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# An explicit derivation of a relation between magnetization $\mathbf{M}$ and saturation magnetization $M_s$

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## ABSTRACT

An explicit relationship between a magnetization vector  $\mathbf{M}$  and its saturation magnetization  $M_s$  is derived using the definition of  $\mathbf{M}$  along with assumptions of the continuum exchange theory. The obtained expression is found to be an extension of the commonly used fixed-length constraint and represents the continuous analog of it for the elementary moment per unit volume. The derivation of this relation is carried out in detail and important potential implications relating to equations for  $\mathbf{M}$  are also highlighted.

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## 1. Introduction

Continuum micromagnetics describes the continuous magnetization vector field  $\mathbf{M}(\mathbf{x},t)$ , where  $\mathbf{x}$  is a position vector and  $t$  is time. Well known formulations such as the Landau–Lifshitz [1] or Landau–Lifshitz–Gilbert [2] equations are also known to preserve the magnitude of  $\mathbf{M}$ , locally, as a function to time. This constraint is more formally given by [3]

$$|\mathbf{M}|^2 = M_s^2 \quad (1-1)$$

While there are many problems well described using the constraint given in (1-1), there are also known experimental conditions that are at odds with it. For example, in the case of ferromagnetic materials transitioning to paramagnetic behavior in finite temperature, it is probable that this constraint is not met strictly below the Curie temperature, since it is clearly not met by paramagnetic materials, which are capable of spontaneously forming nonzero  $\mathbf{M}$  upon application of an external field. Sample size has also been shown to affect nearly all magnetic material parameters, which includes reductions in measurements of  $|\mathbf{M}|$  [4,5], relative to known saturated values of the bulk. More generally, these results suggest

$$|\mathbf{M}|^2 \leq M_s^2 \quad (1-2)$$

There are important technological developments where these points are of immediate interest, for example, in heat assisted magnetic recording (HAMR) [6], where heat is functional in the operation of the magnetic system. Several efforts have been made

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to address these kinds of concerns, primarily, with temperature. One example [7] has used the Fokker–Planck equation to obtain a Landau–Lifshitz–Bloch type equation, which inherently removes the condition in (1-1) by appending a longitudinal relaxation term. It has been deployed by some, e.g. [8]. Atomistic and stochastic approaches appear to be a more common approach in avoiding the LLG, which conserves  $|\mathbf{M}|$ , e.g. [9]. Our interest in this problem is demonstrated by taking a ‘step back’ to examine condition (1-1) more directly. From where does (1-1) originate? It follows from the observed behavior of an electron spin [10,11]. Under the assumption that the driving magnetic field is macroscopic, it is a direct extension of equations for electron spins (with phenomenological damping), thus also satisfying (1-1) for  $\mathbf{M}$ . However, a macroscopic measurement, which spans over a local region of a material, measures a moment density, rather than a spin’s moment directly. One may inquire about the square of the moment per unit volume and whether it really does inherit the condition of (1-1). One of the key points of this work is to show that, in fact, it does not inherit the condition of (1-1). Using assumptions and existing concepts introduced by the continuum exchange theory along with the definition of  $\mathbf{M}$  (dipole moment per unit volume or elementary moment), a constraint relation between  $\mathbf{M}$  and  $M_s$  is explicitly derived. From this analysis, we find a relationship that appears to be a natural extension to the condition given in (1-1) for the quantity defined as the moment per unit volume, and it is also shown to be consistent with (1-2). Important potential implications of this extended constraint are also discussed.

The paper is, thus, organized as follows. In Section 2, a review of the continuum exchange theory is given highlighting essential points that are used in the derivation of the constraint. In Section 3, the relation between  $\mathbf{M}$  and  $M_s$  is derived. In Section 4, the potential implications of the obtained relation are briefly mentioned, and finally in Section 5, summary remarks are given.

## 2. Review of the continuum exchange theory

The ferromagnetic exchange energy arises from a mechanism whose origins are on an atomic or subatomic length scale. Specifically, there exists a form of energy associated with atomic interactions between electron spins giving rise to preferred alignment. This ordering only includes nearest neighbors that may possess overlapping wave functions with the spin  $\mathbf{S}_k$  (see Fig. 2.1) [12].

A representation of the total exchange energy for a collection of spins is given in the Heisenberg form by

$$E_X = -2J \sum_{i>k} \mathbf{S}_i \cdot \mathbf{S}_k \quad (2-1)$$

$J$  is the (scalar) exchange integral for each interaction  $(i,k)$ , which is assumed isotropic [13]. It is a measure of the degree of exchange coupling strength between each pair of overlapping wave functions [12]. This convention, relevant to ferromagnetism, expresses the exchange energy so that parallel spins have a lower energy (more negative) than the antiparallel spins.

