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Nucleation modes in ferromagnetic prolate spheroids

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Abstract. Magnetization reversal in a perfect ferromagnetic prolate spheroid, with no surface anisotropy, is known to start from nucleation either by coherent rotation (for small radii), or by the magnetization curling mode (above a certain size), but the possibility of a third mode has never been ruled out. It is rigorously proved here that there can be no third switching mode if the aspect ratio is not larger than 500:1, and even for larger ratios it may at most exist for a very limited size range.

1. Introduction

When a sufficiently large magnetic field is applied to a ferromagnetic *ellipsoid*, it becomes saturated, that is all of the spins are aligned along the direction of this field. Therefore, it is convenient to start the calculations of the hysteresis curve from this well-defined saturated state in a large field, from which the field is then reduced. Thus, the first step of the theory is to calculate the field at which some sort of deviation from the saturated state just starts, and this step is known [1] as the *nucleation problem*.

In the particular case of an ellipsoid of revolution, with the magnetic field applied parallel to its long axis, which is also an easy axis for the magnetocrystalline anisotropy, and when there is no surface anisotropy, the nucleation problem has been reduced to three possible eigenmodes. That is, it has been *proved* analytically [1] that out of the infinite number of possible modes, nucleation can at most take place in one of these three eigenmodes. One of them is known as the 'coherent rotation' mode, and another is called the 'magnetization curling' mode. The third one will be referred to here as the 'buckling mode', for lack of a better name, even though this name was originally used [1] to describe a certain configuration in an *infinite* cylinder only.

It has also been proved that the third, or buckling, mode is physically inaccessible for all oblate spheroids, *and* for prolate spheroids whose aspect ratio is less than 4.6:1 [1], leaving only the curling and the coherent rotation as possible reversal modes. For more elongated prolate spheroids, the question of which mode may take place remained essentially open, even though there were some indications [2] that the buckling *may* be ruled out. The problem of what might actually happen in more elongated ellipsoids remained dormant, but it has become more practical now, with some recent experiments [3–5] on very small, isolated ferromagnetic particles, which are also extremely elongated.

It is the purpose of the present paper to extend the proof of the non-existence of a third nucleation mode in a prolate spheroid to much larger aspect ratios than in [2]. The technique used here is similar to the one in [2], and uses a very powerful tool originally invented

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[6, 7] by Brown. It is based on calculating a rigorous *lower bound* to the magnetostatic energy, thus avoiding the highly complicated evaluation of its actual value. The present lower bound proves that nucleation by this buckling mode is more difficult than by curling or by coherent rotation, if the aspect ratio is less than about 500:1, which includes all prolate spheroids that may be made in practice. Even this limit is not essential, and a method is given here which allows a relatively easy extension to still larger aspect ratios, if it ever becomes necessary.

2. Nucleation

Consider a homogeneous, ferromagnetic prolate spheroid, whose semi-minor axis is R, and whose aspect ratio is m. Let a homogeneous magnetic field, $\boldsymbol{H}$, be applied parallel to the long ellipsoidal axis, which is taken as the z-axis in a system of cylindrical coordinates, r, z, and ϕ. It is assumed that this z is also an easy axis for the (volume) anisotropy, and that there is no surface anisotropy.

The basic definition of the nucleation process calls for applying first a field along $+z$, which is large enough to saturate the ellipsoid in that direction. This field is slowly reduced to zero, after which it is slowly increased along $-z$, until a nucleation field, H_{n}, is *first* encountered. The important point is that only the mode which has the least negative H_{n} can ever take place, because after reversal has already started at that field, the initial conditions of a saturated ellipsoid do not exist any more for modes with more negative nucleation fields.

The ϕ-dependence of any mode can be expressed as the Fourier expansion of the components of the magnetization vector, $\boldsymbol{M}$,

$$\begin{aligned} M_r &= M_s A_r(r,z)\cos(k\phi - \phi_k) \\ M_\phi &= M_s A_\phi(r,z)\sin(k\phi - \phi_k) \end{aligned} \tag{1}$$

where M_s is the saturation magnetization of the ferromagnetic material, k is an integer, and ϕ_k is a constant which depends on the value of k. It has been shown, however [8], that all the modes with $k \geqslant 2$ have more negative eigenvalues than the easiest one for $k = 0$, which is the curling mode. Therefore, the discussion here is limited to the case in which

$$k = 1 \tag{2}$$

for which it is more convenient [8] to replace the functions in (1) by the linear combinations

$$B_1(r,z) = A_r + A_\phi \qquad \text{and} \qquad B_2(r,z) = A_r - A_\phi. \tag{3}$$

