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1998 J. Phys.: Condens. Matter 10 9495

(http://iopscience.iop.org/0953-8984/10/42/015)

J. Phys.: Condens. Matter **10** (1998) 9495–9505. Printed in the UK PII: S0953-8984(98)94549-0

Periodic walls in very thin films

Amikam Aharoni†

Department of Electronics, Weizmann Institute of Science, 76100 Rehovoth, Israel

Received 26 May 1998, in final form 6 August 1998

Abstract. Analytic formulae are given for the coefficients needed for computing the magnetostatic energy of a domain wall with a periodic magnetization structure, for the case of a film sufficiently thin that there is no dependence on the coordinate along the film thickness. A method is given for reducing the computational time of the magnetostatic energy, which can also be used in other wall computations carried out by the LaBonte method. Several typographical errors in the published coefficients for a magnetization structure with cylindrical symmetry in a sphere are corrected.

1. Introduction

There are three types of 180° domain wall in thin ferromagnetic films, among which the least understood is [1] the Néel wall. This wall is known to be observed in very thin films, but its structure is not known, or at least there has been no reliable computation for such a wall structure. In particular, none of the existing computations obeys [1] any self-consistency test, such as the one given in section 5 here.

A thin film may be taken as a plate which is infinite in both the x- and z-directions, and has a thickness $2b$ in the y-direction. For a certain range of values of b, two-dimensional computations of wall structures that depend on x and y but not on z are [1] very successful in all respects. For thinner films it is obvious that z must also be included [1], and computations become too difficult because a present-day computer cannot handle three-dimensional wall structures to the required accuracy. For still thinner films, some attempts to obtain results for one- and two-dimensional walls have totally failed, and have not even indicated where the correct answer should be looked for. There are some indications [1] that these walls have periodic variations along z, but it seems hopeless to try the full, three-dimensional computations, which do not quite work even for the cross-tie walls in somewhat thicker films.

The solution suggested here is computing a two-dimensional structure of a wall which depends on x and z but not on y. At least for sufficiently thin films, a y-dependence involves a large exchange energy. It is therefore likely to be fairly insignificant, and it is hoped that if there is a weak dependence on y, its effect will be negligible. This assumption makes all the difference, because a large body of experience has already accumulated in the computation of two-dimensional walls. The dependence on z must be periodic, if one wants to retain the assumption that the film is infinite in the z-direction. This periodicity does not make any difference for the other energy terms, but it complicates the calculation of the magnetostatic energy term somewhat, because magnetostatic interaction is a long-range

† E-mail: a.aharoni@ieee.org.

0953-8984/98/429495+11$19.50

force, and the summation converges very slowly. Still, certain periodic structures, such as stripe domains [2, 3], have been studied before. In the present case at any rate, this complication of the periodicity can be handled quite easily, as is seen in the following.

Analytic expressions are given in the next section for the coefficients needed for computing the magnetostatic energy in the LaBonte [4] method. There are some, such as Yan and Della Torre [5] or Chen *et al* [6], who prefer to compute such coefficients numerically by evaluating a multiple integral, since they have to be computed only once. I prefer formulae, whenever it is possible to derive them, which are not specific to one particular computer. Others can evaluate the coefficients from the same formulae in accordance with their particular preference of a subdivision size. An aid for convergence of the evaluation of the coefficients is then described in section 3. In section 4, a method is outlined for reducing the computational time, which can be helpful not only in this particular case, but also in all LaBonte-type computations. The self-consistency test, already used for other walls, is applied in section 5 to the present case of a periodic wall. Finally, I take this opportunity to list corrections to some typographical errors in the published [7] coefficients of the magnetostatic energy of a *sphere*.

2. Magnetostatic energy

This energy, which originates from the classical dipolar interactions among lattice sites, is the largest of all of the energy terms which play a role in the wall structure. As such, it is the term which determines most of the structural details of the wall, and hence it is important to compute it rigorously. All of the approximations ever tried [1] have proved to be unsatisfactory, and in fact only the LaBonte method, which is used here, is sufficiently accurate for the purpose.

A ferromagnetic plate is considered, which is infinite in the x- and z-directions and extends from $-b$ to $+b$ in the y-direction. The part where $|x| \leqslant a$ is assumed to be a wall, separating two domains which are magnetized along $\pm z$ at $x = \pm a$. It is also assumed that the magnetization vector

$$\boldsymbol{m} = \boldsymbol{M}/M_s \tag{1}$$

is independent of y, and that the wall is *periodic* in the z-direction, with a period $2c$—that is, that

$$\boldsymbol{m}(x, z) = \boldsymbol{m}(x, z + 2nc) \tag{2}$$

for any integral value of n. It should be noted that the 'classical', one-dimensional Néel wall is included as a particular case. If there is no energetic advantage to this periodicity, the energy minimization should converge to a structure with no z-dependence. For such a case, there is no meaning to c, which can be any number, but this ambiguity cannot affect a minimization process which starts with a pre-assigned value of c. If a z-dependence does emerge, the value of c should be adjusted so that the lowest energy minimum is obtained.

