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

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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

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simplified via Monge parameterization and admissible linearization process (Agrawal and Steigmann 2009). Within this setting, we obtained reasonably simple (and therefore, practically affordable) forms of exact analytical solutions describing the deformations of lipid membranes subjected to the boundary excitation (e.g., moments, displacements etc…). In particular, we show that, in the case of membrane-substrate interaction problems with an elliptical cross section, obtaining complete analytical solution is possible without the adaptation of Mathieu's function in the limit of those ellipses with 'small' deviations from a circular shape.

2. The energy potential

A well-known model for lipid membranes due to Helfrich (Helfrich 1973) is

$$W(H,K;\theta^\alpha) = kH^2 + \bar{k}K, \tag{1}$$

where are k and $\bar{k}$ empirical constants in the case of films with uniform properties. We note that k has positive values, yet $\bar{k}$ could have both signs. The sign of $\bar{k}$ is hard to determine, since it is related to Lagrangian (not appearing in energy minimization conditions). H and K represent Mean and Gaussian curvatures of surfaces, respectively.

The Helfrich potential can be obtained (without rigorous mathematical derivation) by considering thickness-wise expansions of energy density function $W(H, K;\theta^\alpha)$. However, unlike the usual deformation gradient tensor (F), H, and K have length unit that $H \propto 1/L$, $K \propto 1/L^2$. Thus we introduce membrane thickness "t" to get the following dimensionless curvatures.

$$\bar{H} = tH, \bar{K} = t^2K \tag{2}$$

Similarly, we define dimensionless energy functions $\bar{W}$ as

$$W(H,K;\theta^\alpha) = E\bar{W}(\bar{H},\bar{K};\theta^\alpha), \tag{3}$$

where E is a constant having the same unit as W so that $\bar{W}$ becomes dimensionless. Now, by noticing the fact that both H are K the function of θ^α, we expand $\bar{W}$ at the point of flat surface ($\bar{H} = \bar{H}_0, \bar{K} = \bar{K}_0$) and obtain

$$\bar{W} = \bar{W}(\bar{H}_0,\bar{K}_0) + \bar{W}_{\bar{H}}\bar{H} + \bar{W}_{\bar{K}}\bar{K} + \frac{1}{2}\bar{W}_{\bar{H}\bar{H}}\bar{H}^2 + \frac{1}{2}\bar{W}_{\bar{K}\bar{K}}\bar{K}^2 + \cdots, \tag{4}$$

where subscripts denotes partial derivatives (e.g., $\overline{(*)}_{\bar{H}} = \partial\overline{(*)}/\partial\bar{H}$). Since the thickness of lipid membranes (t) is much smaller than their lateral length scale, we conclude that $\bar{H} \ll 1$ and $\bar{K} \ll 1$. Therefore, it is reasonable to take the terms in Eq. (4) up to the second order of 't' (i.e., $\bar{H}^2 = t^2H^2$ and $\bar{K} = t^2K$; the remainder terms can be practically negligible). Further, the first term in Eq. (4) can be identically vanish (i.e., $\bar{W}(\bar{H}_0,\bar{K}_0) = 0$) in the case of flat surface. Consequently, we obtain

$$\bar{W} = a\bar{H} + b\bar{K} + c\bar{H}^2, \tag{5}$$

where constants a, b, and c are the evaluated values of partial derivatives of $\bar{W}$. In particular, for those membranes with symmetric structures about a mid-plane (bilayers), the proposed energy potential must satisfy

$$\bar{W}(\bar{H},\bar{K}) = \bar{W}(-\bar{H},\bar{K}) \tag{6}$$

Thus, we find constant *a* need to be vanished and Eq. (5) can be re-written as

$$W = kH^2 + \bar{k}K \tag{7}$$

where constant *E* in Eq. (3) is now suppressed with constants *b* and *c*. The above procedure is, in fact, compatible to the reduction of 3D liquid crystal theory into the 2D liquid film (see Remark 1.). In practice, *H* and *K* need to be replaced by $\bar{H}/t$ and $\bar{K}/t^2$, respectively (typical thickness of lipid membranes are 5 *nm*-10 *nm* (see for example, Hianik and Passechnik 1995). With the aid of differential geometry, Mean and Gaussian curvature can be evaluated as (Sokolnikoff 1951)

$$H = \frac{1}{2}a^{\alpha\beta}b_{\alpha\beta}, K = \frac{1}{2}\varepsilon^{\alpha\beta}\varepsilon^{\lambda\mu}b_{\alpha\lambda}b_{\mu\beta}, \tag{8}$$

where $a^{\alpha\beta}$ is the inverse of the metric $a_{\alpha\beta}$. Together, they consist of dual metric basis. $\varepsilon^{\alpha\beta} = e^{\alpha\beta}/\sqrt{a}$ is the permutation tensor with a=det($a^{\alpha\beta}$). Here Greek indices take values of 1 and 2. Thus for example, we evaluate $e^{\alpha\beta}$ as e^{11}=e^{22}=0 –e^{21}=1. Einstein summation is applied for the repeated indices. $b_{\alpha\beta}$ is the coefficients of the second fundamental form. The contravariant cofactor of the curvature is defined by

$$\tilde{b}^{\alpha\beta} = \varepsilon^{\alpha\lambda}\varepsilon^{\beta\mu}b_{\lambda\gamma}, \tag{9}$$

and also satisfies

$$b_\mu^\beta\tilde{b}^{\mu\alpha} = Ka^{\beta\alpha}. \tag{10}$$

b_μ^β are the mixed components of the curvature (covariant and contravariant). In the case of symmetric curvature tensors, we have

$$b_\mu{}^\beta = b^\beta{}_\mu \equiv b_\mu^\beta \; for \; \boldsymbol{b} = \boldsymbol{b}^T. \tag{11}$$

