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NOTE

Removal of Apparent Singularity in Grid Computations

1. INTRODUCTION

A self-consistency test for magnetic domain wall models was suggested by Aharoni [1]. The test consists of evaluating the ratio $S = \varepsilon_{wall}/\varepsilon'_{wall}$, where ε_{wall} is the wall energy, and ε'_{wall} is the integral of a certain function of the direction cosines of the magnetization, α, β, and γ, over the volume occupied by the domain wall. If the computed configuration is a good approximation to one corresponding to an energy minimum, the ratio is close to 1. The integrand of ε'_{wall} contains terms that are inversely proportional to γ, and since γ passes through zero at the centre of the domain wall, these terms have a singularity at these points. Nevertheless, the integral is finite, and its evaluation does not usually present any problems when the direction cosines are known in terms of continuous functions. However, in many cases, significantly better results for magnetization configurations of domain walls can be obtained by computations using finite element methods, as first shown by LaBonte [2]. The direction cosines are then only known at a set of discrete (grid) points, and integration over the domain wall is replaced by summation over these points. Evaluation of ε'_{wall} becomes inaccurate if the terms in the summation are taken to be the values of the integrand at the grid points, because of the large contribution of points close to where γ changes sign. The self-consistency test has recently been generalised to a larger number of cases [3], and as finite element computations of magnetization configurations are popular at present, it is important to have a reliable check of the validity of their results.

The purpose of this paper is to suggest a method of improving the accuracy of the evaluation of integrals in such cases. Since the self-consistency test has so far only been applied to two-dimensional magnetization configurations, the problem and its solution will be presented for that specific case. Generalisation to three or more dimensions is straightforward, although the derivation of the formulae becomes increasingly laborious as the number of dimensions increases.

2. METHOD OF COMPUTATION

We require an approximation to the integral

$$T = \int_{a_2}^{b_2} \int_{a_1}^{b_1} \frac{f(\gamma)}{\gamma}\, dx_1\, dx_2. \tag{1}$$

However, only a finite set of values of γ are known, which will be referred to as $\gamma(r_1, r_2)$, with $r_i = 1, 2, ..., n_i$, $i = 1, 2$, where the argument r_i refers to points whose x_i-coordinate is

$$x_i = a_i + (2r_i - 1)\, \Delta_i \tag{2}$$

and

$$\Delta_i = \frac{b_i - a_i}{2n_i}. \tag{3}$$

A simple approximation to T is the summation

$$T' = \sum_{r_2=1}^{n_2} \sum_{r_1=1}^{n_1} \frac{f(r_1, r_2)}{\gamma(r_1, r_2)} \tag{4}$$

over the grid points. This approximation is good enough except near points, where $\gamma = 0$, which always exist in the problem discussed here. Because of the difficulties caused by these points, it is better to use instead

$$T'' = \sum_{r_2=1}^{n_2} \sum_{r_1=1}^{n_1} F(r_1, r_2), \tag{5a}$$

where

$$F(r_1, r_2) = \int_{-\Delta_2}^{\Delta_2} \int_{-\Delta_1}^{\Delta_1} \frac{f_0 + g_1 \xi_1 + g_2 \xi_2}{\gamma_0 + \delta_1 \xi_1 + \delta_2 \xi_2}\, d\xi_1\, d\xi_2, \tag{5b}$$

is the *local* integral between grid points, and f_0, g_1, g_2, γ_0, δ_1, and δ_2 are the values of f, $\partial f/\partial x_1$, $\partial f/\partial x_2$, γ, $\partial \gamma/\partial x_1$, and $\partial \gamma/\partial x_2$, respectively, at the point (r_1, r_2). (To simplify the notation, the arguments r_1, r_2 have been omitted from f_0, g_1, g_2, γ_0, δ_1, and δ_2.) The partial derivatives can be calculated by using the values of f and γ at the neighbouring grid points. We can then write

$$F(r_1, r_2) = f_0 P + g_1 Q_1 + g_2 Q_2, \tag{6}$$

where

$$P = \int_{-\Delta_2}^{\Delta_2} \int_{-\Delta_1}^{\Delta_1} \frac{d\xi_1\, d\xi_2}{\gamma_0 + \delta_1 \xi_1 + \delta_2 \xi_2} \tag{7a}$$

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and

$$Q_i = \int_{-\Delta_2}^{\Delta_2} \int_{-\Delta_1}^{\Delta_1} \frac{\xi_i \, d\xi_1 \, d\xi_2}{\gamma_0 + \delta_1 \xi_1 + \delta_2 \xi_2} \tag{7b}$$

for $i = 1, 2$; the arguments r_1, r_2 have been omitted from P and Q_i. If $\gamma_0 + \delta_1 \xi_1 + \delta_2 \xi_2$ does not change sign within the region of integration, evaluation of the integrals is straightforward, and it can easily be shown that the results are given by logarithms, except for an extra polynomial term in Q_i. For numerical computation, it is convenient to convert the logarithms to inverse hyperbolic tangents, which can be computed more accurately in cases where the argument of the logarithm is close to 1. However, if $\gamma_0 + \delta_1 \xi_1 + \delta_2 \xi_2$ changes sign within the region of integration, then the absolute value of the arguments of some of the inverse hyperbolic tangents may be greater than 1. In order to deal with these cases, we define

$$G(u, v) = \operatorname{arc\,tanh}\left(\frac{2uv}{u^2 + v^2}\right), \tag{8}$$

and use the fact that

$$G(u, v) = 2 \operatorname{arc\,tanh}(u/v) \quad \text{if} \quad u < v \tag{9a}$$

and

$$G(u, v) = 2 \operatorname{arc\,tanh}(v/u) \quad \text{if} \quad u > v. \tag{9b}$$

