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Bose–Einstein integrals and domain morphology in ultrathin ferromagnetic films with perpendicular magnetization

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Abstract. We demonstrate how the stripe-domain configuration which is the most stable one in thin ferromagnetic films with perpendicular magnetization can be easily analysed in terms of Bose–Einstein integrals. Exact values for the equilibrium thickness of stripes as well as for the minimal free energy of the domain configuration in ultrathin samples are derived from little-known asymptotic expansions of the Bose–Einstein integrals. It is found that, due to an incidental cancellation, the lowest-order results for the stripe structure are exact also to the next order in the small parameter (the ratio of thickness to domain width). The minimization equation for the determination of the equilibrium quantities of interest is cast in a form that makes it applicable *analytically* to films which are not necessarily ultrathin and that allows one to control quantitatively the approximations made. The analytic solution, valid to a high order in the small ratio, is also given.

1. Introduction

Because of the significant practical implications, domain structure in thin and ultrathin ferromagnetic films has recently been the object of vigorous experimental and theoretical investigation [1, 2]. In principle, micromagnetism provides the tools, but not always the solution, for the analysis of possible domain patterns [3–5]. A special group of ever-increasing interest among these are arrays of domains with their magnetization perpendicular to the surface of the specimen (cf [6] and references therein).

Theoretical progress in describing perpendicular domain patterns exhibits an astonishing feature: only cases which seemed realistic from the contemporary technological point of view were examined. Kittel set up the magnetostatic framework in principle, but examined the energetics of a sample whose thickness T was much larger than the typical domain width D ($T/D \gg 1$), neglecting the dipolar interaction of the surface poles [7]. Rowlands [8] and, independently, Malek and Kambersky [9] solved the classic magnetostatic problem for the striped array. The latter authors examined also the case of thin films where thickness and domain width became comparable ($T/D \sim 1$) [9]. Kooy and Enz [10] solved the more general problem of striped perpendicular domain arrays with an external magnetic field applied perpendicular to the surface and taking account of the μ-effect [11]. Regular arrays of perpendicular domains in very thin and ultrathin films ($T/D \ll 1$) have been examined in sufficient detail only recently as the reproducible tailoring of structural and magnetic properties of ultrathin ferromagnetic films responded to increased practical interest. The analysis of Yafet and Gyorgy showed that the striped pattern is of lower overall energy

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than the checkerboard one [12], while Kaplan and Gehring confirmed this conclusion by involved numerical analysis [13] and settled an apparent contradiction with the results of Czech and Villain [14] for the energetics of domain arrays in Ising-like ferromagnetic films.

2. The model and its relation to Bose–Einstein (BE) integrals

Given a regular array of stripe domains of perpendicular magnetization in zero applied field and assuming that the thickness of the domain walls is negligible compared against D, the magnetostatic solution for the total energy of the pattern is given by the expression [8, 9, 13]:

$$E_{tot} = E_{wall} + E_{dip} \tag{1}$$

where the domain wall contribution is

$$E_{wall} = \gamma x \tag{2}$$

while the dipolar (self-energy) contribution is given by

$$E_{dip} = E_0 \bar{S}(x). \tag{3}$$

The notation is chosen to facilitate further manipulations: $\gamma = \sigma_w/\pi$ with σ_w being the domain wall energy density per unit area; $E_0 = 2\pi T M_s^2$ with M_s denoting the spontaneous magnetization; and

$$x \equiv \pi \frac{T}{D} \tag{4}$$

while

$$\bar{S}(x) \equiv S(x) \Big/ \left[\frac{3}{4}\zeta(2)\right] \tag{5}$$

is a normalized quantity with the zeta-function $\zeta(2) = \pi^2/6$ and

$$S(x) \equiv \frac{1}{x} \sum_{k=0}^{\infty} \frac{1 - \mathrm{e}^{-(2k+1)x}}{(2k+1)^3}. \tag{6}$$

The energy $E_0 = \lim_{x\to 0} E_{dip}$ is the energy of the homogeneously perpendicularly magnetized film in the ultrathin limit ($T \to 0$). In the opposite limit $x \to \infty$ ($T \to \infty$), the self-energy is negligible.

The deceptively simple sum $S(x)$ poses difficulties in the limit $x \to 0$. The nature of these difficulties is best revealed by exposing the connection of the quantity $S(x)$ to the BE integrals which has obviously escaped attention: one completes the sum in equation (6) to run over *all* positive integers by adding and subtracting the corresponding sum over *even* positive integers. The generic quantity which arises in the process is

$$\sigma(x) = \sum_{n=1}^{\infty} \frac{\mathrm{e}^{-nx}}{n^3} \tag{7}$$

and, by applying Wheelon's summation technique [15] or by simply recalling known results from applications of BE statistics [16, 17], one finds that

$$\sigma(x) = \mathcal{B}_2(-x) \qquad (x > 0) \tag{8}$$

and, consequently,

$$S(x) = \frac{1}{x}\left\{\frac{1}{8}\left[\mathcal{B}_2(-2x) - \mathcal{B}_2(0)\right] - \left[\mathcal{B}_2(-x) - \mathcal{B}_2(0)\right]\right\} \tag{9}$$

where we have taken up Dingle's definition for the BE integrals of integer order p [18]:

$$\mathcal{B}_p(\mu) = \frac{1}{p!}\int_0^\infty \frac{\mathrm{d}u\ u^p}{\mathrm{e}^{u-\mu}-1}. \tag{10}$$

Note that $\mathcal{B}_p(0) = \zeta(p+1)$.