These terms furnish the well-known Gauss and Weingarten equation

$$\boldsymbol{a}_{\alpha;\beta} = b_{\alpha\beta}\boldsymbol{n}, \qquad \boldsymbol{n}_{,\alpha} = -b_\alpha^\beta\boldsymbol{a}_\beta. \tag{12}$$

Here, $\boldsymbol{a}_\alpha = \boldsymbol{r}_{,\alpha} = \partial\boldsymbol{r}/\partial\theta^\alpha$ are the tangent vectors to the deformed surface w induced by the parameterization $\boldsymbol{r}(\theta^a)$ the position in 3D space of a point on the surface with coordinates θ^a. Then the unit normal vector field to the local surface orientation can be defined as

$$\boldsymbol{n}(\theta^\alpha) = \frac{1}{2}\varepsilon^{\alpha\beta}\boldsymbol{a}_\alpha \times \boldsymbol{a}_\beta \tag{13}$$

In addition, covariant component of a surface matric can be calculated using the inner product of tangents vectors (i.e., $\boldsymbol{a}_\alpha\cdot\boldsymbol{a}_\beta = \boldsymbol{a}_{\alpha\beta}$). Semi-colon in Eq. (12) denotes surface covariant differentiation. For example, $\boldsymbol{a}_{\alpha;\beta}$ is given by (Sokolnikoff 1951)

$$\boldsymbol{a}_{\alpha;\beta} = \boldsymbol{a}_{\alpha,\beta} - \Gamma_{\alpha\beta}^\lambda\boldsymbol{a}_\lambda, \tag{14}$$

where $\Gamma_{\alpha\beta}^\lambda$ are the Christoffel symbols induced by the surface coordinate on *w* defined as

$$\Gamma_{\alpha\beta}^\lambda = \boldsymbol{a}_{\alpha,\beta}\cdot\boldsymbol{a}^\lambda. \tag{15}$$

Here $\boldsymbol{a}^{\lambda}$ is the dual basis on the deformed surface ($\boldsymbol{a}^{\alpha}=a^{\alpha\beta}\boldsymbol{a}_{\beta}$;$(a^{\alpha\beta})=(a_{\alpha\beta})^{-1}$).

In conclusion, Helfrich model (Eq. (1)) can be used safely for those membranes with sufficiently small thickness comparing to their lateral length scale, uniform distributions in lipid molecules over the membrane and symmetric structures about the mid-surface where tails group is aligned. In other words, Eq. (1) should be used with care in the study of non-symmetric and/or non-uniform lipid membranes (modification of the Helfrich potential may be necessary).

Remark 1

We note here that equilibria of 2D membrane is the limiting case of 3D liquid crystal theory which valid for the case when the thickness of the membrane is much smaller than the lateral length scale. In this case, the thickness-wise expansions of full 3D liquid crystal molecules (provided sufficient regularity in the corresponding trajectory field) are essentially identical to those of 2D membrane (with vanishing thickness) up to the leading order (see more details in Steigmann 2013)

3. Equilibrium and shape equation

We note that for the analytical simplicity, it is assumed that deformed surfaces can be covered by a single coordinated patch. In more general cases, large deformations in particular, it may be necessary to cover the deformed surface by the union of a finite number of patches. This requires connecting boundary information across the neighboring patches. The potential energy of the deformed surface is defined by

$$E = \int_{w} W(H, K; \theta^{\alpha})\, da. \tag{16}$$

In general, it cost lots of energy to induce volume change. Thus, we assume there is no volume change under deformations (incompressibility). To accommodate incompressibility, we consider the following augmented energy functional (Agrawal and Steigmann 2009)

$$E = \int_{\Omega} W(H, K; \theta^{\alpha}) + \lambda(\theta^{\alpha})(J-1)dA, \qquad \because JdA = da, \tag{17}$$

where $\lambda(\theta^{a})$ is a Lagrange-multiplier field. J is the local areal stretch from a fixed reference (Ω) to the deformed surface (w) defined as

$$J = \sqrt{a/A}\,. \tag{18}$$

Here a and A are the corresponding areas of w and Ω, respectively.

