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Morphology change in nematic membranes induced by defects

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ABSTRACT. The cell membrane is one of the most important structures of living organisms. This is due to the many functions attributed to it such as permeable selectivity, protection, anchoring to the cytoskeleton and so many others. Any change in the shape of the cell membrane may affect directly the properties and abilities. In this article, we study how defects in the liquid crystalline organization of a membrane can change its shape. For performing this, we consider a membrane with orientational order, i.e., a nematic membrane, which can happen in biological membranes, nematic films and other systems and study how a defect in this order can change the shape of the membrane when the bending rigidity is considered. We find that depending on the ratio of rigidity and elastic constant, buckling of this membrane may happens and turn it into pseudo-spheres.

Keywords: +1 defects, nematic liquid crystals, bending rigidity, buckle.

Mudança de morfologia em membranas nemáticas induzida por defeitos

RESUMO. A membrana celular é uma das estruturas mais importantes dos seres vivos. Isto se deve aos vários fatores atribuídos a ela como permeabilidade seletiva, proteção, ancoramento ao citoesqueleto e vários outros. Qualquer mudança no formato da membrana celular pode afetar diretamente suas propriedades e habilidades. Neste artigo, estudamos como defeitos na organização liquido cristalina de uma membrana pode mudar o seu formato. Isto é feito considerando-se uma membrana com ordem orientacional, isto é, uma membrana nemática, o que pode ocorrer em membranas biológicas, filmes nemáticos e outros sistemas e estudamos como defeitos nesta ordem podem mudar o formato da membrana quando a rigidez da membrana é levada em conta. É encontrado que dependendo da razão entre rigidez e constante elástica, curvaturas desta membrana podem ocorrer levando a formatos conhecidos como pseudo-esferas.

Palavras-chave: defeitos +1, cristais líquidos nemáticos, rigidez, curvatura.

Introduction

The biomembrane is one of the most intriguing structures in nature. The plasma membrane is made of lipids, having amphiphilic nature, just as liotropic liquid crystals (JAKLI; SAUPE, 2006). There are several functions attributed to it, such as permeable selectivity, protection, anchoring to the cytoskeleton and so many others (ALBERTS et al., 2002). All these functions can be greatly affected by external factors, which include changes in the membrane morphology, often described by geometry and topology (FRANK; KARDAR, 2008). In fact, shape change in membranes has been subject of great effort in condensed matter. Very often, these shapes are investigated by analyzing the coupling between geometrical shape and orientational order. These studies include oriententional order and defects in deformable vesicles (LUBENSKY; PROST, 1992; HIRST et al., 2013; JIANG et al., 2007; NYUGEN et al., 2013; PARK et al., 1992; RAMAKRISHNAN et al., 2010) and cytoskeletal filaments (NÉDÉLEC et al., 1997; SURREY et al., 2001). Furthermore, vector fields on a surface or nematic membranes, are considered simplified models to describe membranes that are more complex. These include any flexible sheet with ordered road-like constituents (SHALAGINOV, 1996; SPECTOR et al., 1993; YOUNG et al., 1978).

In this work, we investigate the problem of a flat membrane with coupled nematic order when defects of the +1 kind appear. In regular nematic cells, it is expected that the bulk will buckle into the third dimension when defects are present (CLADIS;

KLEMAN, 1972; JAKLI; SAUPE, 2006; MEYER, 1973). By using a simple model composed of nematic order and bending rigidity in covariant form, we are able to determine that a second-order like transition may guide the buckling of the membrane depending on the ratio of the parameters involved. Furthermore, we obtain an analytical result for the shape of the membrane, which buckles into pseudo-spheres.

Material and methods

In order to model the membrane, the Monge parameterization (NELSON, 2004) was used, which defines a surface, mapped on a plane defined by the variables σ_1 and σ_2 with height $h(\sigma_1,\sigma_2)$. The position vector then can be written as $\vec{r}(\sigma_1,\sigma_2)=[\sigma_1,\sigma_2,h(\sigma_1,\sigma_2)]$, which defines the tangent vectors as $\hat{t}_i=\partial_{\sigma_i}\vec{r}(\sigma_1,\sigma_2)$, with $i=1,2$.

