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A liquid crystal model for early cell division

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A variational principle based on the curvature energy of a two dimensional liquid crystal membrane is constructed to determine the equilibrium shape of a cell with given surface area and volume. A sequence of the forms, calculated numerically, displays the process of cell division.

1. Introduction

The interesting characteristics of liquid crystals make them important from both practical and theoretical points of view. Considerable technological use is made of liquid crystals and a number of natural phenomena are explained by the liquid crystal nature of one or other of the materials involved in them. Perhaps, biological phenomena provide the majority of such examples. Living membranes, which are very important in physiology, have many traits which may be understood with the help of the theory of liquid crystals. The transformations of the cell membrane of the red blood cell [1], pore formation and stability [2], changes in transport behaviour [3], etc., are explained in such ways. The balance of edge and curvature energy of a lipid bilayer plays an essential role in the model given by Helfrich [4] for vesicle formation. The Helfrich model also contributes to our knowledge about the origin of life. In this paper, we point out that the curvature energy of a lipid bilayer membrane can govern the proliferation of very simple cells having no internal structure or organels. The model given here may turn out to be useful when studying the origin of life.

In the model presented we follow Helfrich [1, 4, 5] and Frank [6] and suppose that the free energy of a deflected membrane is a quadratic function of the two principal curvatures. The free energy per unit area is then

$$F_c = K_0(c_1 + c_2 - a^*)^2 + K_1 c_1 c_2, \tag{1}$$

where c_1 and c_2 are the principal curvatures, K_0 and K_1 are elastic constants and a^* is the spontaneous curvature. Their actual values depend on the chemical composition of the membrane and of the liquids inside and outside, as well as on the temperature, the pressure, etc. F_c will be referred to as the curvature energy.

The curvature energy can be the consequence of molecular alignment, but it can be explained in a different way as well. During deflection, the areas of the two sides of the membrane vary in different ways, so the space for the units will be different on the two sides; in consequence the quantity a^* can change when the molecular units exchange position by chance from one side to the other (thermal motion); this is often referred to as the flip-flop motion of the membrane units.

The proliferation of the rudimentary cells must follow a very simple mechanism because they have no organels which could control the processes. The two dimensional liquid–crystal line nature of the cell membrane suggests that it could be the

appropriate explanation. Numerical computations investigating this possibility have proved that the minimal value of the curvature energy can belong to the shape of a proliferating cell. The series of shapes calculated make sure that a real explanation is found.

2. The mechanism of cell profileration

The calculations presented here are based on a similar analysis to those in [4, 5] but a different representation of the variables employed makes the equations easier to solve. For the sake of simplicity, surfaces of revolution are taken into account. We assume a cartesian coordinate system in a plane with a curve set in it. If the curve does not intersect itself and crosses the y axis orthogonally, a smooth surface will be formed by revolving the curve about the y axis. The shape of the proliferating cell is determined by the minimum of the curvature energy at constant volume and constant interfacial area. To calculate it, we need the two principal curvatures which are measured in meridional and normal sections. Their values are given by

$$c_1 = \frac{d\alpha}{ds} \quad \text{and} \quad c_2 = \frac{\sin\alpha}{x}, \tag{2}$$

where s is the arc length of the curve from the bottom to the given point while α is the angle between the tangent of the curve and the x axis (see figure 1.) Using these we obtain the curvature energy as

$$F_c = \int\left[K_0\left(\frac{d\alpha}{ds} + \frac{\sin\alpha}{x} - a^*\right)^2 + K_1\frac{\sin\alpha}{x}\frac{d\alpha}{ds}\right]2\pi x\, ds, \tag{3}$$

where the integration is extended from the bottom of the curve to the top. The equilibrium outline of the cell is determined by the function $\alpha(s)$, minimizing the functional in equation (3) at constant volume and constant surface area. The function $x(s)$ is determined by

$$\frac{dx}{ds} = \cos\alpha. \tag{4}$$

The surface area and the volume are given as

$$\Omega = \int 2\pi x\, ds \quad \text{and} \quad V = \int \pi x^2 \sin\alpha\, ds. \tag{5}$$