The equilibrium state of the membrane can be derived through the variation of the energy. To compute energy variation, it is necessary to evaluate the variational derivatives of J, H and K induced by the virtual displacement $\boldsymbol{u}(\theta^{\alpha}) = \dot{\boldsymbol{r}}$. Here $r(\theta^{a})$ refers equilibrium position filed of the deformed surface and superscript "·" is small deformations (virtual displacements) of the membrane which here simply indicated by the derivative with respect to a parameter $\in$(e.g., $(\dot{*}) = \partial(*)/\partial\epsilon$). In addition, the dot notation states the derivatives at a fixed value of parameter associated with the particular equilibrium state considered (here we set $\in$=0). Therefore, $\boldsymbol{u}(\theta^{\alpha}) = \frac{\partial}{\partial\epsilon}\boldsymbol{r}(\theta^{\alpha};\epsilon)|_{\epsilon=0}$. The same meaning applies to any variables bearing a superposed dot ($\dot{H} =$

$\frac{\partial}{\partial\epsilon}H(\theta^{\alpha};\epsilon)|_{\epsilon=0}, etc$ ...). In order to evaluate total energy variation of membranes, it is essential to account both tangential and normal variations u^{a} and u. This can be done by decomposing the virtual displacement into the normal and tangential components as

$$\boldsymbol{u} = u^{\alpha}\boldsymbol{a}_{\alpha} + u\boldsymbol{n}. \tag{19}$$

We note here that Eq. (19) is the variation of the position of a fixed material point θ^{a} and the coordinate point θ^{a} furnish one to one correspondence to each lipid molecule of the membrane in consideration. Thus, the induced energy variation is given by

$$\dot{E} = \int_{\Omega} \left[J\dot{W} + \dot{J}(W + \lambda)\right]dA. \tag{20}$$

Using Eq. (17), the above can be re-written as

$$\dot{E} = \int_{w} [\dot{W} + (W + \lambda)\dot{J}/J]da, \tag{21}$$

where

$$\dot{W} = W_{H}\dot{H} + W_{K}\dot{K}\ . \tag{22}$$

The week form of the equilibrium equation is given by the virtual-work statement (see for example, Truesdell and Toupin 1960, Mindlin and Tiersten 1962)

$$\dot{E} = P, \tag{23}$$

where P is the virtual work of the applied work.

Under the tangential variations, formulations for the variations of H, J and K are given by (Steigmann *et al*. 2003)

$$\frac{\dot{J}}{J} = u^{\alpha}_{;\alpha}, \dot{H} = u^{\alpha}H_{,\alpha}, \text{and } \dot{K} = u^{\alpha}K_{,\alpha}\ . \tag{24}$$

For example, the second of Eq. (24) can be obtained $\dot{H} = \frac{\partial H}{\partial \epsilon} = \frac{\partial H}{\partial \theta^{\alpha}}\frac{\partial \theta^{\alpha}}{\partial \epsilon} = \frac{\partial H}{\partial \theta^{\alpha}}\frac{\partial \theta^{\alpha}}{\partial \boldsymbol{r}}\cdot\frac{\partial \boldsymbol{r}}{\partial \epsilon} = H_{,\alpha}a^{\alpha}\cdot\boldsymbol{u} = u^{\alpha}H_{,\alpha}$. Thus using Eqs. (23)-(24), we obtain from Eq. (21) that

$$\dot{E} = \int_{w} [u^{\alpha}\left(W_{H}H_{,\alpha} + W_{K}K_{,\alpha}\right) + (W + \lambda)u^{\alpha}_{;\alpha}]da\ . \tag{25}$$

Since $(W+\lambda)u^{\alpha}_{;\alpha} = [(W+\lambda)u^{\alpha} - u^{\alpha}(W+\lambda)_{,\alpha}]$ (i.e., applying integration by parts and $\lambda_{;\alpha} = \lambda_{,\alpha}$ for scalar valued λ), the above can be re-written as

$$\dot{E} = \int_{w} u^{\alpha}\left(W_{H}H_{,\alpha} + W_{K}K_{,\alpha} - W_{,\alpha} - \lambda_{,\alpha}\right)da + \int_{\partial w}(W + \lambda)u^{\alpha}\upsilon_{\alpha}]ds\ . \tag{26}$$

The second term in the above is the result of Green-stoke's theorem and υ_{a} are the covariant components of the exterior unit normal to the boundary (∂w) of the tangent plane w. The orientation of υ_{a} is in the direction of increasing arc length s lying on the tangent plane w. Thus the associated Euler equation (Equilibrium) is the vanishing condition of the parenthetical term in the first integral. Here, we utilize $W_{,\alpha} = W(H,J;\theta^{\alpha})_{,\alpha} = W_{H}H_{,\alpha} + W_{K}K_{,\alpha} + \partial W/\partial\theta^{\alpha}$ and obtain from Eq. (26) as

$$\lambda_{,\alpha}(\theta^{\alpha})_{,\alpha} = -\partial W/\partial\theta^{\alpha} \tag{27}$$

Eq. (27) implies the possible non-uniformity of lipid membranes. In general (except some local parts of the membranes where intra membrane proteins and/or other sub-structures are in present), lipid molecules are distributed over membranes in a fairly uniform manner. In this special case, energy density function W does not depend explicitly on the coordinates θ^a leading to the conclusion λ=constant.