We consider the free energy of the system to come from two contributions: the field, which wants to make all the vectors on the surface of the membrane parallel one to each order, supposing initial flat membrane, and the bending rigidity term. In a configuration with a defect, the flat configuration cannot minimize the free energy of the system, and the membrane has to bend, changing its shape. However, it has to pay a price for bending. The total free energy of the system, in the absence of surface tension (RAMAKRISHNAN et al., 2011), can be written in covariant form as:

$$F=\int\left[\frac{\kappa}{2}H^2\right]dS+\int\frac{K_A}{2}\sqrt{g}g^{uv}g_{py}\nabla_u n^p\nabla_v n^y, \quad (1)$$

where:
κ is the bending rigidity, H is the mean curvature, K_A is the nematic elastic constant (elastic isotropy approximation), n^y represent the components of the director field and g is the metric tensor. The director field, in the presence of defects of $+1$ kind can be written as

$$\vec{n}=\cos(\beta)\hat{t}_{\sigma_1}+\sin(\beta)\hat{t}_{\sigma_2} \quad (2)$$

where:
β is a parameter used to distinguished defects asters ($\beta=0$) and vortices ($\beta=\pi/2$), which is shown in Figure 1.

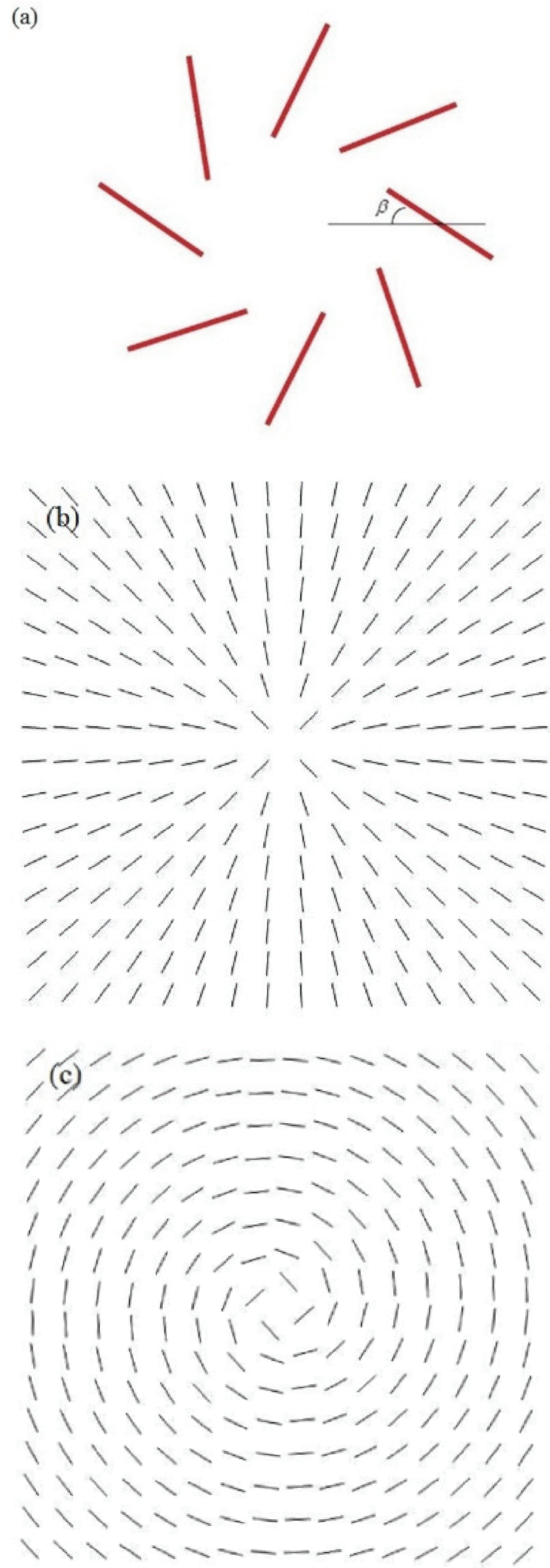

Figure 1. (a) orientation of director field depending on the parameter β. (b) aster configuration ($\beta=0$) and (c) vortices ($\beta=\pi/2$).