The surface of the ellipsoid is taken as $\xi = \xi_0$ in the system of prolate spheroidal coordinates, ξ, η, ϕ, defined by

$$z = f\xi\eta \qquad \text{and} \qquad r = f\sqrt{(\xi^2-1)(1-\eta^2)} \tag{4a}$$

where f is half the distance between the foci. In this system, the semi-minor axis of the ellipsoid is

$$R = f\sqrt{\xi_0^2 - 1} \tag{4b}$$

and the semi-major axis is $f\xi_0$, making the aspect ratio

$$m = \frac{\xi_0}{\sqrt{\xi_0^2 - 1}}. \tag{4c}$$

In the following, the semi-minor axis, R, and the applied field, H, are expressed in terms the reduced quantities S and h respectively, defined as

$$S = RM_s\sqrt{\frac{2}{C}} \qquad \text{and} \qquad h = \frac{H}{2\pi M_s} + \frac{K_1}{M_s^2} - \frac{N_z}{2\pi} \tag{5}$$

where C is the exchange constant, K_1 is the coefficient of either uniaxial or cubic magnetocrystalline anisotropy, and N_z is the demagnetizing factor of the ellipsoid parallel to the z-axis. With this notation, the anisotropy energy, E_a, and the energy of the interaction with the applied field, E_H, at the *start* of any deviation from the saturated state, can be written as

$$\frac{4}{\pi Cf}(E_a + E_H) = \frac{\pi S^2 h}{\xi_0^2 - 1}\int_{-1}^{1}\int_{1}^{\xi_0}(\xi^2 - \eta^2)(B_1^2 + B_2^2)\,\mathrm{d}\xi\,\mathrm{d}\eta. \tag{6}$$

It should be noted that according to equation (5), this expression already contains the contribution of the demagnetizing field in the saturated state, before nucleation. Similarly, the exchange energy of the deviation from the saturated state can be written as

$$\frac{4E_{ex}}{\pi Cf} = \int_{-1}^{1}\int_{1}^{\xi_0}\left\{(\xi^2 - 1)\left[\left(\frac{\partial B_1}{\partial \xi}\right)^2 + \left(\frac{\partial B_2}{\partial \xi}\right)^2\right] + (1 - \eta^2)\left[\left(\frac{\partial B_1}{\partial \eta}\right)^2 + \left(\frac{\partial B_2}{\partial \eta}\right)^2\right] + \frac{4(\xi^2 - \eta^2)B_1^2}{(\xi^2 - 1)(1 - \eta^2)}\right\}\mathrm{d}\xi\,\mathrm{d}\eta. \tag{7}$$

To complete the expression for the total energy, it is still necessary to add the magnetostatic self-energy term to (6) and (7).

3. Magnetostatic energy

This energy term is much more difficult to calculate [9] than the other terms. For this reason, it is often neglected, even though neglecting it is hardly ever justified, because in most cases it is the *largest* energy term in a ferromagnet. Here it is not neglected, but its calculation is still avoided by underestimating it, namely replacing it with an expression which is known to be *smaller* than its real value. The point is that by using a smaller energy barrier for a certain mode, nucleation by that mode becomes *easier* than when the correct energy is calculated, thereby making its nucleation field more positive than it is for the correct mode. But the only mode which has a physical meaning is the one which has the largest (i.e. the least negative) eigenvalue. Therefore, if such a *lower bound* for the nucleation field of a certain mode A is proved to be more negative than the true value of another mode B, then the existence of mode A can be ruled out, because the true value of its nucleation field is certainly more negative than that of mode B.

The calculation of a lower bound for the magnetostatic energy of the buckling mode is based on a general theorem of Brown. He proved [6, 7] that the magnetostatic energy, E_m, of a magnetization distribution $\boldsymbol{M}(\boldsymbol{r})$, in a ferromagnetic body or bodies, always satisfies the inequality

$$E_m \geqslant \int \boldsymbol{M}\cdot\nabla U\,\mathrm{d}\tau - \frac{1}{8\pi}\int(\nabla U)^2\,\mathrm{d}\tau \tag{8}$$

where the first integral is over the ferromagnetic material, and the second one is over all space. The equals sign in (8) is valid if and only if U is identical to the correct magnetostatic potential for $\boldsymbol{M}(\boldsymbol{r})$.

In this theorem, U can be any arbitrary, continuous function of space, with the only constraints that it is regular at infinity, and that it has continuous first derivatives *inside* the ferromagnetic body (or bodies). Discontinuities of the derivative outside, or on the boundary of, the ferromagnetic material are allowed. In the present study, however, two other constraints are imposed. One is the obvious requirement that the function U has the ϕ-dependence of the buckling mode, as implied by equations (1) and (2), namely

$$U(r, z, \phi) = V(r, z)\cos(\phi - \phi_1). \tag{9}$$

The other is that this V is such that $\nabla^2 V = 0$ everywhere. In the prolate spheroidal coordinates, this requirement is

$$\left[\frac{\partial}{\partial\xi}(\xi^2 - 1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1 - \eta^2)\frac{\partial}{\partial\eta} - \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)}\right] V = 0. \tag{10}$$

This choice, already made in [2], is a matter of convenience. It allows analytic integration of the second term in equation (8).

