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Notes on superposed incremental deformations in the mechanics of lipid membranes

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Abstract
We present an analysis of the superposed incremental deformations of lipid membranes in contact with a circular substrate. A complete analytical solution describing the morphological transitions of lipid membranes is obtained via Monge parametric representation and admissible linearization. The corresponding solution demonstrates smooth and bounded behavior within the finite domain of interest (annular) and, more importantly, shows excellent stability as it approaches the boundary of the circular substrate with the radius of convergence compatible with a few nanometers. Under the prescription of the superposed incremental deformations, a complete analysis of the necessary boundary conditions, the anchoring condition of the lipid molecules on an edge, and other geometrical quantities of the membrane is illustrated for the case of the circular substrate–membrane system.

Keywords
Lipid bilayers, shape equation, substrate–membrane interaction, analytic solution, finite domain.

1. Introduction

In materials perspective, lipid membranes are not ‘simple’ in the sense of Noll [1] due to their distinct lipid molecule configuration (phospholipids). The orientation of lipid molecules is, in general, accounted for by introducing a director field ‘$\mathbf{d}$’ in the constitutive modeling level (see, for example, [2]) further requiring the computation of the strain gradient at each material point. This, together with the complex nature of lipid membrane systems, results in highly non-linear coupled partial differential equations (PDEs), often referred to as membrane shape equations. Despite their inherent complexity, unlike other non-linear PDE systems, membrane shape equations enjoy a wide variety of numerical solutions with ensuing ‘smooth/stable’ behavior regardless of the choice of boundary conditions (Neumann, Dirichlet and/or mixed). This is mainly attributed to the positive definiteness of the Helfrich energy potential [3] through the virtual work statement of liquid crystals dictated by Ericksen [4, 5] and the elastic stability of the membranes with respect to uniqueness theorems [6]. The aforementioned results further promote theoretical study of the mechanics of lipid membranes and the resulting numerical models successfully predict various important cellular functions/phenomena such as substrate–membrane interactions [7], thickness distensions [8] and vesicle formations [9, 10]. However, little work has been devoted to the analytical aspects, since, in most cases, it is extremely difficult to determine analytical potentials of the corresponding PDE system satisfying the desired boundary conditions. A limited number of analytical solutions are reported within the prescription of superposed incremental deformations [11] and the Monge parametric surface representations (see, for example, [7, 10]), yet their practical implications may be limited, since the solutions are defined on an unbounded infinite domain. This is due to the imposition of

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an asymptotic decay condition on a 'remote' boundary (physically infinite) in an effort to obtain smooth and bounded solutions within the domain of interest (on the neighborhood of a substrate).

In this manuscript, we demonstrate a rigorous analysis of the superposed incremental deformations of lipid membranes subjected to substrate interactions. Monge parameterization of a surface is adopted through which a coupled PDE system is reduced to a single PDE solving the surface elevation of the membrane. In particular, we adopt physically more deterministic boundary conditions, rather than imposing asymptotic decay conditions on an external boundary, and obtain a complete analytic solution covering the finite domain of interest. The resulting solution is smooth and bounded within a finite annular domain and demonstrates excellent stability even when the radius of the inner boundary (substrate) converges to an order compatible with the nanoscale, further indicating its ensuing practical applicability (e.g. membrane tethering experiments). In addition, a complete analysis of the necessary boundary conditions is presented (including lipid anchoring conditions on an edge) under the description of superposed incremental deformations in order to give clarity when applied to similar kinds of problem. Lastly, we show that under a 'small' deformation regime there are no clear distinctions between the membrane surface (current/deformed configuration) and the projected plane (reference configuration).

