe that $E_\beta[f] = \sup_{u \in H^1(R^d)} \mathcal{E}_\beta[f, u]$, and consequently

$$\inf_f E_\beta[f] = \inf_f \sup_u \mathcal{E}_\beta[f, u] \geq \sup_u \inf_f \mathcal{E}_\beta[f, u].$$

Note that the infimum is taken over the densities f that satisfy constraints (1.13) and also relations (1.10) together with (1.14). For a fixed u we can construct the minimizer of $\mathcal{E}_\beta[f, u]$ over f by varying the probability density f using suitable push-forward maps (see [12,13]) that preserve the constraints (1.13). Then the minimizer M_u, $\mathcal{E}_\beta[M_u, u] = \min_f \mathcal{E}_\beta[f, u]$ for given, fixed u satisfies

$$M_u(x, v) = \frac{1}{Z_\beta(x)} e^{-\beta[\Psi(v) + v(\nabla u(x) - J * m_u(x))]}, \quad (3.2)$$

where $Z_\beta(x)$ is the corresponding partition function and $m_u(x) = \int_{S^2} v\, M_u(x, v)\, dv$. Note that $a_\beta(\nabla u - J * m_u) = 1/\beta \log Z_\beta(x)$. Straightforward calculations show that

$$m_u(x) = \partial_p a_\beta(J * m_u - \nabla u). \quad (3.3)$$

The existence of m_u satisfying (3.3) follows from minimizing the functional

$$-\int_\Omega \frac{1}{2}(J * m)\, m\, dx + \int_\Omega m \nabla u\, dx + \int_\Omega a_\beta^*(m)\, dx.$$

Hence we obtain that

$$\mathcal{E}_\beta[M_u, u] = \min_f \mathcal{E}_\beta[f, u] = -\int_{R^d} \frac{1}{2}|\nabla u|^2\, dx +$$

$$+ \int_\Omega \frac{1}{2}(J * m_u)\, m_u\, dx - \int_\Omega a_\beta(\nabla u - J * m_u)\, dx.$$

Using the duality between a_β and a_β^* we have

$$\sup_u \inf_f \mathcal{E}_\beta[f, u] = \sup_u \mathcal{E}_\beta[M_u, u] = \inf_{m\,\&\,(1.10)} F_\beta[m].$$

Closer inspection of the functional F_β proves that the last infimum is attained and that a minimizer $\bar{m}$ satisfies

$$\bar{m} = \partial_p a_\beta(J * \bar{m} - \nabla \bar{u})$$

and $\bar{m}$, $\bar{u}$ are related by (1.10). The expression (3.2) also implies the equilibrium Maxwellian $M(x, v)$ given by (1.8). Using the constructed fields $\bar{m}(x)$, $\bar{u}(x)$ and $M(x, v)$ we can check that, in fact,

$$\inf_f E_\beta[f] = \inf_f \sup_u \mathcal{E}_\beta[f, u] = \sup_u \inf_f \mathcal{E}_\beta[f, u] =$$

$$= \min_{m\,\&\,(1.10)} F_\beta[m] = F_\beta[\bar{m}].$$

Thus the minimizer of the new Ginzburg-Landau energy $F_\beta[m]$ provides the minimum value of the energy functional $E_\beta[f]$ as well as it describes, through the Maxwellian density $M(x, v)$ the structure of the most-probable macrostate. The rigorous treatment of all steps outlined in the previous sections is described in [8].

IV. DISCUSSION

A natural question is how the presented model relates to the Landau-Lifschitz theory ([2,3]) and how it can be interpreted in view of recent studies of domain formation based on Monte Carlo simulations ([1,5]). First we address the former issue: we expand the convolution $J * m$ in the free energy (1.9), $J * m = J_0 m + J_2/2\, \Delta m + \ldots$, where $J_0 = \int_\Omega J(r)\, dr$, $J_2 = \int_\Omega |r|^2 J(r)\, dr$, and after substituting into (1.9) we obtain

$$\tilde{F}_\beta[m] = \int_\Omega \frac{J_2}{2}|\nabla m|^2\, dx + \int_{R^d} \frac{1}{2}|\nabla u|^2\, dx +$$