Some particular solutions of equation (10) were used in [2], and a more general expression was already given in equation (38) there. After correcting the typographic error, that general solution for the inside of the ellipsoid can be written in the form

$$V = b_n\sqrt{(\xi^2 - 1)(1 - \eta^2)}\,\frac{\mathrm{d}P_n(\xi)}{\mathrm{d}\xi}\,\frac{\mathrm{d}P_n(\eta)}{\mathrm{d}\eta} \qquad \text{for } \xi \leqslant \xi_0. \tag{11a}$$

Here P_n is the Legendre polynomial of order n and b_n is a constant. At this stage, n is just an arbitrary integer. It will be determined later. Outside the ferromagnetic spheroid, the regularity at infinity is obtained by using the spherical harmonics of the second kind, Q_n, instead of P_n. Thus, the solution which passes continuously to (11*a*) at $\xi = \xi_0$ is

$$V = b_n\sqrt{(\xi^2 - 1)(1 - \eta^2)}\,\frac{P_n'(\eta)Q_n'(\xi)P_n'(\xi_0)}{Q_n'(\xi_0)} \qquad \text{for } \xi \geqslant \xi_0 \tag{11b}$$

where the prime denotes the derivative. It is readily seen by substitution and differentiations that this V satisfies the differential equation (10), as well as all of the continuity requirements of Brown's theorem. The only discontinuity is that of $\partial V/\partial\xi$, and only on the boundary, $\xi = \xi_0$. It should be particularly noted that any linear combination of such solutions, with different values of n, is also a solution, because the differential equation (10) is linear.

When all of these equations are substituted into (8), the integration over ϕ is obvious. After integrating by parts over ξ and η, and using the well-known relations

$$\int_{-1}^{1} P_n(\eta)P_k(\eta)\,\mathrm{d}\eta = \frac{2}{2n + 1}\delta_{k,n} \tag{12a}$$

where δ is the Kronecker symbol, and

$$(\xi^2 - 1)\left[P_n(\xi)Q_n'(\xi) - Q_n(\xi)P_n'(\xi)\right] = -1 \tag{12b}$$

the second term of (8) can be fully expressed in a closed form. The result is

$$\frac{4}{\pi C f}E_{\mathrm{m}} \geqslant W_{\mathrm{LB}} = \frac{2\pi S b_n}{\sqrt{\xi_0^2 - 1}}F_n(\xi_0) + \frac{2\pi n^2(n + 1)^2}{2n + 1}b_n^2\frac{P_n'(\xi_0)}{Q_n'(\xi_0)} \tag{13a}$$

where

$$F_n = \int_{-1}^{1}\int_{1}^{\xi_0}\left[g_n(\xi, \eta)B_1(\xi, \eta) + n^2(n + 1)G_n(\xi, \eta)B_2(\xi, \eta)\right]\,\mathrm{d}\xi\,\,\mathrm{d}\eta \tag{13b}$$

with

$$g_n(\xi,\eta) = (\xi^2-1)(1-\eta^2)\left[\xi P_n'(\eta)P_n''(\xi) - \eta P_n'(\xi)P_n''(\eta)\right] \quad (13c)$$

and

$$G_n(\xi,\eta) = \xi P_n(\xi)P_{n-1}(\eta) - \eta P_n(\eta)P_{n-1}(\xi). \quad (13d)$$

It should be noted that the term with b_n^2 in (13*a*) is negative, because normally $P_n'(\xi)$ is positive and $Q_n'(\xi)$ is negative. Therefore, b_n can be chosen so that it maximizes the lower bound, in order to get the best out of the chosen arbitrary U. The result is

$$W_{\mathrm{LB}} = 2c_n[F_n(\xi_0)]^2 \quad (14a)$$

where

$$c_n = -\frac{(2n+1)\pi S^2}{4n^2(n+1)^2(\xi_0^2-1)}\frac{Q_n'(\xi_0)}{P_n'(\xi_0)}. \quad (14b)$$

4. Energy minimization

Adding this *lower bound* (14*a*) for the magnetostatic energy to the other energy terms in (6) and (7), and then minimizing the sum for all possible functions B_1 and B_2, leads to the differential equations

$$\left[\nabla^2 - \frac{4(\xi^2-\eta^2)}{(\xi^2-1)(1-\eta^2)} - \frac{\pi S^2 h}{\xi_0^2-1}(\xi^2-\eta^2)\right]B_1 = 2c_nF_ng_n(\xi,\eta) \quad (15a)$$

and

$$\left[\nabla^2 - \frac{\pi S^2 h}{\xi_0^2-1}(\xi^2-\eta^2)\right]B_2 = 2c_nn^2(n+1)F_nG_n(\xi,\eta) \quad (15b)$$

where the two-dimensional Laplacian in the coordinates ξ and η is

$$\nabla^2 = \frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} \quad (15c)$$

and where g_n and G_n are defined in (13*c*) and (13*d*) respectively. It also leads to the boundary conditions

$$\left(\frac{\partial B_1}{\partial\xi}\right)_{\xi=\xi_0} = \left(\frac{\partial B_2}{\partial\xi}\right)_{\xi=\xi_0} = 0. \quad (15d)$$

Consider first the case in which $F_n = 0$, for which the differential equations (15*a*) and (15*b*) are homogeneous. In this case B_1 should vanish, because it has been proved [8] that *all* of the non-zero solutions of the homogeneous equation for B_1 have eigenvalues which are more negative than that of the curling mode. The solution of B_2 can be expanded in Legendre polynomials, and the most general solution of the homogeneous case can thus be written as

$$B_1 = 0 \qquad \text{and} \qquad B_2 = \sum_{k=0}^{\infty}\psi_k(\xi)P_k(\eta). \quad (16)$$