In the case of normal variation (u^a=0), we have (Steigmann *et al*. 2003, Steigmann 1999)

$$\dot{J}/J = -2Hu, 2\dot{H} = \Delta u + u(4H^2 - 2K), \dot{K} = 2KHu + (\tilde{b}^{\alpha\beta}u_{,\alpha})_{;\beta}, \tag{28}$$

where $\Delta(*)=a^{\alpha\beta}(*)_{;\alpha\beta}$ is the Laplace-Beltrami operator defined on the surface. Thus the partial derivative of the energy function can be computed as (see also Agrawal and Steigmann 2009, Kim and Steigmann 2014)

$$2W_H\dot{H} = u[(4H^2 - 2K) + (W_H)_{;\beta\alpha}a^{\beta\alpha}] + (W_H\tilde{b}^{\alpha\beta}u_{,\alpha})_{;\beta} - [(W_H)_{,\beta}a^{\alpha\beta}u]_{;\alpha}, \tag{29}$$

$$W_K\dot{K} = u[(W_K)_{;\beta\alpha}\tilde{b}^{\alpha\beta} + 2KHW_K] + (W_K\tilde{b}^{\alpha\beta}u_{,\alpha})_{;\beta} - [(W_K)_{,\beta}\tilde{b}^{\alpha\beta}u]_{;\alpha}\,. \tag{30}$$

Combining Eqs. (28)-(30) furnish

$$\begin{aligned}\dot{W} &= W_H\dot{H} + W_K\dot{K}\\ &= u\left[W_H(2H^2 - K) + \Delta\left(\frac{1}{2}W_H\right)\right] + \frac{1}{2}(W_Ha^{\alpha\beta}u_{,\alpha})_{;\beta} - \frac{1}{2}[(W_H)_{,\beta}a^{\alpha\beta}]_{;\alpha}\\ &\quad + u[(W_K)_{;\beta\alpha}\tilde{b}^{\alpha\beta} + 2KHW_K] + (W_K\tilde{b}^{\alpha\beta}u_{,\alpha})_{;\beta} - [(W_K)_{,\beta}\tilde{b}^{\alpha\beta}u]_{;\alpha}\,.\end{aligned} \tag{31}$$

It should be noted here that the derivations of Eqs. (28)-(31) is not trivial. Careful review of the processes may be necessary particularly, when considering energy density functions containing other parameters. Consequently, from Eq. (21) the induced normal energy variation can be obtained as

$$\begin{aligned}\dot{E} = &\int_w u\left[\Delta\left(\frac{1}{2}W_H\right) + (W_K)_{;\beta\alpha}\tilde{b}^{\alpha\beta} + W_H(2H^2 - K) + 2KHW_K - 2H(W + \lambda)\right]da\\ &+ \int_{\partial w}\left[\frac{1}{2}W_H v^{\alpha}u_{,\alpha} - \frac{1}{2}(W_H)_{,\alpha}v_{\beta}u + W_K\tilde{b}^{\alpha\beta}v_{\beta}u\right]ds.\end{aligned} \tag{32}$$

Here $\upsilon^a=\alpha^{\alpha\beta}\upsilon_\beta$ is the contravariant components of the exterior unit normal to the boundary. Suppose the membrane is impermeable and enclosing a volume of incompressible liquids. Then the corresponding internal power (pressure from the inside resulting membrane deformations) is given by

$$\int_w uPda\,, \tag{33}$$

where P is pressure per unit area. Accordingly, the Euler equations are grad P=0. This indicates that uniform pressure is applied on the membrane (w). Thus the equivalent state of the equilibrium is $\int_w u[(*) - P]da = 0$. Since u always has non-zero values, we must have P=(*). Applying the results into the first term of Eq. (32) and obtaining

$$\Delta\left(\frac{1}{2}W_H\right) + (W_K)_{;\beta\alpha}\tilde{b}^{\alpha\beta} + W_H(2H^2 - K) + 2KHW_K - 2H(W + \lambda) = P. \tag{34}$$

Eq. (34) together with the Helfrich energy potential (Eq. (7)), we obtain the following shape equation for the membranes as

$$k[\Delta H + 2H(H^2 - K)] - \lambda H = P. \tag{35}$$

Eq. (35) is one of the most commonly used shape equation (Agrawal and Steigmann 2008, Ou-Yang *et al*. 1999, Rosso and Virga 1999) in the analysis of uniform and symmetric lipid membranes.

4. Solutions to the membranes under the boundary excitations

In this section, we present affordable analytical solutions for lipid membranes (rectangular patch) subjected to special classes of boundary loadings. This requires Monge parameterization of the surface mapping function and admissible linearization of the shape Eq. (35). The procedures are essential in the derivation of linearized shape equations. However, details are somewhat standardized and well documented in other literatures (see for example, Agrawal and Steigmann 2009, Belay *et al*. 2015). Thus for the purpose of our study, here we simply adopt the resulting equations as

$$\frac{1}{2}k\Delta_P(\Delta_P z) - \lambda\Delta_P z \tag{36}$$

and

$$H \approx \frac{1}{2}\Delta_P z,\ K = 0, \tag{37}$$

where z represents deformed configuration of the membrane and Δ_p is surface Laplacian and H and K are the linearized mean and Gaussian curvatures. Eq. (36) is a forth order partial differential equation which requires two sets of boundary conditions in order to fully determine unknown constants. Common boundary conditions are prescribed displacements (z), clamping ($\partial z/\partial\theta^\alpha$) and curvature/bending ($\partial^2 z/\partial(\theta^\alpha)^2$). We note here that boundary conditions must be carefully chosen from the admissible boundary sets. Determining admissible boundary conditions is not trivial and requires rigorous derivations using virtual-work statement (Agrawal and Steigmann 2009, Kim and Steigmann 2014).