We then obtain the generally applicable formulae

$$\begin{aligned} P = {} & \frac{\gamma_0}{\delta_1 \delta_2} G(2\delta_1 \delta_2 \Delta_1 \Delta_2, \delta_1^2 \Delta_1^2 + \delta_2^2 \Delta_2^2 - \gamma_0^2) \\ & + \frac{\Delta_1}{\delta_2} G(2\gamma_0 \delta_2 \Delta_2, \gamma_0^2 - \delta_1^2 \Delta_1^2 + \delta_2^2 \Delta_2^2) \\ & + \frac{\Delta_2}{\delta_1} G(2\gamma_0 \delta_1 \Delta_1, \gamma_0^2 + \delta_1^2 \Delta_1^2 - \delta_2^2 \Delta_2^2) \end{aligned} \tag{10a}$$

and

$$\begin{aligned} Q_i = {} & \frac{\delta_i^2 \Delta_i^2 - \delta_{3-i}^2 \Delta_{3-i}^2 - \gamma_0^2}{2\delta_i^2 \delta_{3-i}} \\ & \times G(2\delta_i \delta_{3-i} \Delta_i \Delta_{3-i}, \delta_i^2 \Delta_i^2 + \delta_{3-i}^2 \Delta_{3-i}^2 - \gamma_0^2) \\ & - \frac{\gamma_0 \Delta_{3-i}}{\delta_i^2} G(2\gamma_0 \delta_i \Delta_i, \gamma_0^2 + \delta_i^2 \Delta_i^2 \\ & - \delta_{3-i}^2 \Delta_{3-i}^2) + \frac{2\Delta_i \Delta_{3-i}}{\delta_i} \end{aligned} \tag{10b}$$

for $i = 1, 2$. If $\delta_{3-i} = 0$, Eqs. (10) are reduced to the one-dimensional case,

$$P = \frac{2\Delta_{3-i}}{\delta_i} G(\gamma_0, \delta_i \Delta_i), \tag{11a}$$

$$Q_i = \frac{4\Delta_i \Delta_{3-i}}{\delta_i} - \frac{2\gamma_0 \Delta_{3-i}}{\delta_i^2} G(\gamma_0, \delta_i \Delta_i), \tag{11b}$$

$$Q_{3-i} = 0, \tag{11c}$$

and if $\delta_1 = \delta_2 = 0$,

$$P = \frac{4\Delta_1 \Delta_2}{\gamma_0}, \tag{12a}$$

$$Q_1 = Q_2 = 0. \tag{12b}$$

It should be noted that Eq. (4) cannot be computed numerically if γ is exactly zero at any grid point. Equations (5) can still be computed in that case, but not in the case when $\gamma \pm \delta_1 \Delta_1 \pm \delta_2 \Delta_2$ is exactly zero for any grid point, because that causes the absolute value of the argument of one of the inverse hyperbolic tangents to be exactly one. However, for a set of values of γ obtained by numerical computation, either of these cases is very unlikely to occur.

If $|u/v|$ is close to 1, it is better to compute $G(u, v)$ from the formula

$$G(u, v) = \ln\left|\frac{u + v}{u - v}\right|, \tag{13}$$

since in these cases it is less sensitive to rounding errors than Eq. (8).

3. NUMERICAL RESULTS

The improved accuracy obtainable from using Eqs. (5) rather than Eq. (4) is seen from the results shown in Table I. The values were computed for a 180° domain wall in an iron film of thickness 200 nm and correspond to case 1 in Table I of Ref. [4], in which the values of the relevant parameters and the method of computation of the magnetization configuration are given. A two-dimensional grid of $n_1 = 201$

TABLE I

Comparison of Values of $\varepsilon'_{\text{wall}}$ and S Calculated (a) Using Eq. (4) and (b) Using Eqs. (5), for Two Walls with Very Similar Structure and $\varepsilon_{\text{wall}}$

Wall	$\varepsilon_{\text{wall}}$	$\varepsilon'_{\text{wall}}$ (a)	S (a)	$\varepsilon'_{\text{wall}}$ (b)	S (b)
1	1.68243143	1.176	1.430	1.66765	1.00886
2	1.68243113	1.691	0.995	1.66755	1.00892

Note. Values of ε are energies per unit area in erg cm^{-2}.

and $n_2 = 40$ points parallel and perpendicular, respectively, to the surfaces of the film was used. The values of ε'_{wall} were computed from formulae [3] that include a term $C\gamma^{-1}\nabla^2\gamma$, where C is the exchange constant. Wall 2 was obtained from wall 1 by a slight rotation of the magnetization vectors (determined by interpolation), appropriate to a displacement of the wall by 0.05 nm, i.e., 0.01 of the distance between neighbouring grid points. It is seen that the change in the values of ε'_{wall} and S corresponding to a small displacement of the wall are much smaller when the relevant term is calculated using Eqs. (5), indicating that these values are much more accurate than those based on Eq. (4). A detailed check of the computations showed that the inaccuracy of values (a) was caused by grid points at which γ was close to 0.

It is concluded, therefore, that reliable values of the self-consistency parameter [1, 3] for magnetization configurations computed at a discrete set of points cannot be obtained by using a straightforward summation of terms. The improved method suggested in this paper has, however, been found to give reliable results in all cases.

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