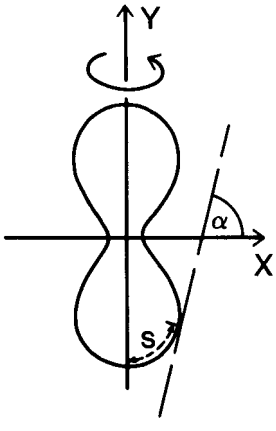

Figure 1. An explanation for the quantities x, y, s and α, which are used in the equations.

The desired functions are determined by the methods of variational calculus. The lagrangian for the constrained variational problem is

$$F^* = \left[K_0\left(\frac{d\alpha}{ds} + \frac{\sin\alpha}{x} - a^*\right)^2 + K_1\frac{\sin\alpha}{x}\frac{d\alpha}{ds}\right]2\pi x + \lambda_1 2\pi x + \lambda_2\pi x^2\sin\alpha + \mu(s)\left(\frac{dx}{ds} - \cos\alpha\right). \tag{6}$$

Here λ_1, λ_2 and $\mu(s)$ are lagrangian multiplers. The physical meaning of λ_1 is analogous to the ordinary surface tension and λ_2 is the underpressure inside the cell. The Euler equations are

$$\left.\begin{aligned} x\frac{d^2\alpha}{ds^2} + \cos\alpha\frac{d\alpha}{ds} - \frac{1}{x}\sin\alpha\cos\alpha &= \frac{\lambda_2}{4K_0}x^2\cos\alpha + \frac{\mu}{4\pi K_0}\sin\alpha, \\ \left(\frac{d\alpha}{ds} - a^*\right)^2 - \left(\frac{\sin\alpha}{x}\right)^2 + \frac{\lambda_1}{K_0} + \frac{\lambda_2}{K_0}x\sin\alpha &= \frac{1}{2\pi K_0}\frac{d\mu}{ds}, \\ \frac{dx}{ds} &= \cos\alpha. \end{aligned}\right\} \tag{7}$$

Because the arc length s does not appear explicitly in the lagrangian and the upper limit of the integral in equation (3) is arbitrary, a first integration of Euler's equations can be obtained in general form as

$$F^* - \frac{d\alpha}{ds}\frac{\partial F^*}{\partial\frac{d\alpha}{ds}} - \frac{dx}{ds}\frac{\partial F^*}{\partial\frac{dx}{ds}} = 0, \tag{8}$$

(see, for example, [7]) which now reads

$$K_0 2\pi x\left[\left(\frac{\sin\alpha}{x} - a^*\right)^2 - \left(\frac{d\alpha}{ds}\right)^2\right] + 2\pi\lambda_1 x + \pi\lambda_2 x^2\sin\alpha - \mu\cos\alpha = 0. \tag{9}$$

Replacing the second equation in (7) and eliminating the auxiliary function $\mu(s)$ we obtain the system of differential equations to be solved as

$$\left.\begin{aligned} \frac{d^2\alpha}{ds^2} &= \left(\frac{\sin\alpha}{x} - \frac{d\alpha}{ds}\right)\frac{\cos\alpha}{x} + \frac{\sin\alpha}{2\cos\alpha}\left[\left(\frac{\sin\alpha}{x} - a^*\right)^2 - \left(\frac{d\alpha}{ds}\right)^2 + \frac{\lambda_1}{K_0} + \frac{\lambda_2}{2K_0}\frac{x}{\sin\alpha}\right], \\ \frac{dx}{ds} &= \cos\alpha. \end{aligned}\right\} \tag{10}$$