Results and discussion

The first approach for solving this problem is to try some specific shape for the membrane that would minimize the energy of the membrane (SEUNG; NELSON, 1998). One could argue that the actually shape for minimizing a +1 defect configuration would be a cone shape, and we can find how deep the cone goes by minimizing the free energy with respect to the angle α between the cone side and the z axis (in cylindrical coordinates), going from $\alpha = \pi/2$ for a flat membrane until $\alpha = 0$. For this configuration, the tangent vectors may be defined everywhere in terms of α as:

$$\hat{t}_{\sigma_1} = \hat{t}_r = \hat{r}\cos[\pi/2-\alpha] + \hat{z}\sin[\pi/2-\alpha] \text{ and } \hat{t}_{\sigma_2} = \hat{t}_\phi = \hat{\phi}. \tag{3}$$

The element of area for a conic surface is given by $dS = rdrd\phi\csc[\alpha]$. Furthermore, the mean curvature of a cone is given by $H = \cos[\alpha]/2r$. Therefore, the free energy's first term is described by the following equation

$$F_1 = \int\left[\frac{\kappa}{2}H^2\right]dS = \int_0^{2\pi}\int_{r_{\min}}^{r_{\max}} rdrd\phi\left[\frac{1}{2}\kappa\left(\frac{\csc[\alpha]}{2r}\right)\right] \tag{4}$$

so,

$$F_1 = \frac{1}{4}\kappa\pi\left[\frac{r_{\max}}{r_{\min}}\right]\frac{\cos[\alpha]^2}{\sin[\alpha]}. \tag{5}$$

In equation (5), $r_{\min}$ and $r_{\max}$ are the distances from the core of the defect to the size of the membrane. The second term of the free energy becomes

$$F_2 = \frac{1}{2}K_A\int_0^{2\pi}\int_{r_{\min}}^{r_{\max}} rdrd\phi\csc[\alpha]\,|\nabla n|^2 = \frac{1}{2}K_A\int_0^{2\pi}\int_{r_{\min}}^{r_{\max}} rdrd\phi\csc[\alpha] \times\frac{\sin[\alpha]^2\cos[\beta]^2+\sin[\beta]^2}{r^2} \tag{6}$$

or

$$F_2 = \frac{1}{2}K_A\pi\ln\left[\frac{r_{\max}}{r_{\min}}\right]\left(\sin[\alpha]\cos[\beta]^2+\sin[\beta]^2\right) \tag{7}$$

Therefore, the total free energy is

$$F = F_1 + F_2 = \frac{1}{2}\pi\ln\left[\frac{r_{\max}}{r_{\min}}\right] \times\left(\frac{1}{2}\kappa\frac{\cos[\alpha]^2}{\sin[\alpha]} + K_A\left(\sin[\alpha]\cos[\beta]^2+\frac{\sin[\beta]^2}{\sin[\alpha]}\right)\right) \tag{8}$$

Let us first examine the case for a defect of the "aster" configuration, which means, $\beta = 0$. In this case, the equilibrium situation is found by setting $\partial F/\partial\alpha = 0$. We find:

$$\left(\frac{K_A}{\kappa}\cos[\alpha] - \frac{1}{4}\cos[\alpha] - \frac{1}{4}\cot[\alpha]\csc[\alpha]\right) = 0. \tag{9}$$

Clearly, $\alpha = \pi/2$ is solution, which means a flat membrane. Nonetheless, the solution for α is

$$\alpha = \arccos\left[\sqrt{1-\frac{1}{4K_A/\kappa-1}}\right] \tag{10}$$

which is a minimum only when $K_A/\kappa > 1/2$. Therefore, there is a ratio between elastic constant and bend rigidity that determines the buckling of the membrane. If the ratio is smaller than $1/2$, than the stable configuration is the one where the membrane remains flat. However, as the ratio grows larger than $1/2$, the system smoothly changes from flat to buckled, in a second order-like change transition. In Figure 2, we show the plot of $F' = 2F/(\pi\ln[r_{\max}/r_{\min}])$ against the angle α.

Notice that in Figure 2(a), we have $K_A/\kappa = 1$, resulting in a buckled configuration whose angle $\alpha = 35.3°$. In Figure 2(b), $K_A/\kappa = 0.2$, so the membrane lies flat with $\alpha = 90.0°$.