Substituting this solution in the homogeneous equations (15*a*) and (15*b*), and carrying out the differentiations with respect to η,

$$\sum_{k=0}^{\infty}P_k(\eta)\left[\frac{\mathrm{d}}{\mathrm{d}\xi}(\xi^2-1)\frac{\mathrm{d}}{\mathrm{d}\xi} - k(k+1) - \frac{\pi S^2 h}{\xi_0^2-1}(\xi^2-\eta^2)\right]\psi_k(\xi) = 0. \quad (17)$$

Let this equation be multiplied by $P_{k'}(\eta)$, for any arbitrary value of k', and then integrated over η, from -1 to 1. According to equation (12a), for every $k \geqslant 0$,

$$\left[\frac{\mathrm{d}}{\mathrm{d}\xi}(\xi^2-1)\ \frac{\mathrm{d}}{\mathrm{d}\xi} - k(k+1) - \frac{\pi S^2 h}{\xi_0^2-1}\xi^2\right]\psi_k(\xi) + \frac{\pi S^2 h}{\xi_0^2-1}\left[\frac{(k+1)(k+2)}{(2k+3)(2k+5)}\psi_{k+2}(\xi) + \frac{2k^2+2k-1}{(2k-1)(2k+3)}\psi_k(\xi) + \frac{k(k-1)}{(2k-1)(2k-3)}\psi_{k-2}(\xi)\right] = 0. \tag{18}$$

If $h \neq 0$ this relation is a recursion formula, which determines all ψ_k in terms of ψ_0 and ψ_1, using only differentiation and no integration. These functions are also restricted by the boundary condition

$$\frac{\mathrm{d}\psi_k(\xi_0)}{\mathrm{d}\xi_0} = 0 \tag{19}$$

which is obtained by substituting (16) in (15d).

Let equation (18) be multiplied by $P_k(\xi)$, and integrated over ξ from 1 to ξ_0. The term which contains derivatives of ψ_k is integrated by parts twice, using the boundary condition (19) and the differential equation of P_k. In the term which contains ξ^2, the recurrence relation of P_k is used twice. This equation then becomes

$$(\xi_0^2-1)\ \psi_k(\xi_0)\frac{\mathrm{d}P_k(\xi_0)}{\mathrm{d}\xi_0} = \frac{\pi S^2 h}{\xi_0^2-1}\int_1^{\xi_0}\left[\frac{k-1}{2k-1}\Psi_{k-1}(\xi) - \frac{k+1}{2k+3}\Psi_{k+1}(\xi)\right]\ \mathrm{d}\xi \tag{20}$$

where

$$\Psi_k(\xi) = (k+1)\left[\frac{P_{k+1}(\xi)\psi_{k-1}(\xi)}{2k-1} - \frac{P_{k-1}(\xi)\psi_{k+1}(\xi)}{2k+3}\right]. \tag{21}$$

This case, however, should also be consistent with the assumption that $F_n = 0$. Substituting (16) in (13b), the integrations over η can readily be carried out using (12a), if (13d) is first transformed by the recurrence relation of P_n to

$$G_n(\xi,\eta) = \frac{n+1}{2n+1}\left[P_{n+1}(\xi)P_{n-1}(\eta) - P_{n-1}(\xi)P_{n+1}(\eta)\right]. \tag{22}$$

One then obtains

$$\int_1^{\xi_0}\left[\frac{P_{n+1}(\xi)\psi_{n-1}(\xi)}{2n-1} - \frac{P_{n-1}(\xi)\psi_{n+1}(\xi)}{2n+3}\right]\ \mathrm{d}\xi = 0 = \int_1^{\xi_0}\Psi_n(\xi)\ \mathrm{d}\xi. \tag{23}$$

It should be noted that equation (20) applies to every value of the index k, while equation (23) is only valid for the particular value n. This n was used for the definition of the (arbitrary) potential in section 3, but without specifying its value there. It should also be noted that all of the equations here are linear, which implies that more than one value of n may be used, and that expressions with different values of n may be added together. In particular, if both a special value $n = \nu$ *and* $n = \nu + 2$ are taken together in the definition of the potential, equation (23) applies to both of them. For the particular case in which $k = \nu + 1$, the right-hand side of equation (20) vanishes, so $\psi_k(\xi_0) = 0$ for this k. But this result is not compatible with equation (19), because a solution of a second-order differential equation cannot be zero at the same point at which its derivative is zero, unless it is identically zero.

The conclusion is thus that there is no solution to the nucleation problem for the homogeneous case besides the curling mode, and in looking for any other mode it must be assumed that $F_n \neq 0$. It must be emphasized, though, that n is still an *arbitrary* integer. The above proof only requires that either $n+2$ or $n-2$ is *also* considered for every n, but it does not determine this n. In the previous study [2], a combination of *three* values of n was used, but two have just been shown to be sufficient.