The task of finding an exact analytical solution is too hard, so we have to approach the result from several sides, with several methods. First we note that the functions

$$\alpha = \frac{s}{r}, \quad x = r\sin\frac{s}{r}, \tag{11}$$

give a solution describing a sphere, and to which the condition

$$\frac{\lambda_2 r}{2K_0} + \frac{\lambda_1}{K_0} + a^*\left(a^* - \frac{2}{r}\right) = 0 \tag{12}$$

belongs. Here r is an arbitrary constant, the radius of the sphere. As the second step, we study forms slightly different from a sphere. The solution is sought in the implicit form

$$s = r[\alpha + v(\alpha)], \quad x = r\sin\alpha[1 + u(\alpha)], \tag{13}$$

where the functions $v(\alpha)$ and $u(\alpha)$ are small. Linearization of the equations in (10) yields

$$\begin{aligned} \frac{dv}{d\alpha} &= u + \frac{du}{d\alpha} tg\alpha, \\ \frac{d^2v}{d\alpha^2} + \frac{1}{\sin\alpha\cos\alpha}\frac{dv}{d\alpha} + tg\alpha\left(\frac{\lambda_2 r^3}{4K_0} - 1 + ra^* - \frac{\cos^2\alpha}{\sin^2\alpha}\right)u &= 0. \end{aligned} \tag{14}$$

Eliminating $v(\alpha)$ and introducing the new independent variable

$$z = -\cos\alpha,$$

we find

$$(1 - z^2)\frac{d^2u}{dz^2} - \frac{2 + 2z^2}{z}\frac{du}{dz} + \left(\frac{\lambda_2 r^3}{4K_0} + ra^*\right)u = 0. \tag{15}$$

This equation has a regular solution in the closed interval $-1 \leqq z \leqq 1$ if, and only if,

$$\frac{\lambda_2 r^3}{4K_0} + ra^* = n(n + 1), \quad n = 2, 3, \ldots \tag{16}$$

The first proper value is 6 and the solution is

$$u = 1 + 3z^2 = 4 - 3\sin^2\alpha. \tag{17}$$

The linearized equations do not answer the question as to whether the elongated shapes or the flattened ones are preferred. Using a higher order approximation, Deuling and Helfrich [5] proved that the elongated shapes are preferred if the inequality

$$a^*r > -\frac{39}{23} \tag{18}$$

holds.

On the basis of these results, we can describe the early stage of proliferation. Osmotic processes cause some underpressure inside the microsphere. When the underpressure reaches the value given by equation (16) the sphere collapses and becomes elongated if the inequality (18) holds. The validity of the inequality can result from the flip-flop motion of the molecules in the bilayer. The curvature energy of a sphere depends on the material constant a^* and has a minimum if a^* equals $2/r$. It is obvious that transfer of the molecules between the outer and the inner side of the membrane makes the value of a^* tend to $2/r$. The process of increasing from inside has a different effect: it decreases a^*. The result of the two tendencies can make the inequality (18) valid. If the flip-flop motion has a stronger effect, the value of a^* will be just below $2/r$, which turns out to be important.

To learn more about the solutions of equations (10) we had to turn to numerical methods. Before tackling this task some transformations of the equations were useful; we also needed certain initial conditions. Equations (10) contain two auxiliary constants, the values of which are unknown. A similarity transformation reduces the number of unknown quantities in the equations. We introduce new variables x', s',

A, K, defined by

$$x = Dx'; \quad s = Ds'; \quad A = Da^*; \quad K = \frac{\lambda_2}{2K_0} D^3, \tag{19}$$

where D is suitably chosen so that the equality

$$2\lambda_1 + \lambda_2 D = 0 \tag{20}$$

holds. Equations (8) become

$$\frac{d^2\alpha}{ds'^2} = \left(\frac{\sin\alpha}{x'} - \frac{d\alpha}{ds'}\right)\frac{\cos\alpha}{x'} + \frac{1}{2}\frac{\sin\alpha}{\cos\alpha}\left[\left(\frac{\sin\alpha}{x'} - A\right)^2 - \left(\frac{d\alpha}{ds'}\right)^2 - K + K\frac{x'}{\sin\alpha}\right],$$