Now, we can examine the vortex case, where $\beta = \pi/2$. In such case, the total free energy, equation (8), becomes:

$$F = \frac{1}{2}\pi\ln\left[\frac{r_{\max}}{r_{\min}}\right]\left(\frac{1}{2}\kappa\frac{\cos[\alpha]^2}{\sin[\alpha]} + K_A\frac{\sin[\beta]^2}{\sin[\alpha]}\right) \tag{11}$$

By setting $\partial F/\partial\alpha = 0$ we can find the stable solution. In this case, the only α that satisfies the equation is $\alpha = \pi/2$, which means the membrane is always flat if defects of the vortex kind exists. Figure 3(a) shows a 3D curve of $F' = 2F/(\pi\ln[r_{\max}/r_{\min}])$ against α and β for $K_A/\kappa = 3$ plotted from $\alpha = 0$ to π and β from 0 to $\pi/2$. It is possible to observe that buckled configurations happen only for defects near the aster arrangement.

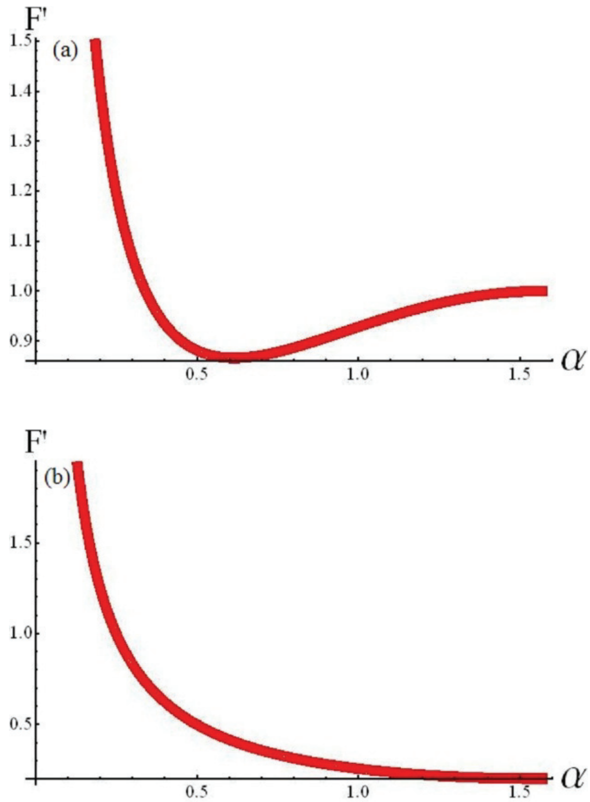

Figure 2. $F' = 2F/(\pi \ln[r_{max}/r_{min}])$ against the angle α for (a) $K_A/\kappa = 1$, and (b) $K_A/\kappa = 0.2$.

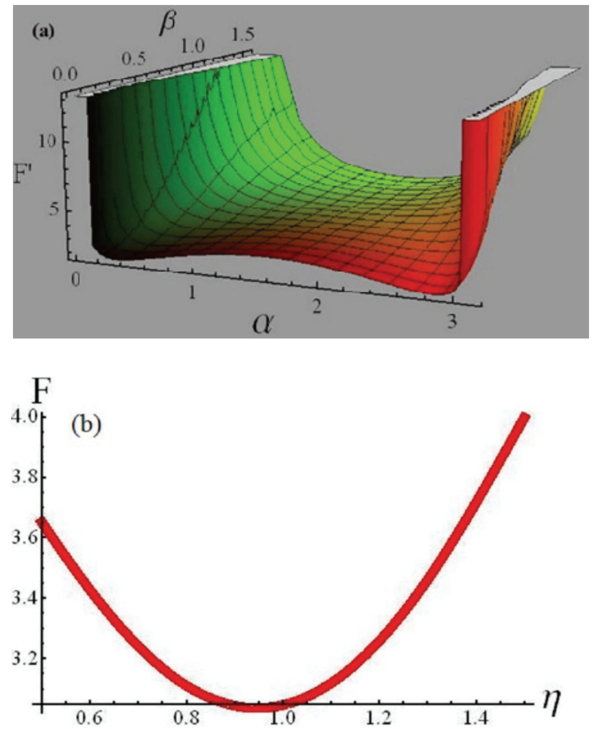

Figure 3. (a) $F' = 2F/(\pi \ln[r_{max}/r_{min}])$ against α and β for $K_A/\kappa = 3$ plotted from $\alpha = 0$ to π and β from 0 to $\pi/2$. (b) Numerical minimization of the free energy when $h = r^{\eta}\cot[\alpha]$, showing that the η coefficient slightly smaller than one leads to lower energy.

