

# Magnetostatic Interaction Fields for a Three-Dimensional Array of Ferromagnetic Cubes

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**Abstract**—An exact analytic formula for the magnetostatic interaction energy of a three-dimensional array of ferromagnetic cubes is presented. The magnetization within each cube is assumed constant but varies in direction from cube to cube. From the expressions for the interaction energy, exact formulas for the effective magnetostatic interaction field are derived. This provides a useful tool for three-dimensional micromagnetic calculations.

## INTRODUCTION

MICROMAGNETIC investigations require a precise knowledge of the magnetostatic field within a ferromagnetic sample [1]. The *total* micromagnetic interaction field encompasses also contributions from several other sources, in particular, the exchange interaction and the crystalline anisotropy. However, these will not be treated in this paper, the sole concern of which is to develop tools for an appropriate treatment of the magnetostatic interaction field in small three-dimensional ferromagnetic samples. A few general remarks on the representation of continuum systems will set the goals and motivation of this work.

Classical micromagnetic analysis has its origin in a continuum formulation of the magnetization field and their associated interactions. This approach is usually quite sufficient to represent the magnetic properties on scales much larger than the scales of the underlying atomic structure. One of the main routes for a mathematical representation is to derive partial differential equations for the magnetization field. The resulting nonlinear coupled partial differential equations are usually called Brown's equations [2]. The great difficulties associated with solving Brown's equations for any realistic situation suggest another approach. The continuum system is replaced by a set of discrete interacting subsystems, whose properties are well defined. Certainly, this introduces a discretization error to the calculation. To control the discretization error properly, the interaction between the specified subsystems has to be handled with great care. Uniformly magnetized cubes have no shape anisotropy [3], their magnetostatic surface charges are easily calculated, and they are space filling. As will be demonstrated, cubical subelements arranged at the sides of a simple cubic lattice

allow for the derivation of exact analytic formulas for the effective magnetostatic interaction field. Hence apart from the inevitable discretization error, no further approximation is introduced to the calculation. From this point of view the exact analytic expressions, as presented in this paper, are quite pleasing. Moreover, the simple cubic array of interacting uniformly magnetized cubes is the simplest possible space-filling discrete representation of a three-dimensional ferromagnetic continuum and therefore of fundamental importance. The work presented in this paper is a continuation of the studies of Brown and LaBonte [4], [5], who investigated one- and two-dimensional ferromagnetic systems. In [5] LaBonte derived the exact analytic interaction integrals for a discretized two-dimensional domain wall. Recently, Della Torre investigated three-dimensional ferromagnetic particles [6]. He did not develop the corresponding three-dimensional magnetostatic interaction integrals, whose exact analytic form will be presented as the main result of this paper.

In the last part of the article a short discussion of the numerical properties of the exact analytic formulas is given. In particular, it is demonstrated that the adoption of simple dipole approximations may introduce large errors for small separation between the interacting cubes. Thus the expressions obtained in this paper are not only of conceptual value, they ensure the numerical correctness of the resulting magnetostatic field, which includes contributions from all neighbors of a given lattice site.

## THE MICROMAGNETIC ARRAY

La Bonte [5] gives a micromagnetic treatment of a two-dimensional ferromagnetic domain wall in a Permalloy film. His approach subdivides the sample into a set of closely packed aligned infinite prisms. It is natural to extend this approach to three-dimensional systems by considering a simple cubic array of ferromagnetic cubes [6]. The cubes are assumed to be sufficiently small so that the magnetization can be taken constant (of magnitude  $M_s$ ) within each cube but may vary in direction from cube to cube. This assumption leads mathematically from the classical continuum approximation of the magnetization distribution to an approximate discrete formalism. The process of dividing the sample into an array of cubes has to be understood as a purely mathematical discretization prescription, which converts the energy functional into an ordinary function of magnetic moments defined at the centers of a simple cubic lattice. Of course, this can only be done at the expense of neglecting magnetic fluctuations

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on scales smaller than the lattice constant of the simple cubic array. On the one hand, the size of the cubes determines the resolution, with which magnetic modes can be calculated in this model. On the other hand, the formulation will cease to be valid as soon as the lattice constant approaches atomic scales. To answer questions involving atomic scales, one would have to give a quantum mechanical treatment. However, the goal of this paper is to develop tools for describing small but nevertheless macroscopic ferromagnetic samples. Therefore, it is assumed that quantum mechanics is accounted for sufficiently in providing the appropriate values of the material constants (e.g., saturation magnetization) characterizing the magnetic properties of the specimen. We arrive at the following formulation.