$$\frac{dx'}{ds'} = \cos\alpha. \tag{21}$$

Expediency suggests that the calculations are started at the waist line, as the equations are singular both at the bottom and the top of the vesicle. Other removable singularities are present where the tangent of the outline is parallel to the axis of the symmetry, especially at the waist. The latter can be avoided if we choose the initial value

$$\left.\frac{d\alpha}{ds'}\right|_0 = \pm\sqrt{\left\{\left(\frac{1}{x_0'} - A\right)^2 - K(1 - x')\right\}}. \tag{22}$$

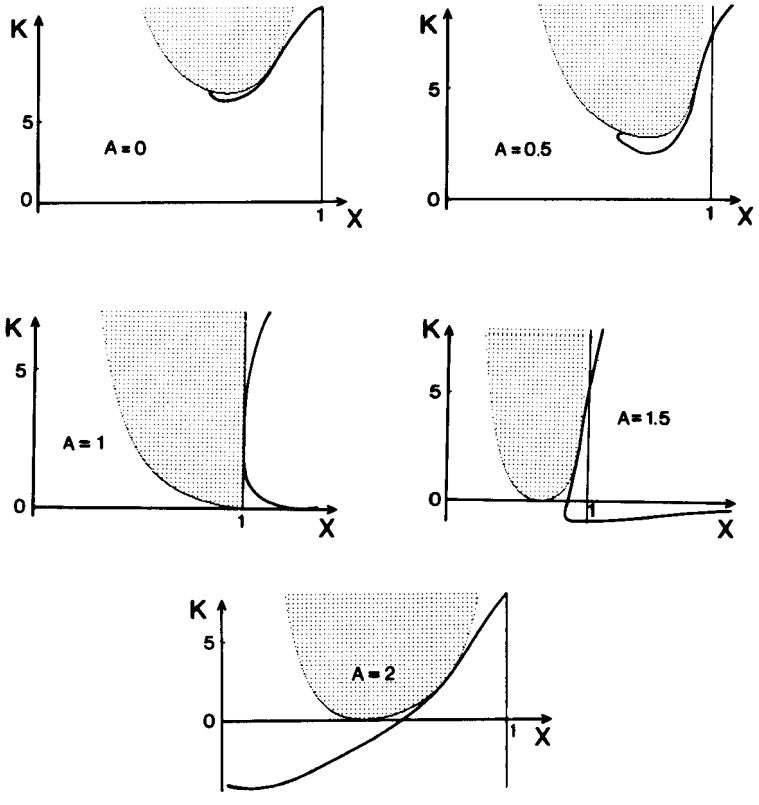

Figure 2. The reduced underpressure inside the dividing cells versus the reduced waist-radius at different spontaneous curvatures, A. The shaded areas are forbidden.