Among various scenarios, we consider a special case that a rectangular membrane subjected to boundary displacements in the form of sinusoidal functions. This problem is of particular interest, since sinusoidal functions can be easily generated in experimental settings and general types of loadings can be also simulated through the combination of each sinusoidal function using Fourier since series (Belay *et al*. 2015).

From the first term of Eq. (37), we have

$$2H = \Delta_P z\,. \tag{38}$$

By substituting Eq. (38) into Eq. (36) yields

$$\Delta H - \mu^2 H = 0;\ \mu^2 = \lambda/k. \tag{39}$$

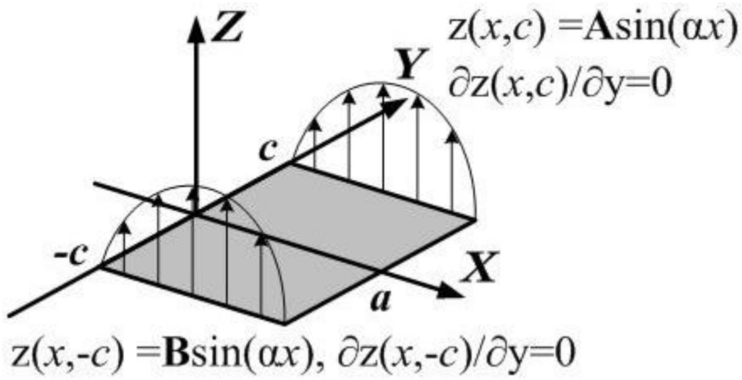

Fig. 1 Schematics of the problem from Eqs. (40)-(42), we obtain the following general solution

Eq. (39) is the modified Helmholtz equation. To get the *z*, we further utilize Eqs. (38)-(39) and obtain (i.e., $\Delta z = 2H = (1/2\mu^2)\Delta H \because \Delta H = \mu^2 H$)

$$z = \left(\frac{2}{\mu^2}\right) H + \varphi, \tag{40}$$

where φ is harmonic function satisfying ($\Delta\varphi$). Since we consider a rectangular shape membrane defined in the cartesian coordinate, the general solution of $H(x,y)$ can be obtained via standard separation of variable method as

$$H(x,y) = \sum_{m=1}^{\infty} (A_m \cos(mx) + B_m\, sin(mx))\,(C_m sinh\sqrt{m^2+\mu^2}y + D_m cosh\sqrt{m^2+\mu^2}y), \tag{41}$$

and φ is the solution of the Laplace equations given by

$$\varphi(x,y) = \sum_{n=1}^{\infty} (A_n \cos(nx) + B_n\, sin(nx))(C_n\, shin(ny) + D_n\, cosh(ny)). \tag{42}$$

$$\begin{aligned} z(x,y) = \left(\frac{2}{\mu^2}\right) \sum_{m=1}^{\infty} (A_m \cos(mx) + B_m\, sin(mx)) \Big(C_m sinh\sqrt{m^2+\mu^2}y \\ + D_m cosh\sqrt{m^2+\mu^2}y\Big) \\ + \sum_{n=1}^{\infty} (A_n \cos(nx) + B_n\, sin(nx))(C_n\, shin(ny) + D_n\, cosh(ny)). \end{aligned} \tag{43}$$

Imposing boundary conditions $z(x,c)$=Asin(αx) and $z(x,-c)$=Bsin(αx), the series expansion in Eq. (43) now reduces

$$\begin{aligned} z(x,-c) = \left(\frac{2}{\mu^2}\right) sin(\alpha x) \Big[-A_1 \sinh\left(\sqrt{\alpha^2+\mu^2}c\right) + B_1 \cosh\left(\sqrt{\alpha^2+\mu^2}c\right) - C_1\, shin(\alpha c) \\ + D_1\, cosh(\alpha c)\Big] = \boldsymbol{A} \sin(\alpha x), \end{aligned} \tag{44}$$

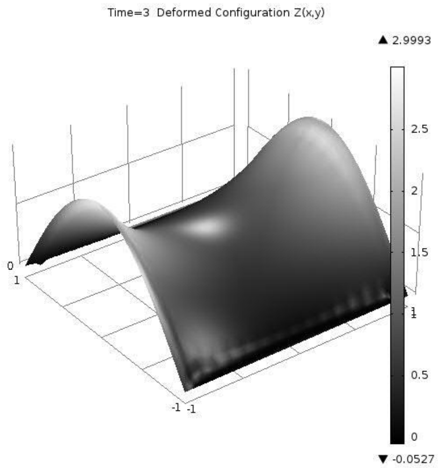

Fig. 2(a) Membrane deformation under sinusoidal loading (2 sides loading)