The basic approach is that of LaBonte [4], which is somewhat modified for the present problem. The wall is subdivided into N_x cells in the x-direction, taking the Ith cell as covering the length

$$-a + 2a(I - 1)/N_x \leqslant x \leqslant -a + 2aI/N_x$$

for $I = 1, 2, \ldots, N_x$. In the z-direction, the *period* $2c$ is subdivided into N_z cells, designated by $J = 1, 2, \ldots, N_z$, where the Jth cell covers the length

$$-c + 2c(J - 1)/N_z \leqslant z \leqslant -c + 2cJ/N_z.$$

These cells are squares if and only if $aN_z = cN_x$, but there is no advantage to the use of this particular case, and it can be assumed that N_x and N_z are chosen independently of each other for any particular study. As is usually the case in such calculations, the magnetization unit vector $\boldsymbol{m}$ is assumed to be a constant in each of these cells. Its value in the (I, J) cell is written as the vector $\boldsymbol{m}(I, J)$.

There is no particular difficulty with the other wall energy terms. The magnetostatic energy per unit wall area per cycle, after one has carried out all of the integrations analytically, has the general form

$$\gamma_{\mathrm{M}} = M_s^2 \sum_{I=1}^{N_x} \sum_{J=1}^{N_z} \sum_{I'=1}^{N_x} \sum_{J'=1}^{N_z} \{A(I, J, I', J') m_x(I, J) m_x(I', J') + B(I, J, I', J') m_y(I, J) m_y(I', J') + C(I, J, I', J') m_z(I, J) m_z(I', J') + D(I, J, I', J')[m_x(I, J) m_z(I', J') + m_z(I, J) m_x(I', J')]\}. \quad (3)$$

Here, the combination of the two terms multiplying D is *not* an assumption. It is the result of calculating each of the two terms separately, and therefore implies

$$D(I, J, I', J') = D(I', J', I, J). \quad (4)$$

Another result from the actual integrations is

$$A(I, J, I', J') + B(I, J, I', J') + C(I, J, I', J') = 0. \quad (5)$$

No physical interpretation can be given for this relation, which is just a mathematical result.

Equation (5) shows that there are only three sets of coefficients, A, B and D, which still need to be specified. It should be noted that these coefficients actually depend only on the distances between each subdivision and the others. Therefore, they depend on the four parameters, I, J, I' and J' only through their differences, $K = I - I'$ and $L = J - J'$, as can be seen from the specific expressions which are given in the following.

If $\mathcal{F}$ denotes one of the sets of coefficients, A, B or D, I have proved that it can be written as the combination

$$\mathcal{F}(I, J, I', J') = 2\overline{\mathcal{F}}(I - I', J, J') - \overline{\mathcal{F}}(I - I' + 1, J, J') - \overline{\mathcal{F}}(I - I' - 1, J, J') \quad (6)$$

and

$$\overline{\mathcal{F}}(K, J, J') = 2\hat{\mathcal{F}}(K, J - J') - \hat{\mathcal{F}}(K, J - J' + 1) - \hat{\mathcal{F}}(K, J - J' - 1) \quad (7)$$

for certain functions $\hat{A}$, $\hat{B}$ and $\hat{D}$. There is some overlap of the functions in $\hat{A}$ and $\hat{B}$, which makes it more convenient to express them as

$$\hat{A}(K, L) = -F_1(K, L) + F_2(K, L) + F_4(K, L) + F_5(K, L) \quad (8)$$

$$\hat{B}(K, L) = -F_2(K, L) - F_3(K, L) + F_4(K, L) + F_6(K, L) \quad (9)$$

where

$$F_1(K, L) = \frac{1}{2} \sum_{n=-\infty}^{\infty} \left(\frac{P}{c} - c\Lambda^2\right) \ln\left(\frac{\sqrt{G} - b}{\sqrt{G} + b}\right) \quad (10)$$

$$F_2(K, L) = \sum_{n=-\infty}^{\infty} \Lambda \left[\left(\frac{P}{b} - b\right) \ln(\sqrt{G} + c\Lambda) - \frac{P}{b} \ln(\sqrt{Q} + c\Lambda)\right] \quad (11)$$

$$F_3(K, L) = \frac{aK}{N_x} \sum_{n=-\infty}^{\infty} \left[\left(\frac{c}{b}\Lambda^2 - \frac{b}{c}\right) \ln\left(\sqrt{G} + \frac{aK}{N_x}\right) - \frac{c}{b}\Lambda^2 \ln\left(\sqrt{Q} + \frac{aK}{N_x}\right)\right] \quad (12)$$

$$F_4(K,L)=\frac{1}{3bc}\sum_{n=-\infty}^{\infty}(G^{3/2}-Q^{3/2}) \tag{13}$$

$$F_5(K,L)=\frac{aK}{N_x}\sum_{n=-\infty}^{\infty}\left[2\Lambda\arctan\left(\frac{bcN_x\Lambda}{aK\sqrt{G}}\right)+\frac{aK}{bcN_x}(\sqrt{Q}-\sqrt{G})\right] \tag{14}$$

and

$$F_6(K,L)=\sum_{n=-\infty}^{\infty}\left[\frac{2aK}{N_x}\Lambda\arctan\left(\frac{acK\Lambda}{bN_x\sqrt{G}}\right)-\frac{b}{c}\sqrt{G}\right]. \tag{15}$$