5. The lower bound

For a non-zero F_n, it can be readily checked by substitution that

$$B_1 = -\frac{2c_n F_n(\xi_0^2 - 1)}{\pi S^2 h(\xi^2 - \eta^2)} g_n(\xi, \eta) \qquad \text{and} \qquad B_2 = -\frac{2c_n F_n n^2(n+1)(\xi_0^2 - 1)}{\pi S^2 h(\xi^2 - \eta^2)} G_n(\xi, \eta) \tag{24}$$

is a solution of the differential equations (15*a*) and (15*b*). But this particular solution does not satisfy the boundary conditions of (15*d*). Therefore, it is necessary to add to it a solution of the *homogeneous* equations to impose the boundary conditions. This addition can be done by means of series expansions of the form

$$B_1 = q_0 \left[\frac{g_n(\xi, \eta)}{\xi^2 - \eta^2} + q_1 \sum_{k=2}^{\infty} f_k^{(1)}(\eta^2)(\xi_0^2 - \xi^2)^k - q_2 \frac{\partial}{\partial \xi_0} \left(\frac{g_n(\xi_0, \eta)}{\xi_0^2 - \eta^2} \right) \right] \tag{25a}$$

and

$$B_2 = q_0 n^2(n+1) \left[\frac{G_n(\xi, \eta)}{\xi^2 - \eta^2} + q_1 \sum_{k=2}^{\infty} f_k^{(2)}(\eta^2)(\xi_0^2 - \xi^2)^k - q_3 \frac{\partial}{\partial \xi_0} \left(\frac{G_n(\xi_0, \eta)}{\xi_0^2 - \eta^2} \right) \right] \tag{25b}$$

where

$$q_0 = -\frac{2c_n F_n(\xi_0^2 - 1)}{\pi S^2 h} \qquad q_1 = \begin{cases} 1 & \text{for odd } n \\ \xi\eta & \text{for even } n \end{cases} \tag{25c}$$

and

$$q_2 = \frac{\xi^2 - \xi_0^2}{2\xi_0} \begin{cases} 1 & \text{for odd } n \\ \dfrac{\xi}{\xi_0} & \text{for even } n \end{cases} \qquad q_3 = \begin{cases} \dfrac{\xi^2 - \xi_0^2}{2\xi_0} & \text{for odd } n \\ \xi - \xi_0 & \text{for even } n. \end{cases} \tag{25d}$$

It obviously satisfies the boundary conditions.

If this solution is substituted in the differential equations (15*a*) and (15*b*), recurrence relations can be worked out for evaluating the coefficients $f_k^{(1)}$ and $f_k^{(2)}$ in terms of F_n. Then F_n has to be found which is consistent with the substitution of these B_1 and B_2 into (13*b*). However, all of this complicated calculation can be bypassed by a method which has already been used in [2]. In this method, equation (15*a*) is multiplied by $g_n(\xi, \eta)/(\xi^2 - \eta^2)$, and (15*b*) is multiplied by $n^2(n+1)G_n(\xi, \eta)/(\xi^2 - \eta^2)$, then these equations are added together, and the result is integrated over ξ from 1 to ξ_0, and over η from -1 to 1. It is seen that the terms which contain $S^2 h$ in the differential equations add up to an expression which is proportional to F_n, according to (13*b*). All of the other terms are also proportional to F_n, when (25*a*) and (25*b*) are used to substitute for B_1 and B_2 in this equation. The condition $F_n \neq 0$ allows a division of the equation by F_n, which is thus eliminated altogether. After obvious integrations by parts where derivatives with respect to ξ and η occur, and after substituting from (14*b*) and (25*c*), the resulting equation can be rearranged as a second-order algebraic equation in h,

$$\frac{h^2}{\Omega_1(\xi_0)} + 2h\Omega_2(\xi_0) - \frac{\Omega_3(\xi_0)}{\pi S^2} = 0 \tag{26}$$

with

$$\Omega_1(\xi) = -\frac{Q_n'(\xi)}{P_n'(\xi)} = \frac{Q_{n-1}(\xi) - Q_{n+1}(\xi)}{P_{n+1}(\xi) - P_{n-1}(\xi)} \tag{27}$$

$$\Omega_2(\xi_0) = \frac{2n+1}{4} \int_{-1}^{1} \int_{1}^{\xi_0} \left[\left(\frac{g_n(\xi, \eta)}{n(n+1)} \right)^2 + (nG_n(\xi, \eta))^2 \right] \frac{\mathrm{d}\xi \, \mathrm{d}\eta}{\xi^2 - \eta^2} \tag{28}$$

and

$$\Omega_3(\xi_0) = \frac{2n+1}{4}(\xi_0^2-1)^2 \frac{\partial}{\partial \xi_0} \int_{-1}^{1} \left[\left(\frac{g_n(\xi_0,\eta)}{n(n+1)(\xi_0^2-\eta^2)} \right)^2 + \left(\frac{nG_n(\xi_0,\eta)}{\xi_0^2-\eta^2} \right)^2 \right] \mathrm{d}\eta. \tag{29}$$

To complete the calculation, it is still necessary to carry out the integrations in these equations, but this part is left for the next section. It is first noted that the quadratic equation (26) already yields the required eigenvalue, without going through the details of the solution of the differential equations. According to this equation, a *lower bound* to the buckling nucleation field is

$$-h_{\mathrm{n}}^{(\mathrm{buck})} = \Omega_1(\xi_0) \left\{ \Omega_2(\xi_0) + \sqrt{[\Omega_2(\xi_0)]^2 + \Omega_3(\xi_0)/\left[\pi S^2 \Omega_1(\xi_0)\right]} \right\}. \tag{30}$$