The next step is to apply operations to (2-1) that are only suitable for continuous functions. However, in its current form, some needed operations are not well defined as it is applied, for example, in the Hamiltonian of the quantum mechanical spin system. However, continuous methods are permissible if the system is assumed to contain a sufficiently large number of spins  $\mathbf{S}$  so that a given finite angle of variation (e.g.  $\varphi \leq \pi$ ) may be achieved across many spins, and the nearest neighbors may, on averaging, have very closely aligned spins [13]. Then, (2-1) becomes

$$E_X = -2JS^2 \sum_{i>j} \boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j = -2JS^2 \sum_n \cos \varphi_n \quad (2-2)$$

Index  $n$  in (2-2) counts the number of interactions. The direction cosines for the spin vector are represented in a vector  $\boldsymbol{\alpha}$  defined by

$$\boldsymbol{\alpha} = \mathbf{S}/S = [\alpha_x \quad \alpha_y \quad \alpha_z]^T \quad (2-3)$$

It is noted that this assumption in the continuum exchange theory consequently leads to the concept of the classical elementary dipole moment given by  $S\boldsymbol{\alpha}$ . This subtle and important step now allows the use of continuum operations.

To express (2-2) as an energy density, expansions of the direction cosines are used. To this end, the direction cosines of all the nearest neighbors, upon expanding, take the general form

$$\alpha_{x,i} = \alpha_{x,k} \pm x_{ik} \frac{\partial \alpha_{x,k}}{\partial x} \pm y_{ik} \frac{\partial \alpha_{x,k}}{\partial y} \pm z_{ik} \frac{\partial \alpha_{x,k}}{\partial z} + \dots$$

$$\frac{1}{2!} \left( \frac{\partial^2 \alpha_{x,k}}{\partial x^2} x_{ik}^2 \pm 2 \frac{\partial^2 \alpha_{x,k}}{\partial x \partial y} x_{ik} y_{ik} + \frac{\partial^2 \alpha_{x,k}}{\partial y^2} y_{ik}^2 \pm \dots \right)$$

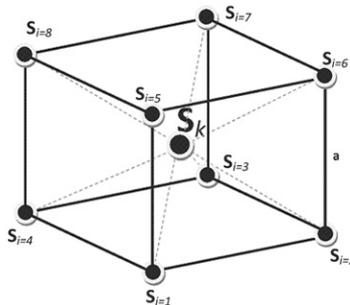


Fig. 2.1. Example of a body-centered cubic (BCC) lattice cell with a central spin with 8 nearest neighbors.

$$2 \left( \frac{\partial^2 \alpha_{x,k}}{\partial y \partial z} y_{ik} z_{ik} + \frac{\partial^2 \alpha_{x,k}}{\partial z^2} z_{ik}^2 \pm 2 \frac{\partial^2 \alpha_{x,k}}{\partial z \partial x} z_{ik} x_{ik} \right) + O(x_{ik} y_{ik} z_{ik}) \quad (2-4)$$

$x_{ik}(y_{ik}, z_{ik})$  is the inter-spin distance along the  $x$  ( $y$ ,  $z$ ) coordinate between spins  $i$  and  $k$ . Using expansions of the form given in (2-4), and truncating all the terms above the 4th order, and taking advantage of cancellations of the odd order terms due to symmetry, a form of the energy as a function of the direction cosine and their spatial derivatives up to 2nd order at moment  $k$  may be obtained. For case of BCC, the form of energy depending on space is given by

$$E_{X,k} = -\frac{JS^2 Na^2}{4} \boldsymbol{\alpha}_k \cdot \nabla^2 \boldsymbol{\alpha}_k \quad (2-5)$$

The final energy density is given by dividing by the volume of the unit cube  $v_0 = a^3$  and substituting  $N=8$  for BCC, leading to

$$e_X = E_X/v_0 = -\frac{2JS^2}{a} \boldsymbol{\alpha} \cdot \nabla^2 \boldsymbol{\alpha} = -A_X^{BCC} \boldsymbol{\alpha} \cdot \nabla^2 \boldsymbol{\alpha} \quad (2-6)$$

In (2-10),  $A_X^{BCC}$  may be defined as the exchange stiffness constant (energy per unit length), i.e.