In the discretized picture the magnetization of the sample is described by the vector field  $\mathbf{M}(x_n, y_n, z_n)$  where  $x_n, y_n,$  and  $z_n$  denote the coordinates of the center of the  $n$ th cube of the simple cubic array. The triples  $\{x_n, y_n, z_n\}$  are chosen to be elements of the set

$$\{0, d, \dots, (N_x - 1)d\} \times \{0, d, \dots, (N_y - 1)d\} \\ \times \{0, d, \dots, (N_z - 1)d\} \quad (1)$$

where  $d$  labels the lattice constant of the simple cubic array.  $N_x, N_y,$  and  $N_z$  characterize the overall shape of the sample. For simplicity, planar boundaries and a closely packed array of cubes are assumed. These assumptions imply that each site of the simple cubic array is indeed occupied by a cube. In principle, voids or irregular boundary shapes can easily be treated by the method presented in this paper. This is due to the fact that the total magnetostatic interaction is taken as a sum of pair interaction terms.

#### THE PAIR INTERACTION ENERGY

The total magnetostatic energy is the sum of the contributions from the pairwise interaction of each cube with every other cube of the array. For simplicity, consider first the magnetostatic interaction energy between one such pair. The system of coordinates is chosen such that the center of the first cube is located at the origin. The displacement vector of the second cube with respect to the origin is given by

$$\mathbf{D} = X, \mathbf{i} + Y, \mathbf{j} + Z, \mathbf{k}, \quad (2)$$

where  $X, Y,$  and  $Z$  are integer multiples of the lattice constant complying with the boundary conditions (1).  $\mathbf{i}, \mathbf{j}, \mathbf{k}$  are the unit vectors in the  $x, y,$  and  $z$  direction, respectively.

It is convenient to introduce the magnetostatic potential due to the magnetostatic surface charges of the first cube. Since a constant magnetization  $\mathbf{M}(x_i, y_j, z_k)$  within each cube is assumed, the magnetostatic surface charge density on a given face of a cube is uniform. It is described by

$$\sigma_l = \mathbf{M}(x_i, y_j, z_k) \cdot \mathbf{n}_l(x_i, y_j, z_k), \quad l = 1, \dots, 6 \quad (3)$$

where  $\mathbf{n}_l(x_i, y_j, z_k)$  is the unit vector corresponding to the surface normal of the cube face under consideration. In (3) the subscript  $l$  takes values from one to six according to the six faces of a given cube. Equation (3) and the subsequent expressions are written in the rationalized CGS system of units.

The magnetostatic potential due to the surface charge density as given by (3) is obtained from

$$V(\mathbf{r}) = \iint \frac{\sigma}{\sqrt{[\mathbf{r} - \mathbf{r}']^2}} d^2 \mathbf{r}'. \quad (4)$$

The integration in (4) is carried out over the six faces of the cube. For convenience, a separate notation for the direction cosines of the magnetization  $\mathbf{M}(x_i, y_j, z_k)$  is introduced:

$$\alpha_{ijk} \equiv \mathbf{M}(x_i, y_j, z_k) \cdot \mathbf{i} \quad \beta_{ijk} \equiv \mathbf{M}(x_i, y_j, z_k) \cdot \mathbf{j} \\ \gamma_{ijk} \equiv \mathbf{M}(x_i, y_j, z_k) \cdot \mathbf{k}. \quad (5)$$