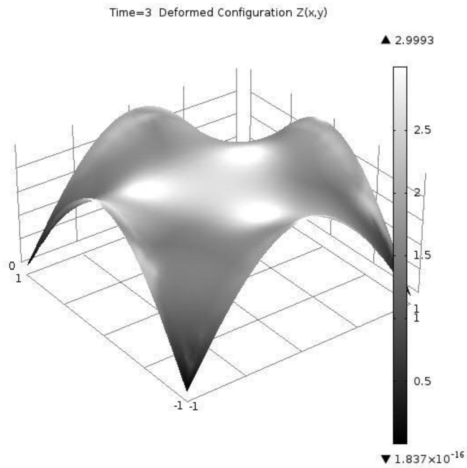

Fig. 2(b) Membrane deformation under sinusoidal loading (superposed solution)

$$z(x,c)=\left(\frac{2}{\mu^2}\right)sin(\alpha x)\left[A_1\sinh(\sqrt{\alpha^2+\mu^2}c)+B_1\cosh(\sqrt{\alpha^2+\mu^2}c)+C_1\,shin(\alpha c)\right.$$
$$\left.+D_1\,cosh(\alpha c)\right] \tag{45}$$
$$=\boldsymbol{B}\sin(\alpha x)\,.$$

Similarly imposing $\partial z(x,c)/\partial y=0$ and $\partial z(x,-c)/\partial y=0$, Eq. (43) yields

$$\partial z(x,-c)/\partial y=\left(\frac{2}{\mu^2}\right)(\cos(\alpha x)+sin(\alpha x))\left[A_1\sqrt{\alpha^2+\mu^2}\cosh\left(\sqrt{\alpha^2+\mu^2}c\right)\right.$$
$$\left.-B_1\sqrt{\alpha^2+\mu^2}\sinh\left(\sqrt{\alpha^2+\mu^2}c\right)-C_1\,\alpha cosh(\alpha c)+D_1\,\alpha sinh(\alpha c)\right]=0, \tag{46}$$

$$\frac{\partial z(x,c)}{\partial y}=\left(\frac{2}{\mu^2}\right)(\cos(\alpha x)+sin(\alpha x))\left[A_1\sqrt{\alpha^2+\mu^2}\cosh(\sqrt{\alpha^2+\mu^2}c)\right.$$
$$\left.+B_1\sqrt{\alpha^2+\mu^2}\sinh(\sqrt{\alpha^2+\mu^2}c)+C_1\,\alpha cosh(\alpha c)+D_1\,\alpha sinh(\alpha c)\right]=0. \tag{47}$$

Thus, unknown constants A_1, B_1, C_1 and D_1 are completely determined and the solution is given by

$$z(x,y)=\left(\frac{2}{\mu^2}\right)sin(\alpha x)\left[-A_1sinh(\sqrt{\alpha^2+\mu^2}y)+B_1\cosh(\sqrt{\alpha^2+\mu^2}y)-C_1\,shin(\alpha y)\right.$$
$$\left.+D_1\,cosh(\alpha y)\right], \tag{48}$$

where $\alpha=\pi/\alpha$ and

$$A_1=(\boldsymbol{B}-\boldsymbol{A})\left(\frac{\mu^2}{4}\right)\left[\frac{\alpha cosh(\alpha c)}{\alpha cosh(\alpha c)\sinh\left(\sqrt{\alpha^2+\mu^2}c\right)-\alpha sinh(\alpha c)\cosh\left(\sqrt{\alpha^2+\mu^2}c\right)}\right],$$

$$B_1 = (\boldsymbol{B}+\boldsymbol{A})\left(\frac{\mu^2}{4}\right)[\frac{\alpha sinh(\alpha c)}{\alpha sinh(\alpha c)\cosh(\sqrt{\alpha^2+\mu^2}c) - \alpha cosh(\alpha c)\sinh(\sqrt{\alpha^2+\mu^2}c}],$$

$$C_1 = (\boldsymbol{A}-\boldsymbol{B})\left(\frac{\mu^2}{4}\right)\left[\frac{\sqrt{\alpha^2+\mu^2}\cosh\left(\sqrt{\alpha^2+\mu^2}c\right)}{\alpha cosh(\alpha c)\sinh\left(\sqrt{\alpha^2+\mu^2}c\right) - \alpha sinh(\alpha c)\cosh\left(\sqrt{\alpha^2+\mu^2}c\right)}\right]$$

$$D_1 = -(\boldsymbol{A}+\boldsymbol{B})\left(\frac{\mu^2}{4}\right)[\frac{\sqrt{\alpha^2+\mu^2}\sinh\left(\sqrt{\alpha^2+\mu^2}c\right)}{\alpha sinh(\alpha c)\cosh(\sqrt{\alpha^2+\mu^2}c) - \alpha cosh(\alpha c)\sinh(\sqrt{\alpha^2+\mu^2}c)}]$$

(Note that in the above analysis, constants appearing in Eq. (43) (e.g., A_m,B_m+...) are now suppressed into A_1, B_1, C_1 and D_1 with given boundary conditions). Eq. (48) offers affordable analytical expressions describing the deformed configurations of the membrane under sinusoidal loading (see Fig. 2(a)). In addition, since the problem in consideration is in linear regime, principles of superposition can be applied to get the solutions of full boundary problems (Fig. 2(b)). With its relatively simple expression, Eq. (48) can be easily adopted in the determination of mechanical responses of lipid membranes subjected to boundary loadings or vice versa (in some cases, minimal modifications may be necessary in order to accommodate the mechanical properties of desired membranes).