$$A_X^{BCC} = \frac{2JS^2}{a} \quad (2-7)$$

Another common form of the exchange energy uses a first order spatial variation, which is easier in applications. This form comes from the following identity with the elementary moments under the assumption that the spin vector length is conserved everywhere, leading to

$$\nabla^2 (\boldsymbol{\alpha} \cdot \boldsymbol{\alpha}) = 0 = 2\boldsymbol{\alpha} \cdot \nabla^2 \boldsymbol{\alpha} + 2\nabla \boldsymbol{\alpha} \cdot \nabla \boldsymbol{\alpha} \quad (2-8)$$

The validity of (2-8) also proves

$$-\boldsymbol{\alpha} \cdot \nabla^2 \boldsymbol{\alpha} \geq 0 \quad (2-9)$$

Under the assumption that (2-8) holds, it leads to the alternative result

$$e_X = A_X \nabla \boldsymbol{\alpha} \cdot \nabla \boldsymbol{\alpha} \quad (2-10)$$

Now let us summarize the key points of the exchange theory that are used in the next section to obtain an explicit relationship between the magnetization and its saturation:

- A sufficiently large number of moments is within a unit volume allowing continuum approximations.
- A classical unit moment vector  $\mathbf{S}$  may be defined from which the magnetization behavior may be found from these elementary moments.
- Using expansions of direction cosines, the final energy expression is found by truncating terms above 3rd order and also assuming high geometrical symmetry of the elementary moments.

## 3. Derivation of an extended relation between $\mathbf{M}$ and $\mathbf{M}_s$

The magnetization vector  $\mathbf{M}$  is defined as the volume average of the magnetic dipole moment or elementary moment,  $\mathbf{m}$ . With this definition,  $\mathbf{m}$  is thus proportional to the continuum spin

vector  $\mathbf{S}$ . For a unit volume  $\nu$  (i.e.  $\nu=1$ ),  $\mathbf{M}$  can be expressed as

$$\mathbf{M} = \frac{1}{N} \sum_{j=1}^N \mathbf{m}_j \quad (3-1)$$

$N$  is the effective number of elementary moments within the unit volume. In the exchange theory, it is the elementary moments that are assumed to have fixed length, denoted by

$$|\mathbf{m}_j| = M_s \quad (3-2)$$

Given (3-1) and (3-2), the relationship between  $\mathbf{M}$  and  $M_s$  is examined. Specifically, using the approximations established in the continuum exchange theory reviewed in the previous section, along with the definition of  $\mathbf{M}$  given in (3-1), a relationship between  $\mathbf{M}$  and  $M_s$  is obtained directly.

Taking a dot product of  $\mathbf{M}$  with itself leads to

$$|\mathbf{M}|^2 = \left[ \frac{1}{N} \sum_{j=1}^N \mathbf{m}_j \right] \cdot \left[ \frac{1}{N} \sum_{k=1}^N \mathbf{m}_k \right] \quad (3-3)$$

The summation in (3-3) may be partitioned into two parts by considering terms with the same and unique indices. This leads to

$$|\mathbf{M}|^2 = \frac{1}{N^2} \left[ \sum_{j=k=1}^N \mathbf{m}_j \cdot \mathbf{m}_j + \sum_{j \neq k} \mathbf{m}_j \cdot \mathbf{m}_k \right] \quad (3-4)$$

Using (3-2) for the elementary moment, (3-4) reduces to

$$|\mathbf{M}|^2 = \frac{M_s^2}{N^2} \left[ N + \sum_{j \neq k} \alpha_j \cdot \alpha_k \right] \quad (3-5)$$

For the second term arising from distinct indices, Taylor series expansions of the direction cosines of  $\alpha_k$  with respect to  $\alpha_j$  may be used in the same way as in the exchange theory, allowing (3-5) to be written as

$$|\mathbf{M}|^2 = \frac{M_s^2}{N^2} \left[ N + \sum_{j=1}^N \sum_{k=1, \neq j}^{N-1} \alpha_j \cdot \left( \alpha_j + \frac{a_{jk}^2}{2!} \nabla^2 \alpha_j \right) \right] \quad (3-6)$$

In (3-6),  $a_{jk}$  represents an effective distance between elementary moment pairs ( $j, k$ ) that possess misalignment within the unit volume. It is, therefore, a function of the atomic structure of the material and in general, its value will be different for distinct cases such as simple cubic, face-centered cubic, body-centered cubic, etc. Because the length scale of the distances between the elementary moments may be near to that of the atomic ordering, we use an average distance  $\tilde{a}$  between the moments within the unit volume and thus (3-6) becomes

$$|\mathbf{M}|^2 = \frac{M_s^2}{N^2} \left[ N + \sum_{j=1}^N \sum_{k=1, \neq j}^{N-1} \alpha_j \cdot \left( \alpha_j + \frac{\tilde{a}^2}{2!} \nabla^2 \alpha_j \right) \right] \quad (3-7)$$

The average distance thus represents a length scale for the variation between the elementary moments.