$$\int_\Omega \left(a_\beta^*(m) - \frac{J_0}{2}|m|^2\right) dx - \int_\Omega h_e m\, dx, \quad (4.1)$$

which can be interpreted as the finite-temperature analogue of the Landau-Lifschitz free energy:

$$F_{LL}[m] = \int_\Omega \frac{A}{2}|\nabla m|^2\, dx + \int_{R^d} \frac{1}{2}|\nabla u|^2\, dx +$$

$$+ \int_\Omega \Psi(m)\, dx - \int_\Omega h_e m\, dx. \quad (4.2)$$

However, the free energy functional F_{LL} is minimized subject to the non-convex constraint $|m| = 1$. In the formulation presented here the direct calculation implies that since $|\partial_p a_\beta(p)| \leq 1$ we have $a_\beta^*(m) = \infty$ for $|m| > 1$ and consequently the energy $\tilde{F}_\beta$ (or F_β) is minimized subject to the constraint $|m| \leq 1$. This remarkable difference from the Landau-Lifschitz theory is caused by the presence of the thermal fluctuations and the averaged nature of the magnetization m in our model. We conclude the discussion on the relation of our proposed finite temperature model to the Landau-Lifschitz theory with an interesting point: one would be tempted to say that a suitable zero-temperature limit (Γ-limit) of the free energy F_β should yield the Landau-Lifschitz model or its relaxation. Indeed, the $\beta \to \infty$ limit of the free energy F_β or $\tilde{F}_\beta$ can be explicitly calculated, at least formally, yielding in (1.9) and (4.1):

$$a_\infty^*(m) = \sup \left\{ f : R^n \mapsto R, f \leq \Psi \text{ on } S^2, f \text{ convex} \right\},$$

if $|m| \leq 1$ and $a_\infty^*(m) = \infty$, if $|m| > 1$. We note that the same energy relaxation was obtained in [14] by a direct minimization of (4.2) over all admissible Young measures, when the energy exchange term $A/2|\nabla m|^2$ is neglected.

Existence of magnetic domains and different types of magnetic walls in the Landau-Lifschitz theory is attributed to the competition of different contributions in the free energy and to the non-convex constraint $|m| = 1$. Due to the thermal agitation incorporated in the finite-temperature free energy F_β (or $\tilde{F}_\beta$) the norm $|m|$ also fluctuates. Although for low temperatures $|m|$ can be close to the unit sphere, in general, we have the convex constraint $|m| \leq 1$. Nevertheless, our model allows for domain formation at finite-temperatures whenever the

exchange energy is strong enough compared to the temperature.

More specifically, in the absence of an external field h_e, the condition that $I - J_0 \partial^2_{pp} a_\beta(0)$ is positive definite guarantees that $m \equiv 0$ and $u \equiv 0$ is the minimizer of F_β (as well as $\tilde{F}_\beta$) implying a uniform state, i.e., no domain formation. When the above condition is violated, then for a suitable domain Ω and anisotropy, there exist nontrivial solutions $m \neq 0$ and $u \equiv 0$ to the Lagrange-Euler equation for the energy $\tilde{F}_\beta$ (or F_β),

$$J_2 \Delta m = -J_0 m + \partial_p a^*_\beta(m), \qquad (4.3)$$

which have lower energy than the uniform state $m \equiv 0$, $u \equiv 0$. Similar steady states on 2D lattices, referred to as many-soliton solutions, were first analytically predicted and also observed in Monte Carlo simulations in [1]. Under simplifying assumptions on the geometry of the domain it is not difficult to calculate the domain-wall profile, as well as its dependence on temperature, the exchange energy and anisotropy energy directly from (4.3). Note that since the magnetization m in our model is computed by averaging over the thermal fluctuations of spins the domains are identified with regions in Ω where $|m(x)| \approx |m^k_\beta| \leq 1$ and m^k_β are non-trivial constant solutions of (4.3). In a forthcoming publication, domain formation and evolution, as well as the corresponding stochastic dynamics are studied both numerically and analytically in the context of the statistical theory developed here.

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