The expression for the magnetostatic potential due to the first cube is

$$V(x, y, z) \\ = M_s \alpha_1 \int_{-d/2}^{+d/2} \int_{-d/2}^{+d/2} \left[ \frac{1}{\sqrt{\left(\frac{d}{2} - x\right)^2 + (y - \eta)^2 + (z - \zeta)^2}} \right. \\ \left. - \frac{1}{\sqrt{\left(\frac{d}{2} + x\right)^2 + (y - \eta)^2 + (z - \zeta)^2}} \right] d\eta d\zeta \\ + M_s \beta_1 \int_{-d/2}^{+d/2} \int_{-d/2}^{+d/2} \left[ \frac{1}{\sqrt{(x - \xi)^2 + \left(\frac{d}{2} - y\right)^2 + (z - \zeta)^2}} \right. \\ \left. - \frac{1}{\sqrt{(x - \xi)^2 + \left(\frac{d}{2} + y\right)^2 + (z - \zeta)^2}} \right] d\xi d\zeta \\ + M_s \gamma_1 \int_{-d/2}^{+d/2} \int_{-d/2}^{+d/2} \left[ \frac{1}{\sqrt{(x - \xi)^2 + (y - \eta)^2 + \left(\frac{d}{2} - z\right)^2}} \right. \\ \left. - \frac{1}{\sqrt{(x - \xi)^2 + (y - \eta)^2 + \left(\frac{d}{2} + z\right)^2}} \right] d\xi d\eta, \quad (6)$$

where  $M_s$  labels the saturation magnetization of the ferromagnetic cubes.  $\alpha_1, \beta_1,$  and  $\gamma_1$  are the direction cosines of the magnetization of the first cube.

Thus the magnetostatic interaction energy between two cubes is

$$\begin{aligned}
 W_{12} = & M_s^2 [\alpha_1 \alpha_2 A(X, Y, Z) + \beta_1 \beta_2 A(Y, Z, X) \\
 & + \gamma_1 \gamma_2 A(Z, X, Y) + \alpha_1 \beta_2 B(X, Y, Z) \\
 & + \beta_1 \gamma_2 B(Y, Z, X) + \gamma_1 \alpha_2 B(Z, X, Y) \\
 & + \beta_1 \alpha_2 B(Y, X, Z) + \beta_2 \gamma_1 B(Z, Y, X) \\
 & + \alpha_1 \gamma_2 B(X, Z, Y)] \quad (7)
 \end{aligned}$$

where  $\alpha_2, \beta_2,$  and  $\gamma_2$  are the direction cosines of the magnetization of the second cube.  $A(X, Y, Z)$  and  $B(X, Y, Z)$  are the fourfold integrals

$$\begin{aligned}
 A(X, Y, Z) = & \int_{z=Z-(d/2)}^{z=Z+(d/2)} \int_{y=Y-(d/2)}^{y=Y+(d/2)} \int_{\xi=-(d/2)}^{\xi=+(d/2)} \int_{\eta=-(d/2)}^{\eta=+(d/2)} \\
 & \cdot \left[ \frac{2}{\sqrt{X^2 + (y - \eta)^2 + (z - \xi)^2}} \right. \\
 & - \frac{1}{\sqrt{(X + d)^2 + (y - \eta)^2 + (z - \xi)^2}} \\
 & - \left. \frac{1}{\sqrt{(X - d)^2 + (y - \eta)^2 + (z - \xi)^2}} \right] \\
 & \cdot d\eta d\xi dy dz, \quad (8)
 \end{aligned}$$

