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Mechanics of lipid membranes subjected to boundary excitations and an elliptic substrate interactions

Chun Il Kim*

Department of Mechanical Engineering, University of Alberta, Edmonton, Alberta, T6G 2G8, Canada

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Abstract. We present relatively simple derivations of the Helfrich energy potential that has been widely adopted in the analysis of lipid membranes without detailed explanations. Through the energy variation methods (within the limit of Helfrich energy potential), we obtained series of analytical solutions in the case when the lipid membranes are excited through their edges. These affordable solutions can be readily applied in the related membrane experiments. In particular, it is shown that, in case of an elliptic cross section of a rigid substrate differing slightly from a circle and subjected to the incremental deformations, exact analytical expressions describing deformed configurations of lipid membranes can be obtained without the extensive use of Mathieu's function.

Keywords: lipid membranes; bilayers; shape equation; substrate-membrane interaction; elliptical contact domain; analytic solution

1. Introduction

Helfrich energy potential (also often referred as Helfrich model (Helfrich 1973) based on 2D liquid crystal theory has become one of the most influential models in lipid membrane study for their simplicity and applicability. The fundamental premise of the model is that the lipid membrane can be regarded as, ideally, a thin film so that the stored energy during the membrane deformations is compatible to the changes of curvatures of the membrane. Despite of the extensive use of the model, its derivations, justifications and limitations are most often overly suppressed which hinder researchers for the more in depth study in this subject. This may be attributed by either the fact that most of recent studies in this subject are mainly focused on practical/empirical aspects of lipid membranes or, perhaps, mathematical complexities arising in the desired derivations.

In this work, we demonstrate tractable mathematical derivations for Helfrich model leading to the well-known shape equation for lipid membranes (see for example, Agrawal and Steigmann 2008, Ou-Yang *et al*. 1999, Rosso and Virga 1999) via the energy variation method. We also briefly discuss the reduction of equilibrium states for 2D membranes from their counterpart in 3D liquid crystal theory. Using the Helfrich energy potential, we proceeds standard energy variation methods (Steigmann 2003) and obtain the corresponding Euler equation which is further

*Corresponding author, Assistant Professor, E-mail: cikim@ualberta.ca

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$$\frac{\partial H_1}{\partial \rho}=\frac{\partial H_1^{(0)}}{\partial \rho}+\frac{\partial H_1^{(1)}}{\partial \rho}=-\frac{\sigma}{k}R\frac{1}{\zeta^2}=-\frac{\sigma R}{k}(cos2\theta+isin2\theta)\ at\ \rho=1. \tag{67}$$

From Eq. (57), we then have

$$\frac{\partial H_1^{(0)}}{\partial \rho}=\sum_{k=-\infty}^{\infty} j_k\, e^{ik\theta}\left(-\frac{\mu R}{2}\right)\left(K_{k+1}(\mu R\rho)+K_{k-1}(\mu R\rho)\right). \tag{68}$$

Now Eq. (65) together with Eqs. (67)-(68) furnish

$$\begin{aligned}\left.\frac{\partial H_1}{\partial \rho}\right|_{\rho=1}&=\left(-\frac{\mu R}{2}\right)\sum_{k=-\infty}^{\infty} j_k\, e^{ik\theta}\left(K_{k+1}(\mu R\rho)+K_{k-1}(\mu R\rho)\right)+\frac{R^3\mu^3F_0}{2}K_0(\mu R\rho)cos2\theta\\&=-\frac{\sigma R}{k}(cos2\theta+isin2\theta).\end{aligned} \tag{69}$$

From the above, we find k=2, −2. Thus Eq. (69) further reduces to

$$\begin{aligned}&\left(-\frac{\mu R}{2}\right)[(j_2e^{i2\theta}+j_{-2}e^{i-2\theta})(K_3(\mu R\rho)+K_1(\mu R\rho))+\frac{R^3\mu^3F_0}{2}K_0(\mu R\rho)cos2\theta\\&=-\frac{\sigma R}{k}(cos2\theta+isin2\theta).\end{aligned} \tag{70}$$

Knowing the fact that $e^{\pm i\theta}=cos\theta\pm i\sin\theta$, Eq. (70) yields two conditions for the real and imaginary parts, respectively. By comparing coefficients of each equation, we obtain

$$j_2=-\frac{\mu R^2\sigma}{2k[K_3(\mu R\rho)+K_1(\mu R\rho)]},j_{-2}=-\frac{\sigma(\mu^2R^2+4)}{\mu[K_3(\mu R\rho)+K_1(\mu R\rho)]}. \tag{71}$$

Consequently, the solution of Eqs. (51), (53) can be found as

$$\begin{aligned}H&=H_0+\varepsilon H_1=H_0+\varepsilon(H_1^{(0)}+H_1^{(1)})\\&=-F_0K_0(\mu R\rho)+\varepsilon[-\frac{1}{2}R^2\mu^2F_0K_0(\mu R\rho)cos2\theta+K_2(\mu R\rho)\left(j_2e^{i2\theta}+j_{-2}e^{i-2\theta}\right),\end{aligned} \tag{72}$$

where F_0, j_2, and j_{-2} are defined in Eqs. (60), (71) and R>0,0<ε<1.

With minor loss of generality, Eq. (72) together with Eq. (40) can be used to determine the deformed configurations of the lipid membranes in contact with an elliptical substrate. In the actual calculations (see Fig. 3), author intentionally exclude the solution of Laplace equation (φ) in the elliptical coordinate, since first, the contribution of Laplace terms in the final deformed configuration is not significant in the case of circular substrate (Agrawal and Steigmann 2009), second, the mathematical expression would then be too complicate that may result obtained solutions practically less efficient and/or interest, last, slight deviations from the experimental data can be easily accommodated by controlling parameter ε.

Remark 2

It is noted that the complete analytical solution for the case with an elliptical cross section is valid for those ellipses with ‘small’ deviations from a circular shape. Otherwise, the corresponding series expansions become merely ‘heavy’ mathematical exercise and/or may produce numerically in accurate results.

6. Conclusions

In this work, we demonstrate relatively simple way of deriving Helfrich potential by considering thickness-wise expansions of the energy density function from the 3D liquid crystal theory. Within Helfrich assumption, we obtained affordable solutions for the deformations of membrane (rectangular shape) when subjected to sinusoidal boundary excitations. The problem is of importance, particularly in practical field, since sinusoidal functions are easily generated under experimental settings and more general types of loadings can be assimilated by combining series of these functions (Fourier series). With its relatively simple expression, the obtained solution can be readily adaptable in testing/measuring the mechanical properties of lipid membranes. Membrane-substrate interaction problems are also considered in the case of an elliptical contact region where semi-analytical solution through Mathieu's function is by far the closest possible alternatives. However, the solution (based on Mathieu's function) still requires numerical aid and therefore, practically less desirable. It is shown that a viable analytical expression describing the deformed configurations of membranes can be obtained via the method of small parameter. The resulting analytical solution demonstrates good agreement with the numerical data in the case of the elliptical contact regions with small deviations from the circular shape. The obtained solution is expected to serve as a feasible alternative in the prediction of the morphological transitions of lipid membranes in contact with non-circular substrate particularly, those subjected to the incremental deformations**.**

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