Obviously, we have now expressed E_{tot} in terms of BE integrals. Moreover, by virtue of

$$\mathcal{B}'_p(\mu) = \mathcal{B}_{p-1}(\mu) \tag{11}$$

the minimization condition $\partial E_{tot}/\partial x = 0$ for the determination of the equilibrium value of the domain width at fixed film thickness T is also compactly expressed in terms of $\mathcal{B}_2$ and $\mathcal{B}_1$:

$$\pi^2\frac{\gamma}{E_0}x^2 + \left[8\mathcal{B}_1(-x) - 2\mathcal{B}_1(-2x)\right]x + \left[8\mathcal{B}_2(-x) - \mathcal{B}_2(-2x) - 7B_2(0)\right] = 0. \tag{12}$$

3. Analysis by implementing the asymptotics for BE integrals

The reason for which one should be pleased to have expressed the domain morphology problem in terms of BE integrals is that the asymptotic expansion of $\mathcal{B}_p$ for $|x| < 2\pi$ was found a long time ago (cf [18] and references therein), the driving force in the development being mathematical curiosity as well as the application to the (nowadays renewedly celebrated) phenomenon of BE condensation.

Following from [18],

$$\mathcal{B}_p(x) = \sum_{k=0\,(k\neq p)}^{\infty}\zeta(p+1-k)\frac{x^k}{k!} - \left[\ln|x| - \psi(p+1) + \psi(1)\right]\frac{x^p}{p!}. \tag{13}$$

Here, $\psi(z) = \mathrm{d}\ln\Gamma(z+1)/\mathrm{d}z$ is the digamma function [19]. This expansion is valid for $|x| < 2\pi$, i.e. for $T/D < 2$. The immediate consequence is that the results which follow apply not only in the ultrathin limit.

We specify the expansion for $p = 2$, whereby we use the known relations

$$\zeta(-2n) = 0 \qquad (n = 1, 2, \ldots) \tag{14}$$

$$\zeta(1-2n) = -B_{2n}/2n \qquad (n = 1, 2, \ldots) \tag{15}$$

where B_{2n} are the Bernoulli numbers. The result now reads

$$\mathcal{B}_2(x) = \zeta(3) + \zeta(2)x + \frac{1}{6}\zeta(0)x^3 + \frac{1}{2}\left(\frac{3}{2} - \ln|x|\right)x^2 - \sum_{n=1}^{\infty}\frac{B_{2n}}{2n}\frac{x^{2n+2}}{(2n+2)!}. \tag{16}$$

Use was made of $\psi(3) - \psi(1) = 3/2$; besides, $\zeta(0) = -1/2$. Substituting in equations (1) and (9) and rearranging terms, one finds the expansion of the total energy of the stripe configuration in the form:

$$E_{tot} = \gamma x + \frac{E_0}{\frac{3}{4}\zeta(2)}\left[\frac{3}{4}\zeta(2) + \frac{1}{4}\left(\ln\frac{|x|}{2} - \frac{3}{2}\right)x - \sum_{n=1}^{\infty}(2^{2n-1}-1)\frac{B_{2n}}{2n}\frac{x^{2n+1}}{(2n+2)!}\right] \tag{17}$$

($|x| < 2\pi$). The terms within the brackets which are not included in the infinite sum have recently been derived by Rowlands in a spectacularly simple way [20].

The dipolar contribution E_{dip} which is given by the second term exhibits an interesting and useful feature. There are no terms of even powers in x. The absence of an $\mathrm{O}(x^2)$-term is due to an *incidental cancellation* at the intermediate stages which is specific to the domain problem in question, while the higher-even-order terms are *systematically absent*. Thus, if the minimization is carried out to a given order, $O(x^{2k+1}, x\ln x)$, the result is automatically correct to one order higher. The condition for the extremum of E_{tot}, derived either via term-by-term differentiation of $E_{tot}(x)$ or from equation (12) combined with equation (13), now takes the form

$$\ln\left(\frac{x}{2}\right) = -3\zeta(2)\frac{\gamma}{E_0} + \frac{1}{2} + \sum_{n=1}^{\infty}(2^{2n-1}-1)\frac{B_{2n}}{n(n+1)}\frac{x^{2n}}{(2n)!}. \tag{18}$$