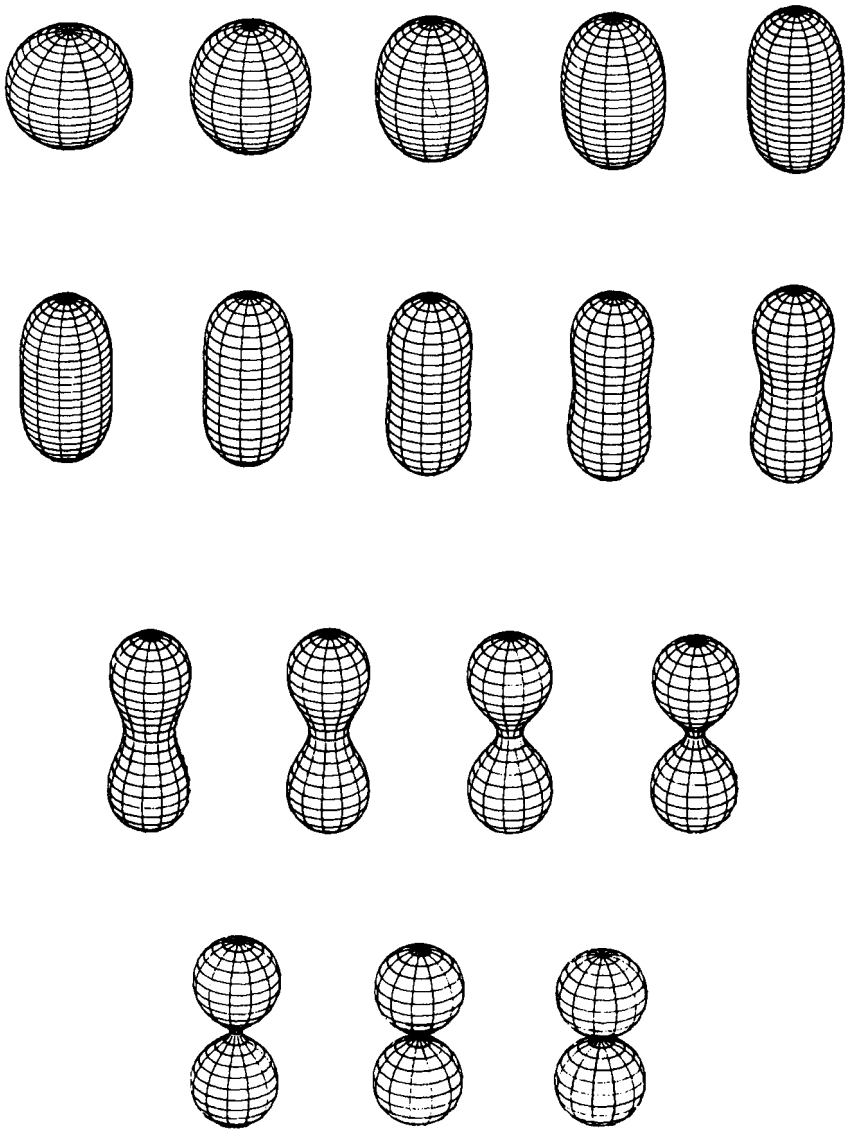

Figure 3. Views of the proliferating cells.

Hence,

$$K \leqslant \frac{(1 - Ax_0')^2}{x_0'^2(1 - x_0')}. \tag{23}$$

The numerical calculations were performed by the Runge–Kutta method. The point of the computations is the fact that for a proper value of K the curve arrives at the symmetry axis perpendicularly, otherwise it curves outward or inward. The proper values were approximated by nested intervals. The inequality (23) shows the feasible values of K. In the limiting case, when the equality in (23) holds, the slim forms join to the bulbous ones, to which the negative and the positive signs occurring in equation (22) respectively belong. The computations were performed with the values of $A = 0$,