2. Preliminary: Surface geometry of lipid membranes

Let $\mathbf{r}(\theta^\alpha)$ define the parametric position vector in three-dimensional space of a point on the membrane surface with coordinates θ^α. The local surface orientation is then given by $\mathbf{n}(\theta^\alpha) = \frac{1}{2}\varepsilon^{\alpha\beta}\mathbf{a}_\alpha \times \mathbf{a}_\beta$, where $\mathbf{n}$ is a unit vector field and $\mathbf{a}_\alpha$ and $\mathbf{a}_\beta$ are the tangent vectors on the deformed surface ω defined by $\mathbf{r}_{,\alpha} = \partial\mathbf{r}/\partial\theta^\alpha = \mathbf{a}_\alpha$; and $\varepsilon^{\alpha\beta} = e^{\alpha\beta}/\sqrt{a}$ is the permutation tensor with $a = \det|a_{\alpha\beta}|$. Together, they consists local curvilinear coordinate of a point on the membrane surface. Here, Greek indices take values of 1 and 2. Thus, for example, we evaluate $e^{\alpha\beta}$ as $e^{11} = e^{22} = 0$, $e^{12} = -e^{21} = 1$. Einstein summation is applied for repeated indices. The surface matric $a_{\alpha\beta}$ is defined by $a_{\alpha\beta} = \mathbf{a}_\alpha \cdot \mathbf{a}_\beta$, where the dot stands for the conventional Euclidean inner product on the enveloping three-dimensional surface. If $a = \det(a_{\alpha\beta}) \neq 0$, the inverse of the matrix surface matric $a_{\alpha\beta}$ exists (i.e. $a^{\alpha\beta} = (a_{\alpha\beta})^{-1}$) and is referred to as the dual matrix components of $a_{\alpha\beta}$. In addition, a semi-colon denotes surface covariant differentiation. For example, $\mathbf{a}_{\alpha;\beta}$ is defined by [12]

$$\mathbf{a}_{\alpha;\beta} = \mathbf{a}_{\alpha;\beta} = \mathbf{a}_{\alpha,\beta} - \Gamma^\lambda_{\alpha\beta}\mathbf{a}_\lambda, \tag{1}$$

where $\Gamma^\lambda_{\alpha\beta}$ are the Christoffel symbols induced by the surface coordinate on ω defined as

$$\Gamma^\lambda_{\alpha\beta} = \mathbf{a}_{\alpha,\beta} \cdot \mathbf{a}^\lambda. \tag{2}$$

Here $\mathbf{a}^\lambda$ is the dual basis on the deformed surface ω and is defined as $\mathbf{a}^\alpha = a^{\alpha\beta}\mathbf{a}_\beta$. These furnish the well-known Gauss and Weingarten equations:

$$\mathbf{a}_{\alpha,\beta} = (\mathbf{a}_{\alpha,\beta} \cdot \mathbf{a}^\lambda)\mathbf{a}_\gamma + (\mathbf{a}_{\alpha,\beta} \cdot \mathbf{n})\mathbf{n} = \Gamma^\lambda_{\alpha\beta}\mathbf{a}_\gamma + b_{\alpha\beta}\mathbf{n}; b_{\alpha\beta} \equiv \mathbf{a}_{\alpha,\beta} \cdot \mathbf{n} \text{ (Gauss)}, \tag{3}$$

$$\mathbf{n}_{,\alpha} = (\mathbf{n}_{,\alpha} \cdot \mathbf{a}_\beta)\mathbf{a}^\beta + (\mathbf{n}_{,\alpha} \cdot \mathbf{n})\mathbf{n} = -b_{\alpha\beta}\mathbf{a}^\beta;\ b_{\alpha\beta} \equiv -\mathbf{n}_{,\alpha} \cdot \mathbf{a}_\beta \text{ (Weingarten)}. \tag{4}$$