$$\begin{aligned}
 B(X, Y, Z) = & \int_{z=Z-(d/2)}^{z=Z+(d/2)} \int_{x=X-(d/2)}^{x=X+(d/2)} \int_{\xi=-(d/2)}^{\xi=+(d/2)} \int_{\eta=-(d/2)}^{\eta=+(d/2)} \\
 & \cdot \left[ \frac{1}{\sqrt{\left(\frac{d}{2} - x\right)^2 + \left(Y + \frac{d}{2} - \eta\right)^2 + (z - \xi)^2}} \right. \\
 & - \frac{1}{\sqrt{\left(\frac{d}{2} + x\right)^2 + \left(Y + \frac{d}{2} - \eta\right)^2 + (z - \xi)^2}} \\
 & - \frac{1}{\sqrt{\left(\frac{d}{2} - x\right)^2 + \left(Y - \frac{d}{2} - \eta\right)^2 + (z - \xi)^2}} \\
 & + \left. \frac{1}{\sqrt{\left(\frac{d}{2} + x\right)^2 + \left(Y - \frac{d}{2} - \eta\right)^2 + (z - \xi)^2}} \right] \\
 & \cdot d\eta d\xi dx dz. \quad (9)
 \end{aligned}$$

The use of the formulation of  $W_{12}$  as given by (7) has reduced the multitude of four-dimensional integrals that need to be evaluated to a set of merely two. The fact that we have to consider two types of integrals arises from the two possible topologies for the magnetostatic interaction, namely, the interaction between two squares that are parallel to each other and those that are perpendicular to each other. The main task is to obtain analytic expressions for the  $A$  and  $B$  integrals as a function of the displacement parameters  $X, Y,$  and  $Z$ . As will be shown, the final result can be represented entirely in terms of elementary functions.

#### NONSINGULAR INTERACTION INTEGRALS

In this section the derivation for the interaction integrals for the general nonsingular case (i.e., where the displacement parameters are nonzero) is outlined. The formulas for the singular cases of one or more of the displacement parameters vanishing may easily be obtained from the nonsingular expressions.

For carrying out the integrations in (8) and (9) it is useful to note that

$$\begin{aligned}
 & \int \ln(\sqrt{\xi^2 + \eta^2 + Z^2} - Z) d\eta \\
 & = \eta \ln(\sqrt{\xi^2 + \eta^2 + Z^2} - Z) \\
 & \quad - \eta + \xi \arctan\left(\frac{\eta}{\xi}\right) \\
 & \quad + \xi \arctan\left(\frac{Z\eta}{\xi\sqrt{\xi^2 + \eta^2 + Z^2}}\right) \\
 & \quad - Z \ln(\sqrt{\xi^2 + \eta^2 + Z^2} + \eta). \quad (10)
 \end{aligned}$$

The integrations over  $z$  and  $\xi$  in (8) yield

$$\begin{aligned}
 A(X, Y, Z) = & 4F_1(X, Y, Z) - 2F_1(X, Y, Z + d) \\
 & - 2F_1(X, Y, Z - d) - 2F_1(X + d, Y, Z) \\
 & + F_1(X + d, Y, Z + d) \\
 & + F_1(X + d, Y, Z - d) \\
 & - 2F_1(X - d, Y, Z) + F_1(X - d, Y, Z + d) \\
 & + F_1(X - d, Y, Z - d), \quad (11)
 \end{aligned}$$

with

$$\begin{aligned}
 F_1(X, Y, Z) = & \int_{y=Y-(d/2)}^{y=Y+(d/2)} \int_{\eta=-(d/2)}^{\eta=+(d/2)} \\
 & \cdot [Z \ln(\sqrt{X^2 + (y - \eta)^2 + Z^2} - Z) \\
 & + \sqrt{X^2 + (y - \eta)^2 + Z^2}] d\eta dy. \quad (12)
 \end{aligned}$$

$F_1$  can be written as

$$F_1(X, Y, Z) = 2F_2(X, Y, Z) - F_2(X, Y - d, Z) - F_2(X, Y + d, Z) \tag{13}$$

where

$$F_2(X, Y, Z) = \frac{Z}{2} (X^2 - Y^2) \ln(\sqrt{X^2 + Y^2 + Z^2} - Z) + \frac{Y}{2} (X^2 - Z^2) \ln(\sqrt{X^2 + Y^2 + Z^2} - Y) - XYZ \arctan\left(\frac{YZ}{X\sqrt{X^2 + Y^2 + Z^2}}\right) + \frac{1}{6} (2X^2 - Y^2 - Z^2) \sqrt{X^2 + Y^2 + Z^2}. \tag{14}$$

Both in (13) and (14) terms linear in Z have been omitted since they will add up to zero in (11) for the A integral.