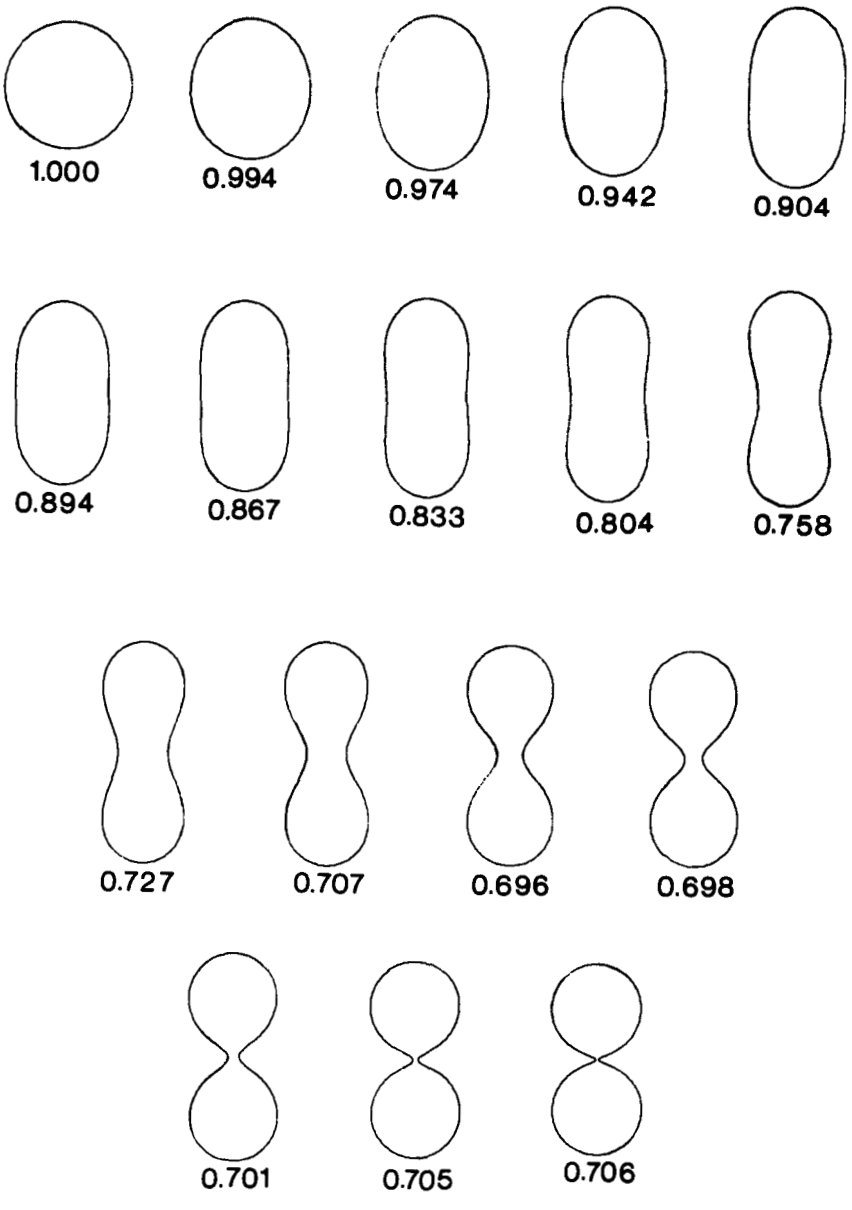

Figure 4. The outlines of the proliferating cells with the ratio of the actual volume to the maximal value with the same envelope.

1/2, 1, 3/2, 2 and also $A = 3$, 5, 10 and 100. The computations showed that the set of the proper values do not denote a way for proliferation if the quantity A is too small. The critical value is slightly smaller than 1·8. The proper values are plotted against the width of the waist in figure 2; the data used in the calculation of the points may be obtained from the author. Figure 3 shows the views of proliferating microspheres. Figure 4 shows their outline, the quantity V/V_0 denotes the ratio of the volume to the maximal value in the same envelope. These values, for the slimmest ones, are about $1/\sqrt{2}$, which corresponds to two smaller spheres.

3. Conclusion

The result of our investigation is that proliferation is the natural behaviour of a two dimensional liquid-crystalline cell membrane and no further regulation is needed. A proper balance of the flip-flop motion of the molecules and the growth from inside demonstrate the quantitative conditions necessary for it. The possible forms in our theory are static in contrast to those given by the theory of Rashevsky [8] or by that of Sorensen [9]; in consequence the speed of cell division is governed by that of growth or by osmotic processes. Nevertheless, the modern cell cannot follow the mechanism proposed here since, first of all, they are set in a tissue or have rigid walls. On the other hand, they have rather complex internal structures the replication of which cannot be ruled in such a simple way so that our idea may be essentially valid for the division of some internal part of a cell the duplication of which can initiate a fission in a modern cell.

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