From equations (1) to (3), we obtain

$$\mathbf{a}_{\alpha;\beta} = b_{\alpha\beta}\mathbf{n}. \tag{5}$$

Further, equation (4) can be rewritten by using the dual matrix $a^{\alpha\beta}$ (e.g. $\mathbf{a}_\alpha a^{\alpha\beta} = \mathbf{a}^\beta$) as

$$\mathbf{n}_{,\alpha} = -b_{\alpha\beta}\mathbf{a}^\beta = -b_{\alpha\gamma}a^{\gamma\beta}\mathbf{a}_\beta = -b^\beta_\alpha\mathbf{a}_\beta, \tag{6}$$

where $b_{\alpha\beta}$ are the coefficients of the second fundamental form and b^β_α are the mixed components of the curvature (covariant and contravariant). For symmetric curvature tensors, we find that

$$b_\alpha{}^\beta = b^\beta{}_\alpha \equiv b^\beta_\alpha \text{ for } \mathbf{b} = \mathbf{b}^{\mathrm{T}}, \tag{7}$$

and, from the identity $(\mathbf{n} \cdot \mathbf{a}_\beta)_{,\alpha} = 0$, the symmetric property of the second fundamental form $(b_{\alpha\beta})$ can be

$$b_{\alpha\beta} = -\mathbf{n}_{,\alpha} \cdot \mathbf{a}_\beta = \mathbf{n} \cdot \mathbf{a}_{\beta,\alpha} = \mathbf{n} \cdot \mathbf{r}_{,\beta\alpha} = b_{\beta\alpha}, \tag{8}$$

given sufficient smoothness of the parametric position vector $\mathbf{r}(\theta^\alpha)$ up to the second-order derivative (i.e $\mathbf{r} \in C$). Consequently, the mean and Gaussian curvatures are given by [12]

$$H = \tfrac{1}{2} a^{\alpha\beta} b_{\alpha\beta} \quad \text{and} \quad K = \tfrac{1}{2} \varepsilon^{\alpha\beta} \varepsilon^{\lambda\mu} b_{\alpha\lambda} b_{\beta\mu}, \tag{9}$$

where the contravariant cofactor of the curvature can be expressed as

$$\tilde{b}^{\alpha\beta} = \varepsilon^{\alpha\lambda} \varepsilon^{\beta\gamma} b_{\lambda\gamma}, \tag{10}$$

and satisfies

$$b^{\beta}_{\mu} \tilde{b}^{\mu\alpha} = K a^{\beta\alpha}. \tag{11}$$

3. Formulations in polar coordinates

Much of the literature simply adopts the following results when linearizing the corresponding shape equations (under Monge representation):

$$\begin{gathered} \mathbf{r}(\theta^\alpha) = \theta + z\mathbf{k}, \\ \frac{1}{2} k \Delta_p (\Delta_p z) - \lambda \Delta_p z = P, \;\; H = \tfrac{1}{2} \Delta_p z, \;\; K = 0 \text{ and} \\ a \cong 1, \;\; \mathbf{n} \cong \mathbf{k} - \nabla_p z, \;\; \mathbf{a}^\alpha \cong \mathbf{e}_\alpha + z_{,\alpha} \mathbf{k} \text{ and } \mathbf{b} \cong \nabla_p^2 z \text{ (up to leading order)}, \end{gathered} \tag{12}$$

where z represents the elevation above the membrane, and Δ_p and ∇_p are the projected Laplacian and gradient on the working coordinate. However, the application of the above results directly in various membrane problems and may produce incorrect results, since equation (12) is sensitive to the working coordinate system. For example, the determinant of a is not $\det|a_{\alpha\beta}| = a \cong 1$; in fact, a is evaluated as $a \cong r^2$ in the polar coordinate system. In addition, the surface Laplacian is often misunderstood as a conventional Laplace operator (Δ), especially when using the linearized formula (we will address this in detail in a later section). This further leads to the incorrect imposition of the necessary boundary conditions. In this section, we present the rigorous derivation of formulae regarding the superposed incremental deformations of lipid membranes in polar coordinates, which are most often adopted in these kinds of problems for their guaranteed smoothness on boundaries.