Here

$$\Lambda=\frac{L}{N_z}-n \qquad P=\left(\frac{aK}{N_x}\right)^2 \qquad Q=c^2\Lambda^2+P \qquad \text{and} \qquad G=Q+b^2. \tag{16}$$

The other function, $\hat{D}$, also has some terms which are the same as, or very similar to, certain terms in the previous functions. However, it does not seem worthwhile to separate them, and therefore they are all put together here as

$$\begin{aligned}\hat{D}(K,L)=\sum_{n=-\infty}^{\infty}\Bigg\{&\frac{aK}{N_x}\left[\Lambda\ln\left(\frac{\sqrt{G}-b}{\sqrt{G}+b}\right)+\frac{1}{3bc}(P-3b^2)\ln(\sqrt{G}+c\Lambda)-\frac{P}{3bc}\right.\\&\times\left.\ln(\sqrt{Q}+c\Lambda)+\frac{2\Lambda}{3b}(\sqrt{G}-\sqrt{Q})\right]+\left(c\Lambda^2-\frac{P}{c}\right)\arctan\left(\frac{abK}{N_xc\Lambda\sqrt{G}}\right)\\&+\frac{1}{c}\left(\frac{b^2}{3}-P\right)\arctan\left(\frac{acK\Lambda}{N_xb\sqrt{G}}\right)+\Lambda\left(\frac{c^2}{3b}\Lambda^2-b\right)\ln\left(\sqrt{G}+\frac{aK}{N_x}\right)\\&-\frac{c^2}{3b}\Lambda^3\ln\left(\sqrt{Q}+\frac{aK}{N_x}\right)\Bigg\}.\end{aligned} \tag{17}$$

In the limit of small b it may be sufficient to consider only the first-order terms in power-series expansions of these expressions. This is not likely to be adequate for many problems, but this first-order approximation is given here anyway:

$$\hat{A}(K,L)=b\sum_{n=-\infty}^{\infty}\left[\frac{\sqrt{Q}}{c}-\Lambda\ln(\sqrt{Q}+c\Lambda)\right]+\mathrm{O}(b^3) \tag{18}$$

$$\hat{B}(K,L)=b\sum_{n=-\infty}^{\infty}\left[\Lambda\ln(\sqrt{Q}+c\Lambda)+\frac{aK}{cN_x}\ln\left(\sqrt{Q}+\frac{aK}{N_x}\right)-\frac{2}{c}\sqrt{Q}\right]+\mathrm{O}(b^3) \tag{19}$$

$$\hat{D}(K,L)=-b\sum_{n=-\infty}^{\infty}\left[\Lambda\ln\left(\sqrt{Q}+\frac{aK}{N_x}\right)+\frac{aK}{cN_x}\ln(\sqrt{Q}+c\Lambda)\right]+\mathrm{O}(b^3). \tag{20}$$

Most of the terms in equation (17) are odd functions of K. As such they vanish for the particular cases in which K is either 0 or ±1, as is the case for $I=I'$. In all of the other terms, the contribution of $K=0$ cancels that of $K\pm1$. It is thus easy to see that

$$D(I,J,I,J')=0. \tag{21}$$

There is no simple relation for the case where $I=I'$ for the other coefficients. LaBonte [4], however, found it more convenient for the minimization process to separate the 'self'-terms, with $(I,J)=(I',J')$, from the 'interaction' terms, with $(I,J)\neq(I',J')$. In some ways it is an artificial and arbitrary separation, because there is no fundamental difference between the two classes. Nevertheless, it is a convenient separation, and is therefore adopted here too, and separate expressions are given for the special case where $(I,J)=(I',J')$.