Partitioning the summation and using the fact that it no longer depends on  $k$  leads to

$$|\mathbf{M}|^2 = \frac{M_s^2}{N^2} \left[ N + \sum_{j=1}^{N^2-N} \alpha_j \cdot \alpha_j + \frac{\tilde{a}^2}{2!} \sum_{j=1}^{N^2-N} \alpha_j \cdot \nabla^2 \alpha_j \right] \quad (3-8)$$

Using (3-2) gives

$$|\mathbf{M}|^2 = \frac{M_s^2}{N^2} \left[ N + (N^2-N) + \frac{\tilde{a}^2}{2!} \sum_{j=1}^{N^2-N} \alpha_j \cdot \nabla^2 \alpha_j \right] \quad (3-9)$$

or

$$|\mathbf{M}|^2 = \frac{M_s^2}{N^2} \left[ N^2 + \frac{\tilde{a}^2}{2!} \sum_{j=1}^{N^2-N} \alpha_j \cdot \nabla^2 \alpha_j \right] \quad (3-10)$$

The following may be observed from (3-10): due to the fact that the second term arises when the second index is not equal to the first (i.e. distinct moments), the derivative terms are therefore generally nonzero, and thus should be retained for determining the relationship between  $\mathbf{M}$  and  $M_s$ . The second term in the sum of (3-10) therefore suggests the source of the contributions to an extension of the current relationship in (1-1).

Since  $j$  is unique only from 1 to  $N$ , (3-10) contains  $N-1$  repeated sums; thus, it may be alternatively written as

$$|\mathbf{M}|^2 = \frac{M_s^2}{N^2} \left[ N^2 + \frac{(N-1)\tilde{a}^2}{2!} \sum_{j=1}^N \alpha_j \cdot \nabla^2 \alpha_j \right] \quad (3-11)$$

The square of  $\mathbf{M}$  is now given by

$$|\mathbf{M}|^2 = M_s^2 + \frac{(N-1)\tilde{a}^2}{2!} \frac{M_s^2}{N^2} \sum_{j=1}^N \alpha_j \cdot \nabla^2 \alpha_j \quad (3-12)$$

For convenience, Eq. (3-12) may also be expressed as

$$|\mathbf{M}|^2 = M_s^2 + \frac{M_s^2(N^2-N)\tilde{a}^2}{2!N^2} \left( \frac{1}{N} \sum_{j=1}^N \alpha_j \cdot \nabla^2 \alpha_j \right) \quad (3-13)$$

Because the coefficient in the second term is positive in (3-13), and given relation (2-9), (3-13) also establishes the inequality given by

$$|\mathbf{M}|^2 \leq M_s^2 \quad (3-14)$$

The expression given in (3-13), however, is not so useful, as the direction cosines correspond to the elementary moment  $\mathbf{m}_j$ . To express it in a relevant form, one needs to determine the relationship between the Laplacian of the elementary moments  $M_s \nabla^2 \alpha$  and its analog for  $\mathbf{M}$ .

Using (3-1), an evaluation of the scalar vector product of  $\mathbf{M}$  and its vector Laplacian  $\nabla^2 \mathbf{M}$  leads to

$$\mathbf{M} \cdot \nabla^2 \mathbf{M} = \frac{M_s^2}{N^2} \left[ \sum_{j=1}^N \alpha_j \right] \cdot \left[ \nabla^2 \left( \sum_{k=1}^N \alpha_k \right) \right] = \frac{M_s^2}{N^2} \left[ \sum_{j=1}^N \alpha_j \right] \cdot \left[ \sum_{k=1}^N \nabla^2 \alpha_k \right] \quad (3-15)$$

Partitioning again leads to

$$\mathbf{M} \cdot \nabla^2 \mathbf{M} = \frac{M_s^2}{N^2} \left[ \sum_{j=1}^N \alpha_j \cdot \nabla^2 \alpha_j + \sum_{k \neq j} \alpha_j \cdot \nabla^2 \alpha_k \right] \quad (3-16)$$

Next, we expand the Laplacian, leading to

$$\mathbf{M} \cdot \nabla^2 \mathbf{M} = \frac{M_s^2}{N^2} \left[ \sum_{j=1}^N \alpha_j \cdot \nabla^2 \alpha_j + \sum_{k \neq j} \alpha_j \cdot \left( \nabla^2 \alpha_j + \frac{\tilde{a}^2}{2!} \nabla^4 \alpha_j \right) \right] \quad (3-17)$$