The lowest-order solution for the equilibrium value $x_0 = \pi T/D_0$ is now found by neglecting the sum on the r.h.s. of the last equation. Thus,

$$x_0 = 2\sqrt{\mathrm{e}}\,\mathrm{e}^{-3\zeta(2)\gamma/E_0} \tag{19}$$

and, consequently,

$$E_{tot}^{min} = E_{tot}(x = x_0) = E_0\left(1 - \frac{1}{3\zeta(2)}x_0\right) = E_0\left(1 - \frac{4\sqrt{\mathrm{e}}}{\pi^2}\mathrm{e}^{-(\pi/2)\sigma_w/E_0}\right). \tag{20}$$

For a given thickness T, the equilibrium domain width D_0 is

$$D_0(T) = \frac{\pi}{2\sqrt{\mathrm{e}}}T\mathrm{e}^{\sigma_w/4M_s^2T}. \tag{21}$$

The *exact* asymptotic coefficients which multiply the exponentials in equations (**??**) and (**??**) can be compared with the numerical results of [13] and one finds that the latter have been determined sufficiently accurately. Below, we give in the first column the exact values and in the second column those of [13] for the numerical coefficients in equations (20) and (21):

$$\frac{4\sqrt{\mathrm{e}}}{\pi^2} = 0.668\,201\,5624 \qquad 0.667 \tag{22}$$

$$\frac{\pi}{2\sqrt{\mathrm{e}}} = 0.952\,736\,1325 \qquad 0.955. \tag{23}$$

The insight that the lowest-order results are in fact valid to $O(x^2)$ in E_{dip} means, in particular, that the formulae derived above are valid under significantly more relaxed experimental conditions; hence, one may use them to address stripe patterns not only in ultrathin films.

In a method of systematic improvement, we now derive the results valid to $O(x^4)$ in the expansion for $E_{dip}(x)$. To this end, one keeps the term of $O(x^2)$ in equation (**??**):

$$\ln\left(\frac{x}{2}\right) = -3\zeta(2)\frac{\gamma}{E_0} + \frac{1}{2} + \frac{1}{24}x^2. \tag{24}$$

This is seemingly a transcendental equation which can, however, be solved exactly for high x by using the 'trick' $\frac{1}{24}x^2 = \ln\left(1 + \frac{1}{24}x^2\right) + O(x^4)$. Hence,

$$\ln\frac{x}{2(1+\frac{1}{24})x^2} = -3\zeta(2)\frac{\gamma}{E_0} + \frac{1}{2} \tag{25}$$

and, upon exponentiating, one finds that

$$\frac{x}{1+\frac{1}{24}x^2} = x_0 \tag{26}$$

with x_0 supplied by the lowest-order solution (equation (**??**)). Thus, the equilibrium values which will now be denoted by a subscript '1' and which are valid to $O(x^4)$ in the dipolar self-energy are given by

$$x_1 = \frac{12}{x_0}\left(1 - \sqrt{1 - x_0^2/6}\right) \approx x_0\left(1 + \frac{1}{24}x_0^2\right) \tag{27}$$

$$D_1 = \frac{\pi}{12}T\frac{x_0}{1 - \sqrt{1 - x_0^2/6}} \approx D_0(T)\left(1 - \frac{\pi^2}{24}\left(\frac{T}{D_0(T)}\right)^2\right) \tag{28}$$

$$E_{tot,1} \approx E_0\left(1 - \frac{2}{\pi^2}x_0 - \frac{1}{36\pi^2}x_0^3\right). \tag{29}$$

The last terms in the equations for x_1, D_1, and $E_{tot,1}$ given above represent the exact corrections including $O(x^4)$ in E_{dip}. Hence, the expressions in equations (28)–(30) would prove practically exact even for ratios as high as $T/D \sim 0.1$. In any case, equation (**??**) allows one to control quantitatively the approximations which are being made.

4. Discussion

We have been able to analyse the energetics of the stripe-domain configuration for thin films with perpendicular magnetization by recognizing the possibility of expressing the problem in terms of the Bose–Einstein integrals of mathematical physics. Systematic use of the properties of these integrals and of their asymptotic expansion for small values of their argument makes possible the explicit derivation of the minimizing equation for the equilibrium value of the ratio of thickness T to domain period D. In the present context, the equation is applicable up to ratios $T/D < 2$. In the first nonnegligible approximation, we have derived the asymptotically exact expressions for E_{tot}^{min} and for $(T/D)^{min}$ which, for a given thickness of the film, lead to the corresponding expression for the equilibrium width of the domain pattern D. The same equilibrium quantities are computed to the second nonnegligible order in the said ratio and this is $O(x^4)$ for E_{dip}. Thus, ultrathin and thin films can be treated analytically on the same footing with any required degree of accuracy.

Provided that sufficient information is obtained experimentally or theoretically about the thickness dependence of the domain wall energy, the analytic advance described above can also be used as a starting point for the quantitative analyses of the maximal density of the domains in this configuration in very thin films and its temperature behaviour. This would certainly shed light on some aspects of the temperature- and thickness-driven reorientations of the magnetization in very thin ferromagnetic films [21, 22]. Besides this, the application of the proposed technique to cases with applied external magnetic fields seems very promising and is currently under consideration.

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