This lower bound has to be compared with the nucleation field for the coherent rotation, which is [2]

$$-h_{\mathrm{n}}^{(\mathrm{rot})} = \xi_0 \left[\xi_0 - \frac{1}{2}(\xi_0^2-1) \ln \frac{\xi_0+1}{\xi_0-1} \right] \tag{31}$$

and with the one for curling, which is [8] proportional to $1/S^2$. The proportionality factor is a rather complicated function of the aspect ratio, m, of the ellipsoid, and for simplicity it is approximated here by a linear function, taking

$$-h_{\mathrm{n}}^{(\mathrm{curl})} = \frac{1.0791 + 0.5287/m}{S^2} \tag{32}$$

which is a good approximation for large values of m. Moreover, the curvature of the exact function, as plotted in figure 6 of [10] or figure 1 of [11], is such that the linear approximation in equation (32) is more negative than the exact eigenvalue, thus making it a rigorous upper bound for the true curling mode. Therefore, no mistake is made in comparing with a lower bound of the buckling mode.

6. Integrations

The main difficulty in carrying out the integrations in (28) and (29) is the existence of the expression in the denominator, which does not look integrable. Therefore, the first step used here is series expansion in Legendre polynomials, namely

$$\frac{g_n(\xi,\eta)}{\xi^2-\eta^2} = n(n+1) \sum_{k=0}^{n-1}{}^{*} (2k+1) P_k(\xi) P_k(\eta) - 2\, \frac{\mathrm{d}P_n(\xi)}{\mathrm{d}\xi}\, \frac{\mathrm{d}P_n(\eta)}{\mathrm{d}\eta} \tag{33a}$$

and

$$\frac{nG_n(\xi,\eta)}{\xi^2-\eta^2} = \sum_{k=0}^{n-1}{}^{*} (2k+1) P_k(\xi) P_k(\eta) \tag{33b}$$

where the star designates summation over odd values of k if n is even, and summation over even values of k if n is odd. These relations were proved by mathematical induction.

When these series are substituted into (28) and (29), the integrations over η involve (12*a*), and other well-known relations, or ones which are readily derived from them. In particular, all of the integrations over η in (28) are

$$\int_{-1}^{1} \eta P_n(\eta) \frac{\mathrm{d}P_n(\eta)}{\mathrm{d}\eta}\, \mathrm{d}\eta = \frac{2n}{2n+1} \qquad \int_{-1}^{1} \left[\frac{\mathrm{d}P_n(\eta)}{\mathrm{d}\eta}\right]^2 \mathrm{d}\eta = n(n+1) \tag{34a}$$

$$\int_{-1}^{1} (1-\eta)^2 \left[\frac{\mathrm{d}P_n(\eta)}{\mathrm{d}\eta}\right]^2 \mathrm{d}\eta = \frac{2n(n+1)}{2n+1} \qquad \int_{-1}^{1} P_{n-1}(\eta) \frac{\mathrm{d}P_n(\eta)}{\mathrm{d}\eta}\, \mathrm{d}\eta = 2. \tag{34b}$$

Using these equations in (28) and rearranging,

$$\begin{aligned}\Omega_2(\xi_0) = \int_1^{\xi_0} \Bigg\{ & n(n+1) P_{n+1}(\xi) P_{n-1}(\xi) + \frac{2}{n(n+1)} \left[\frac{\mathrm{d}P_n(\xi)}{\mathrm{d}\xi}\right]^2 \\ & - \frac{\mathrm{d}P_n(\xi)}{\mathrm{d}\xi} \left[P_{n+1}(\xi) + P_{n-1}(\xi)\right] \Bigg\}\, \mathrm{d}\xi.\end{aligned} \tag{35}$$

Hence,

$$\begin{aligned}\Omega_2(\xi) = & \frac{n(n+1)}{2} \xi P_{n+1}(\xi) P_{n-1}(\xi) - \frac{n(n^2+n+2)}{2(n+1)} \xi [P_n(\xi)]^2 \\ & - \frac{n(n-1)}{2(n+1)} P_n(\xi) P_{n-1}(\xi) + \frac{\xi P_{n-1}(\xi) - P_n(\xi)}{n+1} \frac{\mathrm{d}P_n(\xi)}{\mathrm{d}\xi}\end{aligned} \tag{36}$$

because the derivative of this expression is equal to the integrand of (35), and it is zero at the lower bound, $\xi = 1$. Similarly,

$$\begin{aligned}\frac{\Omega_3(\xi)}{(2n+1)(\xi^2-1)^2} = & \frac{\mathrm{d}P_n(\xi)}{\mathrm{d}\xi} \left[\frac{\xi^2+1}{2\xi} \frac{\mathrm{d}P_n(\xi)}{\mathrm{d}\xi} - \frac{2}{n(n+1)} \frac{\mathrm{d}^2 P_n(\xi)}{\mathrm{d}\xi^2}\right] \\ & - \frac{n P_n(\xi)}{2\xi} \left[n P_n(\xi) + \frac{P_{n-1}(\xi)}{\xi}\right].\end{aligned} \tag{37}$$