In this case, the summation of the various terms in equations (6) and (7) can be performed analytically, thus giving A and B explicitly. Specifically, using the notations

$$\begin{aligned} n_1 &= n + \frac{1}{N_z} & P_1 &= \left(\frac{a}{N_x}\right)^2 \\ Q_0 &= P_1 + c^2n^2 & Q_1 &= P_1 + c^2n_1^2 \\ G_0 &= b^2 + c^2n^2 & G_1 &= b^2 + c^2n_1^2 \\ G_2 &= G_0 + P_1 & G_3 &= G_1 + P_1 \end{aligned} \tag{22}$$

it is possible to write

$$A(I, J, I, J) = -F_1^{(n)} + F_2^{(n)} + F_4^{(n)} + F_5^{(n)} \tag{23}$$

$$B(I, J, I, J) = -F_2^{(n)} - F_3^{(n)} + F_4^{(n)} + F_6^{(n)} \tag{24}$$

with

$$F_1^{(n)} = 4c\sum_{n=1}^{\infty} n^2 \ln\left(\frac{\sqrt{G_0}+b}{\sqrt{G_0}-b}\right) - 2c\sum_{n=-\infty}^{\infty} n_1^2 \ln\left(\frac{\sqrt{G_1}+b}{\sqrt{G_1}-b}\right) + 2\sum_{n=-\infty}^{\infty}\left[\left(\frac{P_1}{c} - cn^2\right)\ln\left(\frac{\sqrt{G_2}+b}{\sqrt{G_2}-b}\right) - \left(\frac{P_1}{c} - cn_1^2\right)\ln\left(\frac{\sqrt{G_3}+b}{\sqrt{G_3}-b}\right)\right] \tag{25}$$

$$F_2^{(n)} = 4\sum_{n=-\infty}^{\infty}\left\{n\left[\frac{P_1}{b}\ln(\sqrt{Q_0}+cn) - b\ln(\sqrt{G_0}+cn) + \left(b - \frac{P_1}{b}\right) \times \ln(\sqrt{G_2}+cn)\right] + n_1\left[b\ln(\sqrt{G_1}+cn_1) + \left(\frac{P_1}{b} - b\right)\ln(\sqrt{G_3}+cn_1) - \frac{P_1}{b}\ln(\sqrt{Q_1}+cn_1)\right]\right\} \tag{26}$$

$$F_3^{(n)} = \frac{2a}{N_x}\sum_{n=-\infty}^{\infty}\left[\left(\frac{b}{c} - \frac{cn^2}{b}\right)\ln\left(\frac{\sqrt{G_2}+a/N_x}{\sqrt{G_2}-a/N_x}\right) + \frac{cn^2}{b}\ln\left(\frac{\sqrt{Q_0}+a/N_x}{\sqrt{Q_0}-a/N_x}\right) + \left(\frac{cn_1^2}{b} - \frac{b}{c}\right)\ln\left(\frac{\sqrt{G_3}+a/N_x}{\sqrt{G_3}-a/N_x}\right) - \frac{cn_1^2}{b}\ln\left(\frac{\sqrt{Q_1}+a/N_x}{\sqrt{Q_1}-a/N_x}\right)\right] \tag{27}$$

$$F_4^{(n)} = \frac{4}{3bc}\sum_{n=-\infty}^{\infty}\left[G_3^{3/2} - G_2^{3/2} - G_1^{3/2} + G_0^{3/2} - Q_1^{3/2} + Q_0^{3/2} + c^3(|n_1|^3 - |n|^3)\right] \tag{28}$$

$$F_5^{(n)} = \frac{4a}{N_x}\sum_{n=-\infty}^{\infty}\left[\frac{a}{bcN_x}(\sqrt{G_2} - \sqrt{G_3} + \sqrt{Q_1} - \sqrt{Q_0}) - 2n\arctan\left(\frac{bcN_xn}{a\sqrt{G_2}}\right) + 2n_1\arctan\left(\frac{bcN_xn_1}{a\sqrt{G_3}}\right)\right] \tag{29}$$

$$F_6^{(n)} = \sum_{n=-\infty}^{\infty}\left\{\frac{4b}{c}(\sqrt{G_2} - \sqrt{G_3} + \sqrt{G_1} - \sqrt{G_0}) + \frac{8a}{N_x}\left[n_1\arctan\left(\frac{acn_1}{bN_x\sqrt{G_3}}\right) - n\arctan\left(\frac{acn}{bN_x\sqrt{G_2}}\right)\right]\right\}. \tag{30}$$

These terms, and therefore A and B as well, do not depend on the values of I and J. This result is as expected, because there can be no difference between one prism and another when it is taken as a separate entity, without the interaction with other prisms. Unlike the case studied by LaBonte [4], the ‘self’-terms here contain a summation over n, because the case where $I = I'$, $J = J'$ does not lead to a single cell. It leads to the basic unit, which is the set of all of the cells with the same (I, J), separated by the periodic length $2c$, including the interactions among them. The actual terms for the isolated cell, as in the ‘self’-terms of [4], are those with $n = 0$ in equations (23) to (30). These terms, however, only lead to the demagnetizing factors of the unit prism, with the dimensions $2a/N_x \times 2b \times 2c/N_z$, which have no particular application to the present problem. The demagnetizing factors of the general prism have already been published [8], and it does not seem necessary to list them here.