Regrouping the summation in (3-17) gives

$$\mathbf{M} \cdot \nabla^2 \mathbf{M} = \frac{M_s^2}{N^2} \left[ \sum_{j=1}^{N^2} \alpha_j \cdot \nabla^2 \alpha_j + \frac{(N-1)}{2!} \left( \sum_{j=1}^N \alpha_j \cdot \tilde{a}^2 \nabla^4 \alpha_j \right) \right] \quad (3-18)$$

The second term on the RHS in the summation of (3-18) involves fourth order terms for the elementary moment, which have fixed length. The theory of exchange already supposes these terms to be negligible as they are truncated. Therefore, truncation leaves us with

$$\mathbf{M} \cdot \nabla^2 \mathbf{M} \approx \frac{M_s^2}{N^2} \sum_{j=1}^{N^2} \alpha_j \cdot \nabla^2 \alpha_j \quad (3-19)$$

Because  $j$  is only unique from 1 to  $N$  it allows (3-18) to be alternatively written as

$$\mathbf{M} \cdot \nabla^2 \mathbf{M} \approx M_s^2 \left( \frac{1}{N} \sum_{j=1}^N \alpha_j \cdot \nabla^2 \alpha_j \right) \quad (3-20)$$

Eq. (3-20) may now be used in Eq. (3-13) leading to the following:

$$|\mathbf{M}|^2 = M_s^2 + \frac{M_s^2(N^2-N)\tilde{a}^2}{2!N^2} \left( \frac{1}{M_s^2} \mathbf{M} \cdot \nabla^2 \mathbf{M} \right) \quad (3-21)$$

After simplifying and taking the limit as  $N$  approaches infinity for a continuum theory, one obtains

$$|\mathbf{M}|^2 = M_s^2 + \frac{\tilde{a}^2}{2} \mathbf{M} \cdot \nabla^2 \mathbf{M} \quad (3-22)$$

The interpretation of the parameter  $\tilde{a}$  as the average distance between misaligned moments within the unit volume also suggests that it correlates with the variation length of the moment vector or an exchange length  $\ell_x$ , which is already estimated in the existing fixed-length micromagnetics theory using parameters such as saturation magnetization  $M_s$ , exchange stiffness  $A_x$ , and/or the anisotropy constant  $K$ . Well known length scales are typically given by the ratio of exchange energy density to other important energy (density) contributions. For example, a well known expression for the exchange length characterizing a Neel wall is given by

$$\ell_x \approx \sqrt{2A_x/\mu_0 M_s^2} \quad (3-23)$$

Using this, (3-22) may also be expressed as

$$|\mathbf{M}|^2 = M_s^2 + \kappa \ell_x^2 \mathbf{M} \cdot \nabla^2 \mathbf{M} \quad (3-24)$$

$\kappa$  is a convenient number on the order of unity.

Eq. (3-22) is a constraint relation between the magnetization vector  $\mathbf{M}$  and  $M_s$ , which follows directly from its definition and the theory of continuum exchange for the elementary moments. It can also be seen that the current constraint of fixed length given in (1-1) is a lower order approximation of (3-22).

#### 4. Potential implications of the extended relation between $\mathbf{M}$ and $M_s$

In magnetism, the constraint for the magnetization vector is imposed in a LaGrangian to obtain the equations of motion that satisfy, both, the energy minimum condition and the constraint simultaneously [14]. As an extended constraint has been found here, the implications are that the extended equations of motion for  $\mathbf{M}$  may be obtained using condition (3-22) instead of (1-1). An early analysis of these effects includes, for example (1) the effect of the parameter  $\tilde{a}$  on equilibrium solutions, for example, many works have been done on the classical calculations that determine transitions from a flower state to a vortex state; thus what effects may be found on the critical sizes like those studied in [15–18], and (2) the effect of a new exchange term on the behavior of the dynamics of a magnetization vector. Although it is not within the scope of this work to address these points, these kinds of questions concerning the equations of motion are also being investigated in future works.

#### 5. Summary and conclusions

We have presented an explicit derivation of a relationship between  $\mathbf{M}$  and  $M_s$  using the existing continuum exchange theory along with the definition of a magnetization vector  $\mathbf{M}$ . The resulting relation is seen to be an extension of the fixed-length constraint, and suggest  $M_s$  as an upper bound for  $|\mathbf{M}|$ .

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