A strategy similar to the one used to obtain the analytic expressions for the A integrals yields

$$B(X, Y, Z) = G_1\left(X, Y + \frac{d}{2}, Z\right) - G_1\left(X, Y - \frac{d}{2}, Z\right), \tag{15}$$

with

$$G_1(X, Y, Z)$$

$$= 4G_2\left(X, Y + \frac{d}{2}, Z\right) - 4G_2\left(X, Y - \frac{d}{2}, Z\right) - 2G_2\left(X, Y + \frac{d}{2}, Z + d\right) + 2G_2\left(X, Y - \frac{d}{2}, Z + d\right) - 2G_2\left(X, Y + \frac{d}{2}, Z - d\right) + 2G_2\left(X, Y - \frac{d}{2}, Z - d\right) - 2G_2\left(X - d, Y + \frac{d}{2}, Z\right) + 2G_2\left(X - d, Y - \frac{d}{2}, Z\right) + G_2\left(X - d, Y + \frac{d}{2}, Z + d\right) - G_2\left(X - d, Y - \frac{d}{2}, Z + d\right)$$

$$+ G_2\left(X - d, Y + \frac{d}{2}, Z - d\right) - G_2\left(X - d, Y - \frac{d}{2}, Z - d\right) - 2G_2\left(X + d, Y + \frac{d}{2}, Z\right) + 2G_2\left(X + d, Y - \frac{d}{2}, Z\right) + G_2\left(X + d, Y + \frac{d}{2}, Z + d\right) - G_2\left(X + d, Y - \frac{d}{2}, Z + d\right) + G_2\left(X + d, Y + \frac{d}{2}, Z - d\right) - G_2\left(X + d, Y - \frac{d}{2}, Z - d\right), \tag{16}$$

with

$$G_2(X, Y, Z) = \int_{\xi=0}^{\xi=X} \left[ YZ \ln(\sqrt{\xi^2 + Y^2 + Z^2} - Z) + \frac{Z^2}{2} \ln(\sqrt{\xi^2 + Y^2 + Z^2} - Y) + \frac{Y}{2} \sqrt{\xi^2 + Y^2 + Z^2} - \frac{\xi^2}{2} \ln(\sqrt{\xi^2 + Y^2 + Z^2} - Y) + \xi Z \arctan\left(\frac{YZ}{\xi\sqrt{\xi^2 + Y^2 + Z^2}}\right) \right] d\xi. \tag{17}$$

The integrals in (17) can be carried out analytically in terms of elementary functions to give the following result:

$$G_2(X, Y, Z) = \left(\frac{Y^3}{6} - \frac{YZ^2}{2}\right) \ln(R + X) + \frac{X}{6} (3Z^2 - X^2) \ln(R - 1) + \frac{XYR}{3} + XYZ \ln(R - Z) + \frac{Y^2Z}{2} \arctan\left(\frac{XZ}{RY}\right) + \frac{Z^3}{6} \arctan\left(\frac{XY}{RZ}\right)$$

$$+ \frac{X^2 Z}{2} \arctan \left( \frac{YZ}{RX} \right) + G_2'(X, Y, Z) \quad (18)$$

where

$$R = \sqrt{X^2 + Y^2 + Z^2} \quad (19)$$

and

$$\begin{aligned} G_2'(X, Y, Z) &= \left( \frac{-Y^3}{12} + \frac{YZ^2}{4} \right) \ln(Y^2 + Z^2) \\ &+ \frac{2}{3} Z^3 \arctan \left( \frac{X}{Z} \right) \\ &+ Y^2 Z \arctan \left( \frac{X}{Y} \right) \\ &- XYZ - \frac{2XZ^2}{3} + \frac{X^3}{18}. \end{aligned} \quad (20)$$

For the purpose of calculating  $B(X, Y, Z)$  terms in (18) that are linear in  $Z$  or independent of  $X$  or  $Y$  may be omitted. This follows from the symmetry of (15) and (16). Therefore, none of the terms in  $G_2'$  contributes to  $B(X, Y, Z)$  and  $G_2'$  can be omitted in (18).