3. Summation over n

All of the expressions in the previous section are rigorous, being calculated by analytic integration, with no approximations. It is clear, however, that the magnetostatic coefficients cannot be computed from these expressions, as written, to any reasonable accuracy, because large computational errors will be encountered for large values of n. Therefore, the summation over n is replaced by an integration over n above a certain value, N_p:

$$F_i(K, L) = \sum_{n=-\infty}^{\infty} \mathcal{G}_i(n) = \sum_{n=-(N_p-1)}^{N_p-1} \mathcal{G}_i(n) + \left[\int_{-\infty}^{-N_p} + \int_{N_p}^{\infty}\right] \mathcal{G}_i(n)\ \mathrm{d}n \tag{31}$$

where the $\mathcal{G}_i$ are the expressions in all of the foregoing definitions of F_i, and similarly for $\hat{D}$. After carrying out all of the integrations, the result is

$$F_i(K, L) = \sum_{n=-(N_p-1)}^{N_p-1} \mathcal{G}_i(n) + \sum_{m=\pm 1} m F_i^*(K, L, -mN_p) \tag{32}$$

and similarly for $\hat{A}$ etc. Since many of the terms occur in more than one of the F_i^*, computing them separately is wasteful. Therefore, the combinations according to equations (8) and (9) are written directly as

$$\begin{aligned}
\hat{A}^*(K, L, n) = {} & \frac{\Lambda}{2}\left(\frac{c}{3}\Lambda^2 - \frac{P}{c}\right) \ln\left(\frac{\sqrt{G} + b}{\sqrt{G} - b}\right) + \frac{\Lambda}{2b|\Lambda|}\Bigg\{P\left(\Lambda^2 - \frac{P}{4c^2}\right)\ln(\sqrt{Q} \\
& + c|\Lambda|) + \left[\Lambda^2(b^2 - P) - \frac{1}{4c^2}\left(\frac{b^4}{3} + 2b^2P - P^2\right)\right]\ln(\sqrt{G} + c|\Lambda|)\Bigg\} \\
& + \frac{aK}{N_x}\left[\left(\frac{P}{3c^2} - \Lambda^2\right)\arctan\left(\frac{bcN_x\Lambda}{aK\sqrt{G}}\right) + \left(\frac{L}{N_z}\right)^2 \frac{\Lambda}{|\Lambda|}\arctan\left(\frac{bN_x}{aK}\right)\right] \\
& + \frac{\Lambda}{4bc}\left[\frac{Q^{3/2} - G^{3/2}}{3} + \frac{5P}{2}(\sqrt{G} - \sqrt{Q}) - \frac{5b^2}{6}\sqrt{G}\right]
\end{aligned} \tag{33}$$

$$\begin{aligned}
\hat{B}^*(K, L, n) = {} & \frac{\Lambda}{2b|\Lambda|}\Bigg\{\left[(P - b^2)\Lambda^2 + \frac{1}{c^2}\left(\frac{b^4}{4} - \frac{b^2}{2}P - \frac{P^2}{12}\right)\right]\ln(\sqrt{G} + c|\Lambda|) \\
& + \left(\frac{P}{12c^2} - \Lambda^2\right)P\ln(\sqrt{Q} + c|\Lambda|)\Bigg\} + \frac{aK}{N_x}\Bigg\{\Lambda\left[\left(\frac{c\Lambda^2}{3b} - \frac{b}{c}\right)\ln\left(\sqrt{G}\right.\right. \\
& \left.\left. + \frac{aK}{N_x}\right) - \frac{c\Lambda^2}{3b}\ln\left(\sqrt{Q} + \frac{aK}{N_x}\right)\right] + \left(\frac{b^2}{3c^2} - \Lambda^2\right)\arctan\left(\frac{aKc\Lambda}{bN_x\sqrt{G}}\right) \\
& + \left(\frac{L}{N_z}\right)^2 \frac{\Lambda}{|\Lambda|}\arctan\left(\frac{aK}{bN_x}\right)\Bigg\} + \frac{\Lambda}{4bc}\Bigg[\frac{Q^{3/2} - G^{3/2}}{3} + \frac{5b^2}{2}\sqrt{G}
\end{aligned}$$

$$+\ \frac{5P}{6}(\sqrt{Q}-\sqrt{G})\bigg]. \tag{34}$$

The second arctangent in each of the equations (33) and (34) is an integration constant that makes the appropriate expression vanish at infinity. Similarly,