5. Substrate Interaction problems with an elliptical contact region

By far, obtaining complete analytical solutions for the membrane-substrate interaction problems are possible only for those substrates with circular cross section (Agrawal and Steigmann 2009). In the case of an elliptical contact region (although this case is more realistic), semi-analytical expressions based on Mathieu's function is the closest possible alternative (Belay *et al*. 2015). Otherwise one has to rely heavily on the numerical analysis to predict the mechanical responses of lipid membranes. However, Mathieu's function itself is not an explicit expression requiring numerical aid to determine each coefficient in the function. Here, we present viable analytical expressions using the method of the small parameter (Kalandiya 1975).

We first define the mapping function that maps (conformally) an elliptic domain (in the z-plane) into a unit circle (in the ζ-plane) as

$$z = \omega(\zeta) = R\left(\zeta + \frac{\varepsilon}{\zeta}\right) = \xi + i\eta, \zeta = \rho e^{i\theta}, |\zeta| = 1, R > 0, 0 < \varepsilon < 1, \tag{49}$$

where $z=x+iy$ is a usual complex variable defined in the z-plane. The major and minor axes of an ellipse are then given by

$$a = R(1+\varepsilon), b = R(1-\varepsilon). \tag{50}$$

From Eq. (49), Eq. (39) transforms into the mapped domain (ζ- plane) as (i.e., $\Delta_{xy} \rightarrow \Delta_{\xi\eta}$)

$$\Delta_{\xi\eta}H - \mu^2|\omega'(\zeta)|H = 0, \omega'(\zeta) = R[1 - \frac{\varepsilon}{\zeta^2}]. \tag{51}$$

Here we suppress the notation of H (i.e., $H(z) = H(\omega(\zeta) = \widehat{H}(\zeta) = H(\zeta))$. We note that, in complex plane, H can be written as $H(z, \bar{z})$, where $\bar{z} = x - iy$ and the Laplace operator satisfies the identity $\Delta=\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}=4\frac{\partial^2}{\partial\zeta\partial\bar{\zeta}}$. Therefore, the modified Helmholtz equation (Eq. (51)) is well defined in the complex domain and the corresponding Laplace operator preserves under the conformal mapping (Muskhelishvili 1953). The substrate-membrane contact boundary conditions (in the case of circular contact region, Agrawal and Steigmann 2009) $\partial H/\partial r=\sigma/k$ now becomes

$$\frac{\partial H}{\partial r}=\frac{\partial H}{\partial\zeta}\frac{\partial\zeta}{\partial z}\frac{\partial z}{\partial r}=\frac{\partial H(\zeta)}{\partial\zeta}\frac{1}{\omega'(\zeta)}e^{i\theta}=\frac{\sigma}{k}. \tag{52}$$

Since $\zeta=\rho e^{i\theta}$ in mapped plane, Eq. (52) further deduces

$$\frac{\partial H(\zeta)}{\partial\zeta}\frac{\partial\zeta}{\partial\rho}=\frac{\partial H(\zeta)}{\partial\rho}=\frac{\sigma}{k}\omega'(\zeta)\equiv h\left(e^{i\theta}\right)\ \because\frac{\partial\zeta}{\partial\rho}=\frac{\partial\rho e^{i\theta}}{\partial\rho}=e^{i\theta}. \tag{53}$$

Thus, the boundary condition in the mapped plane is obtained. The potentials (H, h) satisfying Eqs. (51), (53) are sought in the form of power series in the parameter ε

$$H(\xi,\eta)=\sum_{n=0}^{\infty}\varepsilon^n H_n(\xi,\eta), h\left(e^{i\theta}\right)=\sum_{n=0}^{\infty}\varepsilon^n h_n(\xi,\eta)\,. \tag{54}$$

By substituting Eq. (51) into Eq. (54) and using the expression in Eq. (49), we obtain the following equations in the determination of $H_n(n=0,1,2,\ldots)$

$$\Delta H_0-R^2\mu^2H_0=0,$$

$$\Delta H_1-R^2\mu^2H_1=R^2\mu^2\left[f'(\zeta)+\overline{f'(\zeta)}\right]H_0,\qquad f'(\zeta)=-\frac{1}{\zeta^2}. \tag{54}$$

Further, in view of Eq. (53), $h(e^{i\theta})$ can be found accordingly as

$$h\left(e^{i\theta}\right)=\sum_{n=0}^{1}\varepsilon^n h_n(\xi,\eta)=\frac{\sigma}{k}R+\varepsilon\left(-\frac{\sigma}{k}R\frac{1}{\zeta^2}\right), \tag{56}$$

where it can be easily identified that $h_0=\frac{\sigma}{k}R$ and $h_1=-\frac{\sigma}{k}R\frac{1}{\zeta^2}$.