#### SINGULAR INTERACTION INTEGRALS

The calculation of the total magnetostatic interaction energy of the sample also includes integrals with one or more of the displacement parameters vanishing. The energy, however, cannot be singular, and indeed, these singularities are of the type  $x \ln[x]$ , which are removed in the limit  $x \rightarrow 0$ . Passing to this limit is strictly correct only in the context of the micromagnetics approximation, which uses continuum instead of the actual atomic structure. The justification of this approximation has already been thoroughly discussed in [1] and [4]. The following formulas list the expressions for  $F_2$  and  $G_2$  for the case where at least one of the displacement parameters vanishes:

1)  $X = 0, Y \neq 0, Z \neq 0$ :

$$\begin{aligned} F_2(0, Y, Z) &= -\frac{ZY^2}{2} \ln(R - Z) \\ &- \frac{YZ^2}{2} \ln(R - Y) - \frac{R^3}{6} \end{aligned} \quad (21)$$

$$G_2(0, Y, Z) = \left( \frac{3Y^3}{16} - \frac{11YZ^2}{8} \right) \ln(R); \quad (22)$$

2)  $X \neq 0, Y = 0, Z \neq 0$ :

$$\begin{aligned} F_2(X, 0, Z) &= \frac{ZX^2}{2} \ln(R - Z) \\ &+ \frac{1}{6} (2X^2 - Z^2) R \end{aligned} \quad (23)$$

$$G_2(X, 0, Z) = \left( \frac{XZ^2}{2} - \frac{X^3}{6} \right) \ln(R); \quad (24)$$

3)  $X \neq 0, Y \neq 0, Z = 0$ :

$$\begin{aligned} F_2(X, Y, 0) &= \frac{YX^2}{2} \ln(R - Y) \\ &+ \frac{1}{6} (2X^2 - Y^2) R \end{aligned} \quad (25)$$

$$\begin{aligned} G_2(X, Y, 0) &= \frac{3Y^3}{16} \ln(R + X) \\ &- \frac{X^3}{6} \ln(R - Y) - \frac{Y^3}{96} \\ &\cdot \ln \left( \frac{R + X}{R - X} \right) + \frac{XYR}{3}; \end{aligned} \quad (26)$$

4)  $X = 0, Y = 0, Z \neq 0$ :

$$F_2(0, 0, Z) = -\frac{|Z|^3}{6} \quad (27)$$

$$G_2(0, 0, Z) = 0; \quad (28)$$

5)  $X = 0, Y \neq 0, Z = 0$ :

$$F_2(0, Y, 0) = -\frac{|Y|^3}{6} \quad (29)$$

$$G_2(0, Y, 0) = \frac{3Y^3}{32} \ln(Y^2); \quad (30)$$

6)  $X \neq 0, Y = 0, Z = 0$ :

$$F_2(X, 0, 0) = \frac{|X|^3}{3} \quad (31)$$

$$G_2(X, 0, 0) = -\frac{X^3}{12} \ln(X^2); \quad (32)$$

7)  $X = 0, Y = 0, Z = 0$ :

$$F_2(0, 0, 0) = 0 \quad (33)$$

$$G_2(0, 0, 0) = 0. \quad (34)$$

#### THE MAGNETOSTATIC INTERACTION ENERGY

Equation (7) for the pair interaction energy is generalized to obtain an expression for the total magnetostatic interaction energy. Let  $W_{ijk, i'j'k'}$  denote the interaction energy between the cubes at site  $(i, j, k)$  and  $(i', j', k')$ , respectively.  $W_{ijk, i'j'k'}$  is obtained from (7) by replacing all subscripts 1 by the triple  $(i, j, k)$  and all subscripts 2 by the triple  $(i', j', k')$ .