Using polar coordinates $\mathbf{r}(\theta^\alpha)$ can be expressed as

$$\mathbf{r}(\theta^\alpha) = r\mathbf{e}_r(\theta) + z(r,\theta)\mathbf{k}, \;\; \mathbf{e}_r(\theta) = \cos\theta \mathbf{e}_1 + \sin\theta \mathbf{e}_2. \tag{13}$$

Accordingly, we evaluate

$$\mathbf{a}_1 = \frac{\partial \mathbf{r}}{\partial r} = \mathbf{e}_r(\theta) + z_{,r}(r,\theta)\mathbf{k}, \;\; \mathbf{a}_2 = \frac{\partial \mathbf{r}}{\partial \theta} = r\mathbf{e}_\theta(\theta) + z_{,\theta}(r,\theta)\mathbf{k}, \tag{14}$$

and

$$a_{11} = \mathbf{a}_1 \cdot \mathbf{a}_1 = r^2 + z_{,r}^2, \;\; a_{22} = \mathbf{a}_2 \cdot \mathbf{a}_2 = 1 + z_{,\theta}^2, \;\; a_{12} = \mathbf{a}_2 \cdot \mathbf{a}_1 = \mathbf{a}_1 \cdot \mathbf{a}_2 = z_{,r} z_{,\theta}. \tag{15}$$

Thus, the determinant of the surface matrix can be obtained:

$$\det|a_{\alpha\beta}| = a = r^2(1 + z_{,r}^2) + z_{,\theta}^2, \tag{16}$$

and the components of the inverse matrix ($a^{\alpha\beta} = (a_{\alpha\beta})^{-1}$) are then

$$a^{11} = \frac{r^2 + z_{,\theta}^2}{a}, \;\; a^{22} = \frac{1 + z_{,r}^2}{a}, \;\; a^{12} = a^{21} = -\frac{z_{,r} z_{,\theta}}{a}. \tag{17}$$

Since $\mathbf{a}^\alpha = a^{\alpha\beta} \mathbf{a}_\beta$, we also find a dual basis (from equations (14 and 17))

$$\begin{aligned} \mathbf{a}^1 &= a^{11}\mathbf{a}_1 + a^{12}\mathbf{a}_2 = \frac{1}{a}[(r^2 + z_{,\theta}^2)\mathbf{e}_r - r z_{,r} z_{,\theta} \mathbf{e}_\theta + r^2 z_{,r} \mathbf{k}], \\ \mathbf{a}^2 &= \frac{1}{a}[-r z_{,r} z_{,\theta} \mathbf{e}_r + r(1 + z_{,r}^2)\mathbf{e}_\theta + z_{,\theta} \mathbf{k}]. \end{aligned} \tag{18}$$

In addition, from equation (14), the local surface orientation can be found:

$$\mathbf{n} = \frac{\mathbf{a}^1 \times \mathbf{a}^2}{\sqrt{a}} = \frac{1}{\sqrt{a}}(-z_{,\theta}\mathbf{e}_\theta - rz_{,r}\mathbf{e}_r + r\mathbf{k}). \tag{19}$$

3.1. Curvature tensor, mean and Gaussian curvatures, and Laplace–Beltrami operator

Utilizing the dual basis, the curvature tensor $\mathbf{b}$ can be expressed as

$$\mathbf{b} = b_{\alpha\beta}\mathbf{a}^\alpha \otimes \mathbf{a}^\beta;\ b_{\alpha\beta} = \mathbf{a}_{\beta,\alpha} \cdot \mathbf{n}. \tag{20}$$

Thus, for example, we evaluate

$$b_{11} = \mathbf{n} \cdot \mathbf{a}_{1,1} = \frac{1}{\sqrt{a}} rz_{,rr};\ \mathbf{a}_{1,1} = \frac{\partial(\mathbf{e}_r(\theta) + z_{,r}(r,\theta)\mathbf{k})}{\partial r} = z_{,rr}\mathbf{k}, \tag{21}$$

and similarly for

$$b_{12} = b_{21} = \frac{1}{\sqrt{a}}(rz_{,r\theta} - z_{,\theta}),\ b_{22} = \frac{1}{\sqrt{a}}(r^2 z_{,r} + rz_{,\theta\theta}). \tag{22}$$