For n=0, we have $\Delta H_0-R^2\mu^2H_0=0$ and the corresponding boundary condition is $h_0=\frac{\sigma}{k}R$. The standard solution for the problem is well studied and is given in the complex valued form as

$$H_0=\sum_{k=-\infty}^{\infty}j_kK_k\,(\mu R\rho)e^{ik\theta}\,. \tag{57}$$

Eq. (57) must satisfy the boundary condition h_0

$$\left.\frac{\partial H(z)}{\partial r}\right|_{\rho=1}=\sum_{k=-\infty}^{\infty}j_ke^{ik\theta}\mu R(-\frac{1}{2})(K_{k+1}\,(\mu R)+K_{k-1}(\mu R))=\frac{\sigma}{k}R. \tag{58}$$

Therefore, we find

$$j_0=\frac{\sigma}{k}\left(-\frac{2}{\mu}\right)\frac{1}{K_1(\mu R)+K_{-1}(\mu R)}=-\frac{\sigma}{k\mu K_1(\mu R)}\ \because K_n=K_{-n}\,. \tag{59}$$

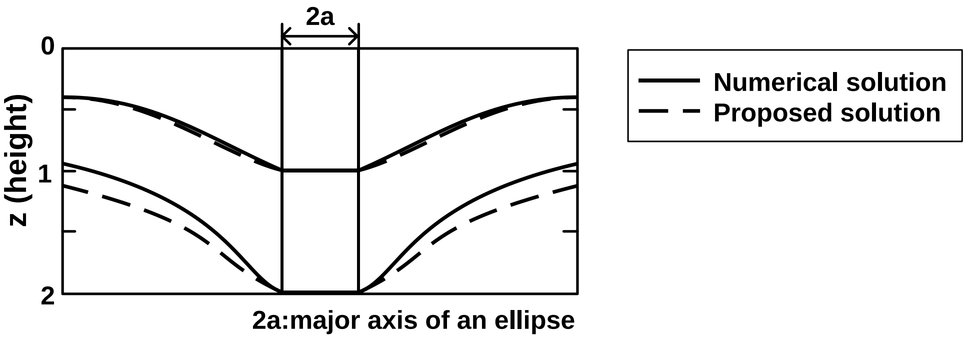

Fig. 3 Membrane deformation under a substrate interaction (elliptic cross section)

Substituting Eq. (59) into Eq. (57) yields

$$H_0 = -F_0 K_0(\mu R\rho);\ F_0 \equiv \frac{\sigma}{k\mu K_1(\mu R)}. \tag{60}$$

For H_1, we have from Eqs. (55), (60) that

$$\Delta H_1 - R^2\mu^2 H_1 = \frac{2R^2\mu^2}{\rho^2} cos2\theta F_0 K_0(\mu R\rho), \qquad \because f'(\zeta) + \overline{f'(\zeta)} = -\frac{2cos2\theta}{\rho^2}. \tag{61}$$

On the basis of the identity (Kalandiya 1975, Muskhelishvili 1953)

$$\frac{d^2 K_n(\mu R\rho)}{d\rho^2} + \frac{1}{\rho}\frac{dK_n(\mu R\rho)}{d\rho} - \left(R^2\mu^2 + \frac{n^2}{\rho^2}\right) K_n(\mu R\rho) = 0. \tag{62}$$

We now consider the following operation for an arbitrary constant $\boldsymbol{A}$

$$\Delta \boldsymbol{A} K_0(\mu R\rho) cos2\theta = \left[\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho}\right) K_0(\mu R\rho) cos2\theta + \frac{1}{\rho^2} K_0(\mu R\rho)\frac{\partial^2}{\partial\theta^2} cos2\theta\right]\boldsymbol{A}. \tag{63}$$

Substituting Eq. (62) (when *n*=0) into Eq. (63) yields

$$\Delta \boldsymbol{A} K_0(\mu R\rho) cos2\theta = \left[R^2\mu^2 K_0(\mu R\rho) cos2\theta - \frac{4}{\rho^2} K_0(\mu R\rho) cos2\theta\right]\boldsymbol{A}. \tag{64}$$

The above equation satisfies $\Delta H_1 - R^2\mu^2 H_1 = \frac{2R^2\mu^2}{\rho^2} cos2\theta F_0 K_0(\mu R\rho)$ when $\boldsymbol{A} = -\frac{1}{2}R^2\mu^2 K_0$. Thus we obtain

$$H_1^{(1)} = -\frac{1}{2} R^2\mu^2 F_0 K_0(\mu R\rho) cos2\theta. \tag{65}$$

Consequently, any solution of Eq. (61) can be represented in the form of

$$H_1 = H_1^{(0)} + H_1^{(1)}, \tag{66}$$

where $H_1^{(0)}$ is the solution of corresponding homogeneous solution (i.e., $\sum_{k=-\infty}^{\infty} j_k e^{ik\theta} K_k(\mu R\rho)$). Similar to Eq. (58), Eq. (66) must satisfy the following boundary condition (h_1) depicted in Eq. (56).

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

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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