Now the total (tot) magnetostatic interaction energy can be written as

$$W_{\text{tot}} = \frac{1}{2} \sum'_{ijk, i'j'k'} W_{ijk, i'j'k'}. \quad (35)$$

The prime on the summation indicates that only terms with  $ijk \neq i'j'k'$  are included in the calculation of the total

energy. The omission of the self-energy is legitimate since the uniformly magnetized cubic elements do not have shape anisotropy. Hence the contribution of the self-terms is independent of the directional cosines  $\alpha_{ijk}$ ,  $\beta_{ijk}$ ,  $\gamma_{ijk}$ .

#### THE EFFECTIVE MAGNETOSTATIC INTERACTION FIELD

The effective interaction field is obtained from the energy expression (35) by regarding the  $\alpha_{ijk}$ ,  $\beta_{ijk}$ , etc., as independent variables. They play the role of generalized coordinates for the energy function (35). The effective interaction fields, on the other hand, are defined to be proportional to the negative gradient of  $W_{\text{tot}}$ , the gradient being taken with respect to the magnetization vector at a given lattice site. The effective interaction field at site  $(i, j, k)$  is given by

$$\begin{aligned} H_x(i, j, k) &= -\frac{1}{M_s d^3} \frac{\partial W_{\text{tot}}}{\partial \alpha_{ijk}}, \\ H_y(i, j, k) &= -\frac{1}{M_s d^3} \frac{\partial W_{\text{tot}}}{\partial \beta_{ijk}}, \\ H_z(i, j, k) &= -\frac{1}{M_s d^3} \frac{\partial W_{\text{tot}}}{\partial \gamma_{ijk}}. \end{aligned} \quad (36)$$

This definition of the effective interaction field is useful since at each site of the lattice there is one quadratic constraint which involves only the magnetization vector of that particular site. The constraints are the condition that  $\alpha_{ijk}^2 + \beta_{ijk}^2 + \gamma_{ijk}^2 = 1$  for each lattice site. To be able to treat the  $\alpha_{ijk}$ ,  $\beta_{ijk}$ , and  $\gamma_{ijk}$  as independent variables during a variational calculation,  $W_{\text{tot}}$  has to be augmented by

$$\sum_{ijk} \lambda_{ijk} (\alpha_{ijk}^2 + \beta_{ijk}^2 + \gamma_{ijk}^2)$$

where the  $\lambda_{ijk}$  are Lagrange multipliers. A necessary condition for the equilibrium configuration is then obtained as the requirement that at each and every lattice site the magnetization be parallel to the effective interaction field.

In terms of  $A$ ,  $B$  integrals and directional cosines of the magnetization, the effective interaction field can be written as

$$\begin{aligned} H_x(i, j, k) &= -\frac{M_s}{d^3} \sum'_{i'j'k'} \alpha_{i'j'k'} A(X, Y, Z) \\ &\quad + \beta_{i'j'k'} B(X, Y, Z) \\ &\quad + \gamma_{i'j'k'} B(X, Z, Y) \end{aligned} \quad (37)$$

$$\begin{aligned} H_y(i, j, k) &= -\frac{M_s}{d^3} \sum'_{i'j'k'} \beta_{i'j'k'} A(Y, Z, X) \\ &\quad + \gamma_{i'j'k'} B(Y, Z, X) \\ &\quad + \alpha_{i'j'k'} B(Y, X, Z) \end{aligned} \quad (38)$$

$$\begin{aligned} H_z(i, j, k) &= -\frac{M_s}{d^3} \sum'_{i'j'k'} \gamma_{i'j'k'} A(Z, X, Y) \\ &\quad + \alpha_{i'j'k'} B(Z, X, Y) \\ &\quad + \beta_{i'j'k'} B(Z, Y, X) \end{aligned} \quad (39)$$