$$\begin{aligned}\hat{D}^{*}(K,L,n) &= \frac{aK}{2N_x}\left(\frac{P}{3c^2}-\Lambda^2\right)\ln\left(\frac{\sqrt{G}-b}{\sqrt{G}+b}\right)+\frac{aK|\Lambda|}{3bcN_x}(3b^2-P)\ln(\sqrt{G}+c|\Lambda|)\\ &\quad+\frac{|\Lambda|}{3bc}\left(\frac{aK}{N_x}\right)^3\ln(\sqrt{Q}+c|\Lambda|)-\left(\frac{b^3}{12c^2}-\frac{b\Lambda^2}{2}+\frac{c^2\Lambda^4}{12b}\right)\ln\left(\sqrt{G}\right.\\ &\quad\left.+\frac{aK}{N_x}\right)+\frac{c^2\Lambda^4}{12b}\ln\left(\sqrt{Q}+\frac{aK}{N_x}\right)-\frac{aK}{4N_xbc^2}(G^{3/2}-Q^{3/2})\\ &\quad+\frac{5}{12bc^2}\left(\frac{aK}{N_x}\right)^3(\sqrt{G}-\sqrt{Q})+\Lambda\left(\frac{P}{c}-\frac{c}{3}\Lambda^2\right)\arctan\left(\frac{abK}{c\Lambda N_x\sqrt{G}}\right)\\ &\quad+\frac{\Lambda}{c}\left(P-\frac{b^2}{3}\right)\arctan\left(\frac{aKc\Lambda}{bN_x\sqrt{G}}\right).\end{aligned} \tag{35}$$

As is the case with equation (21), it can be shown that this part of the total expression for D also vanishes for $I=I'$, whatever J and J' are.

After integration of equations (25)–(30) as in equation (31), and then substitution in equations (23) and (24), one obtains for the case where $(I,J)=(I',J')$

$$A^{(n)*}(I,J,I,J)=f_A(n)-f_A(n_1)-\frac{4an_1}{N_xN_z^2|n_1|}\arctan\left(\frac{bN_x}{a}\right) \tag{36}$$

and

$$B^{(n)*}(I,J,I,J)=f_B(n)-f_B(n_1)-\frac{4an_1}{N_xN_z^2|n_1|}\arctan\left(\frac{a}{bN_x}\right) \tag{37}$$

with

$$\begin{aligned}f_A(n) &= \frac{n}{b|n|}\left\{\left(2n^2-\frac{P_1}{2c^2}\right)P_1\ln(\sqrt{Q_0}+c|n|)-b^2\left(2n^2-\frac{b^2}{6c^2}\right)\ln(\sqrt{G_0}+c|n|)\right.\\ &\quad\left.+\left[2n^2(b^2-P_1)-\frac{1}{2c^2}\left(\frac{b^4}{3}+2b^2P_1-P_1^2\right)\right]\ln(\sqrt{G_2}+c|n|)\right\}\\ &\quad-\frac{2cn^3}{3}\ln\left(\frac{\sqrt{G_0}+b}{\sqrt{G_0}-b}\right)+2n\left(\frac{cn^2}{3}-\frac{P_1}{c}\right)\ln\left(\frac{\sqrt{G_2}+b}{\sqrt{G_2}-b}\right)\\ &\quad+\frac{4a}{N_x}\left(\frac{P_1}{3c^2}-n^2\right)\arctan\left(\frac{bcnN_x}{a\sqrt{G_2}}\right)+\frac{5nP_1}{2bc}(\sqrt{G_2}-\sqrt{Q_0})\\ &\quad+\frac{n}{3bc}\left[G_0^{3/2}-c^3|n|^3+Q_0^{3/2}-G_2^{3/2}+\frac{5b^2}{2}(\sqrt{G_0}-\sqrt{G_2})\right]\end{aligned} \tag{38}$$

and

$$\begin{aligned}f_B(n) &= \frac{n}{b|n|}\left\{\left(\frac{P_1}{6c^2}-2n^2\right)P_1\ln(\sqrt{Q_0}+c|n|)+b^2\left(2n^2-\frac{b^2}{2c^2}\right)\ln(\sqrt{G_0}+c|n|)\right.\\ &\quad\left.+\left[2n^2(P_1-b^2)+\frac{1}{2c^2}\left(b^4-2b^2P_1-\frac{P_1^2}{3}\right)\right]\ln(\sqrt{G_2}+c|n|)\right\}\\ &\quad+\frac{2a}{N_x}\left\{n\left[\left(\frac{cn^2}{3b}-\frac{b}{c}\right)\ln\left(\frac{\sqrt{G_2}+a/N_x}{\sqrt{G_2}-a/N_x}\right)-\frac{cn^2}{3b}\ln\left(\frac{\sqrt{Q_0}+a/N_x}{\sqrt{Q_0}-a/N_x}\right)\right]\right.\end{aligned}$$

$$+ 2\left(\frac{b^2}{3c^2} - n^2\right)\arctan\left(\frac{acn}{bN_x\sqrt{G_2}}\right)\Bigg\} + \frac{5bn}{2c}(\sqrt{G_2} - \sqrt{G_0})$$
$$+ \frac{n}{3bc}\left[G_0^{3/2} - c^3|n|^3 + Q_0^{3/2} - G_2^{3/2} + \frac{5P_1}{2}(\sqrt{Q_0} - \sqrt{G_2})\right]. \quad (39)$$

4. Saving computational time

It can be shown that the foregoing implies that

$$A(I, J, I', J') = A(I', J', I, J) \qquad \text{and} \qquad B(I, J, I', J') = B(I', J', I, J). \quad (40)$$

This relation is a direct result of the definition of A and B as interaction terms in equation (3), because the interaction of a and b is always the same as the interaction of b and a. Similar relations also hold for C and D, according to equations (4) and (5). These symmetry relations can be used to eliminate about half of the terms from the summations in equation (3), thus reducing the computational time required to obtain the magnetostatic energy in each iteration by about a factor of 2.