These expressions complete the calculation of the buckling lower bound of equation (30). In the actual computations they have to be evaluated numerically for ξ which is very nearly 1, for which the advice of [12] on how to compute Q_n is not practical, leading to large errors. Instead, some transformations of the definition in [12] in terms of the hypergeometric function lead to the more practical equation

$$Q_n(x) = \frac{1}{x^{n+1} n!} \sum_{k=0}^{\infty} \frac{(2k+n)!}{2^{2k+1}(k!)^2} \left[\ln\left(\frac{4x^2}{x^2-1}\right) - A_{k,n}\right] \left(\frac{x^2-1}{x^2}\right)^k \tag{38a}$$

with

$$A_{k,n} = \sum_{l=k+1}^{k+[n/2]} \frac{1}{l} + 2 \sum_{l=k+1}^{k+[(n+1)/2]} \frac{1}{2l-1} + \sum_{l=1}^{k} \frac{1}{l(2l-1)} \tag{38b}$$

where the square brackets designate the largest integer included in their argument. A similar usage of the Gauss hypergeometric series yields

$$P_n(x) = \sum_{k=0}^{n} \frac{(n+k)!}{(n-k)!(k!)^2} \left(\frac{x-1}{2}\right)^k \tag{39}$$

which is useful for computing both the Legendre polynomials and their derivatives, when the argument is very nearly 1.

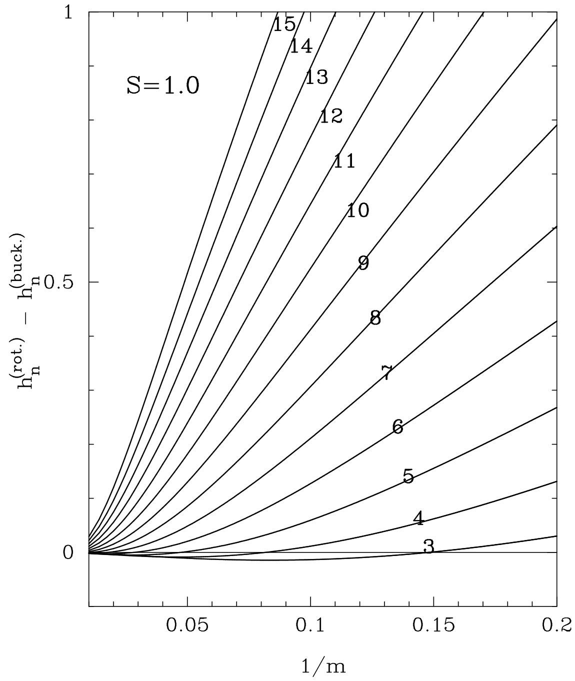

Figure 1. The difference between the eigenvalue for nucleation by coherent rotation and the lower bound for nucleation by the buckling mode, for the reduced semi-minor axis $S = 1.0$, as a function of the aspect ratio, m of a prolate spheroid. The numbers on the curves are the values of the parameter n.

7. Results

The difference thus computed between the eigenvalue for nucleation by coherent rotation, equation (31), and the lower bound for nucleation by the buckling mode, equation (30), is plotted in figure 1 for the particular reduced radius $S = 1.0$, and for various values of the (arbitrary) integer n. It is seen from the figure that this difference is positive (i.e. the coherent rotation has a less negative eigenvalue than the lower bound for the buckling mode) above a certain value of $1/m$. Such a positive value means that buckling cannot take place in that region, and it may only exist for a smaller $1/m$, i.e. for a larger m than the crossover point. It is also clear from the figure that the crossover moves towards smaller values of $1/m$ with increasing n, so the region in which buckling *may* exist keeps shrinking with the use of a larger n. This behaviour is typical, and the figure is qualitatively the same for all values of S.

A similar behaviour is also seen in figure 2, which compares the lower bound for nucleation by the buckling mode with the eigenvalue for nucleation by the curling mode, for the case $S = 1.02$. This value of S is slightly below the turnover from coherent rotation to curling, and for this S the buckling mode should still be compared with the coherent rotation. Only for still larger values of S does curling become an easier mode than the coherent rotation, and the buckling should be compared with it. Such a comparison is plotted in figure 3 for the case where $S = 1.1$, which is well within the region in which curling is easier than coherent rotation. It is seen from the figure that for this S, curling is also easier than the lower bound for the buckling mode. Similar results are obtained for all

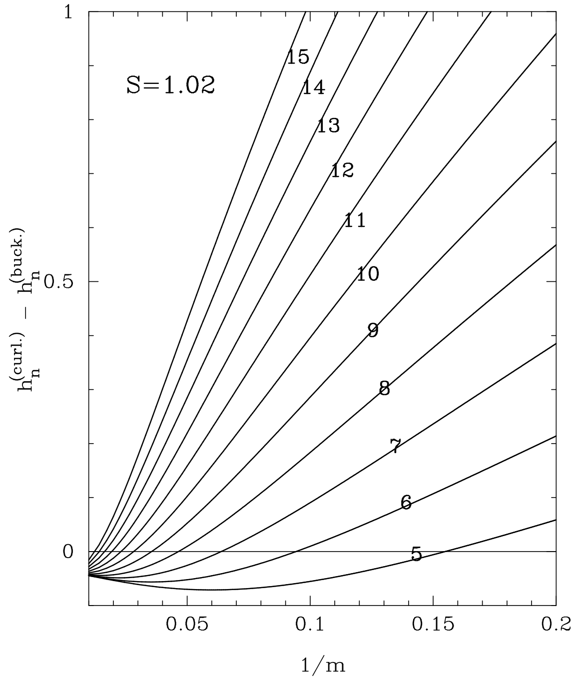

Figure 2. The difference between the eigenvalue for nucleation by curling and the lower bound for nucleation by the buckling mode, for the reduced semi-minor axis $S = 1.02$, as a function of the aspect ratio, m of a prolate spheroid. The numbers on the curves are the values of the parameter n.