A more general solution

In the previous section, we have analyzed the morphology change of a membrane by assuming it would buckle into a cone. This means the function for the height was written as $h = r\cot[\alpha]$. Now, we shall look for profiles that are different from the conical shape. However, it is straightforward to foresee that the actual morphology of a buckled membrane in the presence of $+1$ defects should not differ much from the conical shape. This is indeed expected from the famous scape to the third dimension in bulk nematic (CLADIS; KLEMAN, 1972; JAKLI; SAUPE, 2006; MEYER, 1973). In fact, our first approach is to solve the problem imagining the following situation: $h = r^{\eta}\cot[\alpha]$, where η is a coefficient to be determined. By numerically integrating and finding the minimum of the free energy, equation (11), we encounter that the stable configuration of the buckled membrane happens for $\eta \approx 0.95$, assuming $K_A/\kappa = 1$, $r_{min} = 1$ nm and $r_{max} = 1$ μm. The behavior of F against η is shown in Figure 3(b).

In order to seek for a more general solution of the problem, we assume that height of the surface depends only on the radial distance from the core, or, $h \to h(r)$. In this situation, the tangent vectors, as well as the normal vector $\hat{k}$ are given by

$$\hat{t}_{\sigma_1} = (1,0,h_r)\frac{1}{\sqrt{1+h^2{}_r}},\ \hat{t}_{\sigma_2} = (0,1,0) \text{ and}$$

$$\hat{k} = \hat{t}_{\sigma_1} \times \hat{t}_{\sigma_2} = (-h_r,0,1)\frac{1}{\sqrt{1+h^2{}_r}},$$

where:
$h_r = dh(r)/dr$. The total free energy, equation (1), is then written as

$$F = \frac{1}{2}\kappa\int dr d\phi\left[\frac{\left(h_r(1+h_r{}^2)+rh_{rr}\right)^2}{4r(1+h_r{}^2)^{5/2}}\right] + \frac{1}{2}K_A\int dr d\phi\frac{1}{r(1+h_r{}^2)^{3/2}} \times\left[\begin{array}{l}1+(1+\sin[\beta]^2)h_r{}^2+\sin[\beta]^2 h_r{}^4\\ +r\sin[2\beta]h_r\sqrt{1+h^2{}_r}\,h_{rr}\\ +r^2\cos[\beta]^2 h_{rr}{}^2\end{array}\right]. \quad (12)$$

Now, we perform the following change of variables

$h_r = \tan[\delta(r)],$

where:
$\delta(r)$ is an unknown function of the variable r. Therefore, it follows that $h_{rr} = \sec[\delta]^2 \delta_r$ (we shall now drop the (r) indicating it is a function of r). Furthermore, based on previous results, we look for solutions in the case where $\beta = 0$. Then, equation (11) becomes:

$$F = 2\pi \int dr \frac{1}{16 r \cos[\delta]} \times \begin{bmatrix} 4K_A + \kappa + (4K_A - \kappa)\cos[2\delta] \\ + r\delta_r (2\kappa \sin[2\delta] \\ + r(8K_A + \kappa + \kappa\cos[2\delta])\delta_r) \end{bmatrix}. \quad (13)$$

The profile that minimizes the free energy is the one that satisfies the Euler-Lagrange equation

$$\frac{\partial f}{\partial \delta} - \frac{d}{dr}\frac{\partial f}{\partial \delta_r} = 0, \quad (14)$$

where:
f is the integrand of the total free energy in equation (12). Hence

$$\begin{aligned} &(4K_A - \kappa)\sin[2\delta] - 2\kappa\tan[\delta] \\ &+ 2(8K_A + \kappa + \kappa\cos[2\delta])[r\delta_r + r^2\delta_{rr}] + \\ &+ r^2\delta_r^2 (8K_A \tan[\delta] - \kappa\sin[2\delta]) = 0. \end{aligned} \quad (15)$$