#### DISCUSSION

It is interesting to ask how the exact treatment of the interaction energy between uniformly magnetized cubes compares to a treatment where each cube is replaced by a dipole of strength  $M_s d^3$  at the center of each cube. For simplicity, consider two cubes, one at the origin, the other one displaced in the  $z$  direction by  $n$  lattice constants ( $X = Y = 0, Z = nd$ ). Each of the cubes be uniformly magnetized along the  $z$  direction ( $\alpha = \beta = 0, \gamma = 1$ ). Formula (7) yields for the interaction energy in this case

$$W_{12} = M_s^2 A(nd, 0, 0). \quad (40)$$

Replacing the cubes by dipoles of strengths  $M_s d^3$  pointing in the  $z$  direction at the center of the cubes yields

$$W'_{12} = -2M_s^2 \frac{d^3}{n^3}. \quad (41)$$

The ratio between (41) and (40) is

$$r = \frac{-2d^3}{n^3 A(nd, 0, 0)}. \quad (42)$$

The resulting values of  $r$  for the first nearest neighbors are given in Table I.

Note that the dipole approximation for  $n = 1$  overestimates the interaction energy by more than 17 percent. Thus the dipole approximation may introduce significant errors in the calculation of the magnetostatic interaction field due to nearest neighbors.

To ensure the correctness of the analytic results, elaborate tests have been performed. The symbol manipulation package (SMP) [7] has been used to differentiate the formulas of the integrals to recover the integrands. SMP was also employed initially to obtain parts of the more tedious integrals. Furthermore, numerical evaluations of the various integrals were carried out to test the numerical usefulness of the analytic expressions and to guarantee the accuracy of the final results.

The numerical values of the integrals  $A$  and  $B$  depend critically on the precision to which  $F_2$  and  $G_2$  are obtained. The values of the  $A$  and  $B$  integrals are many orders of magnitude smaller than the contributing terms  $F_2$  and  $G_2$ . This is due to a very delicate cancelation of the  $F_2$  terms involved to yield the values of the  $A$  integrals, and of the  $G_2$  terms which contribute to the value of the  $B$  integrals. For a numerical evaluation of the  $A$  and  $B$  integrals, the  $F_2$  and  $G_2$  functions have to be calculated to sufficient accuracy. Unless the displacement parameters involve very high integer multiples of the lattice constant, ordinary VAX double precision turns out to be quite sufficient. It is also straightforward to expand the  $F_2$  and  $G_2$  functions in Taylor series about the displacement parameters. This may be useful in cases where the available word length of the computational hardware is rather small, or where a very wide range of displacement parameters is involved.

We checked the numerical reliability of the results by comparing the values of the  $A$  and  $B$  integrals as obtained from the analytic formulas with those obtained from a

TABLE I  
COMPARISON OF THE INTERACTION ENERGY BETWEEN TWO CUBES AS  
CALCULATED FROM THE EXACT FORMULAS AND FROM THE DIPOLE  
APPROXIMATION, RESPECTIVELY

$n$	$r$
1	1.1788
2	1.0243
3	1.0052
4	1.0017

Gauss-quadrature procedure over a four-dimensional hypercube [8]. The agreement is quite satisfactory within the accuracy of the numerical integration procedure. The integration over the last free variable yielding  $F_2$  and  $G_2$ , respectively, is the most critical step of the entire calculation. For reasons indicated earlier a small error in the calculation of  $F_2$  or  $G_2$  results in large errors of the  $A$  and  $B$  integrals. The resolution of the four-dimensional numerical integration was limited to a relative error of  $10^{-5}$ . To exclude the possibility of small distortions of the final result, which would go undetected due to the limited accuracy of the four dimensional Gauss-quadrature integration, a one-dimensional 64-point Gauss-Kronrod [9] integration of the integrands of  $F_2$  and  $G_2$ , respectively, was performed. Excellent agreement (relative error  $< 10^{-1}$ ) with the results obtained from the analytic formulas was achieved.

#### CONCLUSION

A method for calculating effective magnetostatic interaction fields from exact analytic formulas has been presented. The use of the exact expressions seems important, in particular, for the calculation of the contribution to the interaction fields arising from the nearest neighbors of a given site in the interacting array of cubes. The formulas

obtained are suitable for use in micromagnetic variational procedures. Research in this direction is currently in progress.

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