To do this, let each sum over I' in equation (3) be broken up into a sum of three terms, one for $I' < I$, one for $I' = I$ and one for $I' > I$. In the sum with $I' > I$, the *order* of the summation over I and I' is changed, together with interchanging of the *labels* $I \leftrightarrow I'$ and $J \leftrightarrow J'$. Using the symmetry relations, it is readily seen that this sum is the same as the one with $I' < I$. Using equations (5) and (21), and the notation

$$R(I, J, I', J') = \left[m_x(I, J)m_x(I', J') - m_z(I, J)m_z(I', J')\right]A(I, J, I', J') \quad (41)$$

$$S(I, J, I', J') = \left[m_y(I, J)m_y(I', J') - m_z(I, J)m_z(I', J')\right]B(I, J, I', J') \quad (42)$$

$$T(I, J, I', J') = \left[m_x(I, J)m_z(I', J') + m_z(I, J)m_x(I', J')\right]D(I, J, I', J') \quad (43)$$

the magnetostatic energy per unit wall area per cycle can be written as

$$\gamma_{\mathrm{M}} = M_s^2 \sum_{J=1}^{N_z} \sum_{J'=1}^{N_z} \Bigg\{ \sum_{I=1}^{N_x} \left[R(I, J, I, J') + S(I, J, I, J')\right]$$
$$+ 2\sum_{I=2}^{N_x} \sum_{I'=1}^{I-1} \left[R(I, J, I', J') + S(I, J, I', J') + T(I, J, I', J')\right]\Bigg\}. \quad (44)$$

The second summation over I starts from $I = 2$, because the sum over I' is empty for $I = 1$. The 'self'-terms of LaBonte [4] are part of the first line, but are not written separately here.

Obviously, this reduction of the number of terms in the four-times summation by a factor of 2 reduces the computational time by about the same factor. Moreover, this time saving is effectively by a factor of two in the total computational time, because almost all of the computer time is spent on computing the magnetostatic energy term in this kind of computation. It should be particularly emphasized that the reduction is not due to any assumption of symmetry in the wall structure. It is a mere manifestation of the general rule that an interaction of a with b is the same as an interaction of b with a, and need not be evaluated twice.

As a general rule it should not be too difficult to apply this to other cases of LaBonte-type computations, which are always very elaborate and time consuming. In particular, in the original two-dimensional wall computations, LaBonte [4] noted the same symmetry relations as are used here, but did not take the next step of eliminating superfluous terms from the summations. Equation (44) can be used for that case, and for other wall computations in the literature, in almost the same form in which it is written here, but this was for some reason not noticed. Researchers have tried to reduce the computational time by certain techniques, such as those described in [9], which are less powerful, less general and more difficult to apply than the present one. Others tried to simplify the computation of the magnetostatic energy term, which takes practically all of the computational time, by making various approximations, listed in [10] and in chapter 11 of [1]. Some still do this, but others realized later that these approximations were not good enough, and reverted to the full LaBonte method as in the case of [5] or, more recently, [11]. The present suggestion could have been more useful.

5. Self-consistency

It is very easy to make mistakes in programming numerical computations, and very difficult to find them. It is therefore necessary to build some tests and checks into any program. One such check, known as the self-consistency test, has been used [1] to eliminate incorrect wall structures. It is based on computing the total energy using two different formulae, which should yield the same results *if the computed structure is at a true energy minimum*. It is thus known that if the results are not nearly the same, there is something wrong with the energy minimization. Having such a self-consistent magnetization structure is only a necessary, and not a sufficient, condition for the computation to be correct, but the test always helps, and is a powerful tool that has already been used successfully.

In the case studied here, the total energy contains two other energy terms, besides the magnetostatic energy. One of them is the exchange energy, which originates from the quantum-mechanical interaction between neighbouring spins. In its classical form, and for the case of no y-dependence, this energy, per unit wall area per cycle, is

$$\gamma_{\mathrm{e}} = \frac{C}{4c} \int_{-c}^{c} \int_{-a}^{a} \left[(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2 \right] \mathrm{d}x \; \mathrm{d}z \tag{45}$$

where C is the exchange constant. The second term is the anisotropy energy, which originates from the spin–orbit interaction that couples the spins (namely, the direction of the magnetization) to certain preferred crystallographic directions. This energy, per unit wall area per cycle, when there is no y-dependence, can be written as

$$\gamma_{\mathrm{a}} = \frac{1}{2c} \int_{-c}^{c} \int_{-a}^{a} w_{\mathrm{a}} \; \mathrm{d}x \; \mathrm{d}z + \gamma_{\mathrm{s}} \tag{46}$$

where w_{a} is the anisotropy energy density and γ_{s} is a surface anisotropy term. There may be different forms for the latter, which need not be specified here. It should only be noted that it is essential to include such an energy term, even though previous studies of domain walls did not consider it. There is clear experimental evidence [12] that very thin films often have a high surface anisotropy.

