Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Journal of Magnetism and Magnetic Materials 285 (2005) L1–L10
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Letter to the Editor

General magnetostatic shape–shape interactions

M. Beleggia[a], M. De Graef[b,*]

[a]Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, USA
[b]Department of Materials Science and Engineering, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213-3890, USA

Received 16 July 2004; received in revised form 1 September 2004
Available online 1 October 2004

Abstract

The magnetostatic interaction energy between two magnetic elements of arbitrary shape is presented as a convolution between the cross-correlation of the particle shapes and the dipolar tensor field. A generalized dipole–dipole interaction is derived, where the magnetic moments associated with the two particles interact through a magnetometric tensor field, carrying all the shape information. Example computations are given in order to verify the correctness of the formalism. The well-known result of the interaction between prisms, employed in most micromagnetic simulations, is correctly retrieved. The numerical accuracy of the method is also compared to a simple analytical result. Finally, one additional example computation, two interlaced interacting rings, is presented to show the generality of the formalism.

PACS: 41.20.Gz; 75.30.Gw; 75.40.Mg; 75.75.+a

Keywords: Magnetostatic energy; Shape amplitude; Magnetic nanoparticles

1. Introduction

The calculation of the magnetostatic interaction energy, E_m, between multiple uniformly magnetized particles of arbitrary shape represents one of the most difficult components of a typical micromagnetic computation. In fact, it requires the evaluation of a six-fold integral for each pair of magnetic elements, as each magnetic moment of the first element interacts with each moment of the second (a first three-fold integration), and then all the moments of the first particle must be considered (another three-fold integration). This must then be repeated for each pair of magnetic elements. For a review of the literature on the topic of magnetostatic energy computations we refer to Chapters 7 and 11 in Ref. [1]. The six-fold integrations can be avoided in principle, by reformulating the equations of micromagnetics in terms of field Lagrangians [2], but this approach is not commonly used in contemporary micromagnetics software.

*Corresponding author. Tel.: +1 412 268 8527; fax: +1 412 268 7596.
E-mail address: degraef@cmu.edu (M. De Graef).

0304-8853/$ - see front matter © 2004 Elsevier B.V. All rights reserved.
doi:10.1016/j.jmmm.2004.09.004

Many micromagnetic simulation packages use rectangular prisms to subdivide the volume of a magnetic shape, and then employ pre-calculated coefficients, based on the functions first derived by Rhodes and Rowlands [3], to compute the pairwise interactions between all prisms. When a different shape is needed for the computations, then these coefficients must be recomputed. For most shapes, the integrals involved can not be solved analytically, so that numerical computations must be used. Simulations of blocking effects and magnetostatic interactions in random particle arrays (i.e., particles not arranged on a periodic lattice) are often carried out by truncating the long-range interactions at an appropriate radius [4]. Ewald summation schemes are also frequently used [5]. In dilute dispersions of single domain Fe particles in an insulating matrix, magnetostatic interactions were shown to be dominant even at packing fractions as low as 10% [5]. In such studies, the actual particle shapes are not taken into account, and all particles are assumed to behave as point dipoles [6], an assumption that has been shown to be inaccurate for small particle separations when the actual particle shape is properly taken into account [7]. Magnetostatic interactions can also be computed indirectly by considering the demagnetizing field; in such an approach, the demagnetizing field at a point in space due to a magnetized object is computed by dividing this object into small (cubic) cells, and then summing over all cells. This procedure is then repeated for all cells in a second body, so that the interaction energy can be computed [8].

It is the purpose of this Letter to introduce a novel theoretical and computational approach which reformulates the magnetostatic interaction energy as a convolution product between a function determined by the shape of the individual particles, and the dipolar interaction tensor field. The approach is very general, and permits evaluation (mostly numerical, but in some cases also analytical) of the shape–shape pair interaction energy. We begin this Letter with an explicit derivation of the new formalism, followed by a series of example computations. We conclude with the outline of a numerical algorithm for the computation of the magnetostatic interaction energy, with a final explicit example: two interlaced magnetized rings.

2. Theoretical model

The theoretical approach employs the concept of the *characteristic function* or *shape function*, $D(\mathbf{r})$, which is a discontinuous function equal to unity inside the particle and zero outside. For a particle with a uniform magnetization state, the magnetization can be expressed as a vector field $\mathbf{M}(\mathbf{r}) = M_0\hat{\mathbf{m}}D(\mathbf{r})$, where M_0 is the saturation magnetization and a hat indicates a unit vector. It was shown in Ref. [9], that the Fourier transform of the shape function, the so-called *shape amplitude* $D(\mathbf{k})$, is a continuous function that can be used to define the demagnetization tensor field $N^{\alpha\beta}(\mathbf{k}) = D(\mathbf{k})\hat{k}^{\alpha}\hat{k}^{\beta}$. We denote vector and tensor components with Greek superscripts. $\hat{k}^{\alpha} = k^{\alpha}/|\mathbf{k}|$ is the direction cosine of the α component of $\mathbf{k}$. The real space representation, $N^{\alpha\beta}(\mathbf{r})$, can be obtained by a three-dimensional (3D) inverse Fourier transformation. The shape amplitude is hence central to the description of the magnetostatic behavior of a uniformly magnetized particle.

It was also shown, in Ref. [7], that the demagnetization tensor field can be written as the convolution between the shape function and the dipolar tensor, $D^{\alpha\beta}(\mathbf{r})$

$$N^{\alpha\beta}(\mathbf{r}) = D(\mathbf{r}) \otimes \mathscr{F}^{-1}[\hat{k}^{\alpha}\hat{k}^{\beta}] = D(\mathbf{r}) \otimes \mathscr{D}^{\alpha\beta}(\mathbf{r}), \qquad (1)$$

where $\otimes$ represents the convolution product, and $\mathscr{F}$ the Fourier transform operator. The dipolar tensor is defined as

$$\mathscr{D}^{\alpha\beta}(\mathbf{r}) \equiv \frac{1}{4\pi r^5}[r^2\delta^{\alpha\beta} - 3r^{\alpha}r^{\beta}], \qquad (2)$$

where $r = |\mathbf{r}|$, and $\delta^{\alpha\beta}$ is the identity matrix. Examples of the computation of the demagnetization tensor field using this approach were described in Refs. [10,11].

Once the demagnetization tensor field (DTF) is known, then the magnetostatic energy can be computed by contracting the tensor with respect to the magnetization unit vector, $m^{\alpha}N^{\alpha\beta}(\mathbf{r})m^{\beta}$ (a summation over repeated superscripts is implied), and integrating over the complete volume of the