First, we notice that if $\delta_r = \delta_{rr} = 0,$ we obtain

$$\frac{(4K_A - \kappa)\sin[2\delta] - 2\kappa\tan[\delta]}{16 r\cos[\delta]} = 0, \quad (16)$$

whose solution is

$$h(r) = r\tan[\arccos\left[\sqrt{1 - \frac{1}{4K_A/\kappa - 1}}\right]], \quad (17)$$

which corresponds to the conical solution. The next step requires solving equation (14). Unfortunately, equation (14) is very complicated and has no analytical solution. Nonetheless, we can use our previous results to infer about solving it. The numerical minimization showed that the actual minimum of energy is slightly different from the conical configuration. Therefore, we assume the solution for equation (16) can be written as

$$h(r) = r\tan[\arccos\left[\sqrt{1 - \frac{1}{4K_A/\kappa - 1}}\right]] + m(r), \quad (18)$$

where:
$m(r)$ is a function to be determined, considered small. By replacing equation (17) in (14), we get an equation depending only on $m(r)$. Since it is small, we can expand this equation and take only linear terms on $m(r)$. The usual minimization procedure allows the following equation for $m(r)$:

$$\begin{aligned} &[m_r + r m_{rr}](16K_A^2 - 4K_A\kappa + \kappa^2) r \\ &- 2m(8K_A^2 - 6K_A\kappa + \kappa^2) = 0, \end{aligned} \quad (19)$$

where:
$m_r = dm/dr.$ Equation (18) is solved by setting $m(r_{\min}) = -r\tan[\alpha],$ where α is given by equation (10), so near the core the membrane remains flat; and $m(r_{\max}) = 0,$ meaning that far away from the core the configuration is basically the same as a cone. Therefore, we find that

$$\begin{aligned} h(r) = &\frac{r}{(8K_A - \kappa)\kappa}\sqrt{\frac{4K_A}{\kappa} - 2}\,\csc[\theta_m] \\ &\times(\sqrt{2(6K_A\kappa - \kappa^2 - 8K_A^2)} \\ &\times\sqrt{-4K_A\kappa + \kappa^2 + 16K_A^2}\cos[\theta] \\ &-(-4K_A\kappa + \kappa^2 + 16K_A^2) \\ &\times\sin[\theta] + (8K_A - \kappa)\kappa\sin[\theta_m]), \end{aligned} \quad (20)$$

where

$$\theta_m = \frac{\sqrt{2(6K_A\kappa - \kappa^2 - 8K_A^2)}(\ln[r_{\max}/r_{\min}])}{\sqrt{-4K_A\kappa + \kappa^2 + 16K_A^2}}, \quad (21)$$

and

$$\theta = \frac{\sqrt{2(6K_A\kappa - \kappa^2 - 8K_A^2)}(\ln[r/r_{\min}])}{\sqrt{-4K_A\kappa + \kappa^2 + 16K_A^2}}. \quad (22)$$

Figure 4 shows a graphic of the height profile, equation (20) as a function of r for $K_A/\kappa = 1$, $r_{\min} = 1$ nm and $r_{\max} = 1$ μm. The profile is known as pseudosphere, with negative Gaussian curvature, in agreement with results reported before (FRANK; KARDAR, 2008).

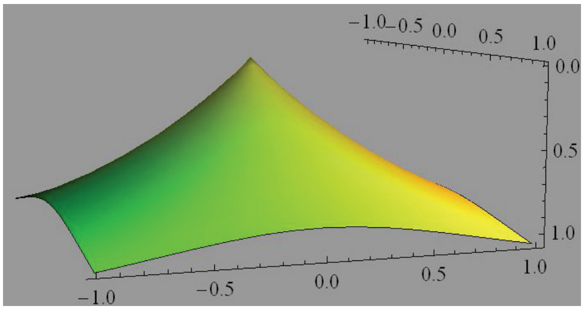

Figure 4. height profile calculated when the membrane buckles due to a +1 defect in the director field. The pseudosphere morphology is the one that minimizes the free energy.

Conclusion

In conclusion, the problem of a membrane with bend rigidity and a nematic vector field (nematic membrane) has been studied when defects of +1 kind exist in the director. We were able to show that the conical shape minimizes, in a first approximation, the free energy of the system when the ratio between the bend rigidity and elastic constant are in the appropriate range and that the transition between the flat and buckled state is second-order like. Further analyzes have shown that without any approximation the lowest energy is slightly different than the cone, which was first numerically calculated. Then, by using a perturbation method, we were able to analytically calculate the shape of the buckled membrane and show that it is a pseudosphere.