values of S above the transition, and on the whole there is no conflict between curling and buckling. Once the curling is easier than coherent rotation, it becomes the only possible nucleation mode. This result is different from the one in the previous study [2], in which buckling could not be completely ruled out above the transition from coherent rotation to curling. The reason is that the values $n = 2$ and $n = 3$, used [2] in that study, turn out to be special cases with an atypical behaviour. For $n > 4$, however, there is a sharp and clear-cut distance between the curves for the curling nucleation field versus m and the one for the buckling, and they do not cross each other.

The results of all the computations are summarized in figure 4. Above a certain curve, which looks like a straight line in the small region shown, only curling is possible. Below that curve, coherent rotation takes over, except for in a small region of a very large aspect ratio m, in which a third mode has not been ruled out, and it *may* be possible. This region keeps shrinking steadily with increasing n, but its border is shown for two cases only, in order to avoid crowding the figure. The cases are $n = 8$ (dotted curve) and $n = 13$ (full curve). The edge of the triangle for the case in which $n = 13$ is at $m \approx 500$, which proves that there cannot be any third mode for prolate spheroids whose aspect ratio is 500:1 or smaller.

It is possible in principle to shrink this region even further by using larger values of n. And it is not particularly difficult to do it with the analytic expressions for all of the integrals. The only difficulty is in handling values of ξ which are very close to 1, which occur when m is large; see equation (4*c*). In plotting figure 4 it was necessary to deal with $\xi = 1+10^{-8}$, and for such values it is necessary to be careful even with the simplest expressions. For

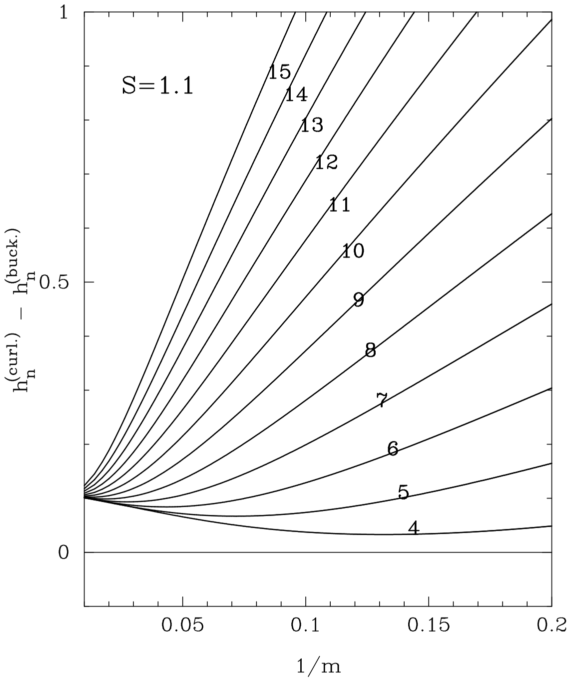

Figure 3. As figure 2, but for a reduced radius $S = 1.1$.

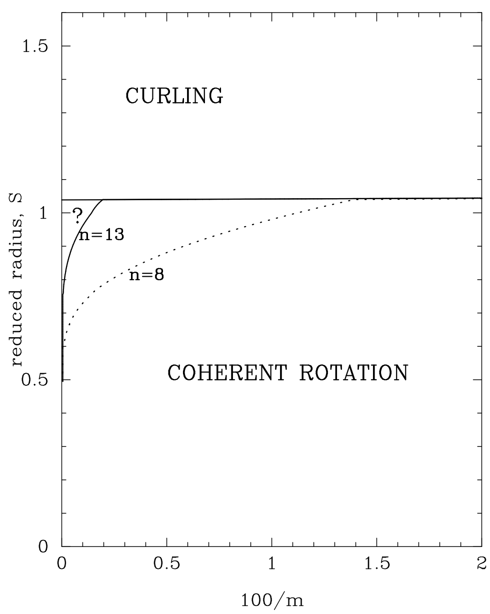

Figure 4. The possible nucleation modes in a prolate spheroid with an aspect ratio (major to minor axis) m, and a reduced semi-minor axis, S, defined in equation (5). Only curling, or coherent rotation, are physically possible in the regions so marked. If any third mode exists at all, it can only be in the little quasi-triangle, around the question mark. Its border has been computed for $n = 13$, but the border for the larger region obtained for $n = 8$ is also shown for comparison, as the dotted curve.

example, $\xi^2 - 1$ is evaluated to a higher accuracy if expressed as $(\xi + 1)(\xi - 1)$, for such a value of ξ. The present program could not handle $\xi = 1 + 10^{-9}$ at all, and it was therefore decided to stop at $n = 13$. Aspect ratios larger than 500:1 are not practical anyway, and the effort needed to extend the theory beyond that limit does not seem justified. But it should be noted that it is not that big an effort, and that it is relatively simple to use larger values of n, if needed.

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