The transformation of these energy terms, with or without adding an interaction with an applied field, is essentially the same as in [4], and need not be specified. Expressing the problem in terms of differential equations, and then integrating a linear combination of them is also the same as the procedure in section 8.4 of [1], and need not be repeated. That derivation did not specify any form for the surface energy term, but the surface energy does not enter the differential equations anyway and affects only the boundary conditions. It can thus be readily seen that if the magnetization is at an energy minimum, the total wall energy should also be equal to

$$\gamma'_{\text{wall}} = \frac{1}{4c}\int_{-c}^{c}\int_{-a}^{a}\left[2w_{\text{a}} - \boldsymbol{m}\cdot\frac{\partial w_{\text{a}}}{\partial \boldsymbol{m}} + \frac{1}{m_y}\left(\frac{\partial w_{\text{a}}}{\partial m_y} - C\,\nabla^2 m_y\right)\right]\mathrm{d}x\ \mathrm{d}z + \gamma_{\text{s}} + \gamma^*_{\text{M}} \tag{47}$$

where

$$\gamma^*_{\text{M}} = \frac{M_s}{8bc}\int_{-c}^{c}\int_{-b}^{b}\int_{-a}^{a}\frac{1}{m_y}\frac{\partial U}{\partial y}\ \mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z \tag{48}$$

and U is the magnetostatic scalar potential. The integrations are the same as some of those that enter the magnetostatic energy, leading to

$$\gamma^*_{\text{M}} = \frac{M_s^2}{4bc}\sum_{I=1}^{N_x}\sum_{I'=1}^{N_x}\sum_{J=1}^{N_z}\sum_{J'=1}^{N_z}\frac{m_y(I', J')}{m_y(I, J)}B(I, J, I', J') \tag{49}$$

with the same B as defined in the foregoing. The computation of the most difficult term in equation (47) is discussed in [13]. This equivalence of γ_{wall} and γ'_{wall} at an energy minimum can serve (as in previous cases) to check the self-consistency of the computations. If γ_{wall} and γ'_{wall} are not nearly the same, the solution is not near a minimum-energy state.

Another such check can be obtained from a different combination of the differential equations, and should be particularly useful for a case in which m_y turns out to be zero. It can be proved that at an energy minimum, γ_{wall} should *also* be equal to

$$\gamma''_{\text{wall}} = \frac{1}{4c}\int_{-c}^{c}\int_{-a}^{a}\left[2w_{\text{a}} - \boldsymbol{m}\cdot\frac{\partial w_{\text{a}}}{\partial \boldsymbol{m}} + \frac{1}{m_z}\left(\frac{\partial w_{\text{a}}}{\partial m_z} - C\,\nabla^2 m_z\right)\right]\mathrm{d}x\ \mathrm{d}z + \gamma_{\text{s}} + \gamma^{**}_{\text{M}} \tag{50}$$

with

$$\gamma^{**}_{\text{M}} = \frac{M_s^2}{4bc}\sum_{I=1}^{N_x}\sum_{I'=1}^{N_x}\sum_{J=1}^{N_z}\sum_{J'=1}^{N_z}\frac{D(I, J, I', J')m_x(I', J') + C(I, J, I', J')m_z(I', J')}{m_z(I, J)}. \tag{51}$$

Appendix A. The sphere

The coefficients of the magnetostatic energy of a sphere, under the constraint of cylindrical symmetry of the magnetization, were published in [7]. They were computed and used correctly in all of the computations which followed, but there are some errors in the *printed* formulae, which have never been pointed out. These errors are listed here in order to make it possible for others to use the correct coefficients.

(i) Equation (8) of [7] should be replaced by

$$M' = \frac{9}{2N_r^3}. \tag{A1}$$

(ii) Equation (16) of [7] should be replaced by

$$g_n(J, J') = \left[\frac{1}{(J-1)^{n-1}} - \frac{1}{J^{n-1}}\right][(J')^{n+2} - (J'-1)^{n+2}]. \tag{A2}$$

(iii) Equation (20) of [7] should be replaced by

$$Y(J) = \frac{1}{6}\left[(J-1)^3\ln\left(\frac{J}{J-1}\right) - J^2 + J - \frac{1}{3}\right]. \tag{A3}$$

(iv) $(n+2)^2$ should be replaced by $(n+2)^3$ in the denominators of both equation (12) and equation (15) of [7].

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