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References

ALBERTS, B.; JOHNSON, A.; LEWIS, J.; RAFF, M.; ROBERTS, K.; WALTER, P. **Molecular Biology of the Cell**. 4th ed. New York: Garland Science, 2002.

CLADIS, P.; KLEMAN, M. Non-singular disclinations of strength S = +1 in nematics. **Journal of Physique**, v. 33, n. 5-6, p. 591-598, 1972.

FRANK, J. R.; KARDAR, M. Defects in nematic membranes can buckle into pseudospheres. **Physical Review E**, v. 77, n. 4, 041705, 2008.

HIRST, L. S.; OSSOWSKI, A.; FRASER, M.; GENG, J.; SELINGER, J. V.; SELINGER, R. L. B. Morphology transition in lipid vesicles due to in-plane order and topological defects. **Proceedings of the National Academy of Sciencies USA**, v. 110, n. 9, p. 3242-3247, 2013.

JAKLI, A.; SAUPE, A. **One- and Two-Dimensional Fluids**: Properties of smectic, lamellar and columnar liquid crystals. Boca Raton: CRC Press, 2006.

JIANG, H.; HUBER, G.; PELCOVITS, R. A.; POWERS, T. R. Vesicle shape, molecular tilt, and the suppression of necks. **Physical Review E**, v. 76, n. 3, 031908, 2007.

LUBENSKY, T. C.; PROST, J. Orientational order and vesicle shape. **J. Phys. II France**, v. 2, n. 3, p. 371-382, 1992.

MEYER, R. B. On the existence of even indexed disclinations in nematic liquid crystals. **Philosophical Magazine**, v. 27, n. 2, p. 405-424, 1973.

NÉDÉLEC, F. J.; SURREY, T.; MAGGS, A. C.; LEIBLER, S. Self-organization of microtubules and motors. **Nature**, v. 389, n. 6648, p. 305-308, 1997.

NELSON, D. **Statistical Mechanics of Membranes and Surfaces**. 2nd ed. Singapore: World Scientific, 2004.

NYUGEN, T. S.; GENG, J.; SELINGER, R. L. B.; SELINGER, J. V. Nematic order on a deformable vesicle: theory and simulation. **Soft Matter**, v. 9, n. 34, p. 8314-8326, 2013.

PARK, J.; LUBENSKY, T. C.; MACKINTOSH, F. C. n -atic order and continuous shape changes of deformable surfaces of genus zero. **Europhysics Letters**, v. 20, n. 3, p. 279-284, 1992.

RAMAKRISHNAN, N.; SUNIL KUMAR, P. B.; IPSEN, JOHN, H. Monte Carlo simulations of fluid vesicles with in-plane orientational ordering. **Physical Review E**, v. 81, n. 4, 041922, 2010.

RAMAKRISHNAN, N.; SUNIL KUMAR, P. B.; IPSEN, JOHN, H. Modeling anisotropic elasticity of fluid membranes. **Macromolecular Theory and Simulations**, v. 20, n. 7, p. 446-450, 2011.

SEUNG, H. S.; NELSON, D. R. Defects in flexible membranes with crystalline order. **Physical Review A**, v. 38, n. 2, p. 1005-1018, 1998.

SHALAGINOV, A. N. Fluctuations and light scattering in free-standing smectic-C films. **Physical Review E**, v. 53, n. 4, p. 3623-3628, 1996.

SPECTOR, M. S.; SPRUNT, S.; LITSTER, J. D. Novel dynamical mode in a tilted smectic liquid-crystal film. **Physical Review E**, v. 47, n. 2, p. 1101-1107, 1993.

SURREY, T.; NÉDÉLEC, F.; LEIBLER, S.; KARSENTI, E. Physical properties determining self-organization of motors and microtubules. **Science**, v. 292, n. 5519, p. 1167-1171, 2001.

YOUNG, C. Y.; PINDAK, R.; CLARK, N. A.; MEYER, R. B. Light-scattering study of two-dimensional molecular-orientation fluctuations in a freely suspended ferroelectric liquid-crystal film. **Physical Review Letters**, v. 40, n. 12, p. 773-776, 1978.

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