Therefore, from equations (18) and (20) to (22), the expression of $\mathbf{b}$ is given by

$$\begin{aligned}\mathbf{b} = & \frac{rz_{,rr}}{a^2\sqrt{a}}[(r^2 + z_{,\theta}^2)\mathbf{e}_r - rz_{,r}z_{,\theta}\mathbf{e}_\theta + r^2 z_{,r}^2\mathbf{k}] \otimes [(r^2 + z_{,\theta}^2)\mathbf{e}_r - rz_{,r}z_{,\theta}\mathbf{e}_\theta + r^2 z_{,r}^2\mathbf{k}] \\ & + \frac{rz_{,r\theta} - z_{,\theta}}{a^2\sqrt{a}}[(r^2 + z_{,\theta}^2)\mathbf{e}_r - rz_{,r}z_{,\theta}\mathbf{e}_\theta + r^2 z_{,r}^2\mathbf{k}] \otimes [-rz_{,r}z_{,\theta}\mathbf{e}_r + r(1 + z_{,r}^2)\mathbf{e}_\theta + z_{,\theta}\mathbf{k}] \\ & + \frac{rz_{,r\theta} - z_{,\theta}}{a^2\sqrt{a}}[-rz_{,r}z_{,\theta}\mathbf{e}_r + r(1 + z_{,r}^2)\mathbf{e}_\theta + z_{,\theta}\mathbf{k}] \otimes [(r^2 + z_{,\theta}^2)\mathbf{e}_r - rz_{,r}z_{,\theta}\mathbf{e}_\theta + r^2 z_{,r}^2\mathbf{k}] \\ & + \frac{r^2 z_{,r} - rz_{,\theta\theta}}{a^2\sqrt{a}}[-rz_{,r}z_{,\theta}\mathbf{e}_r + r(1 + z_{,r}^2)\mathbf{e}_\theta + z_{,\theta}\mathbf{k}] \otimes [-rz_{,r}z_{,\theta}\mathbf{e}_r + r(1 + z_{,r}^2)\mathbf{e}_\theta + z_{,\theta}\mathbf{k}].\end{aligned} \tag{23}$$

Lastly, for H and K, we obtain from equations (9), (17), (21) and (22) that

$$H = \frac{1}{2a^{3/2}}[r^3 z_{,rr} + r^2 z_{,r} + r^2 z_{,r}^3 + rz_{,rr}z_{,\theta}^2 - 2rz_{,r\theta}z_{,r}z_{,\theta} + rz_{,\theta\theta} + rz_{,\theta\theta}z_{,r}^2 + 2z_{,r}z_{,\theta}^2], \tag{24}$$

$$K = \frac{1}{a^2}[r^3 z_{,r}z_{,rr} + r^2 z_{,rr}z_{,\theta\theta} - r^2 z_{,r\theta}^2 + 2rz_{,r\theta} - z_{,\theta}^2]. \tag{25}$$

In the case of Helfrich energy potential, $W(H, K; \theta^\alpha = kH^2 + \bar{k}K)$ [3], the corresponding shape equation is given by [7]

$$k[\Delta H + 2H(H^2 - K) - 2\lambda H] = P, \tag{26}$$

where k is an empirical constant, and λ and P are the local Lagrange multiplier and internal pressure, respectively. The delta operator Δ in equation (26) reads as the Laplace–Beltrami operator. Confusion often arises between the conventional Laplacian and the Laplace–Beltrami operator, especially when dealing with linearized formulae. In the present local curvilinear coordinates, the Laplace–Beltrami operator can be evaluated as

$$\Delta\varphi = \text{div}(\text{grad}\varphi) = \text{tr}((\nabla\varphi)_{,\alpha} \otimes \mathbf{a}^\alpha) = \text{tr}(\varphi_{\alpha;\beta}\mathbf{a}^\beta \otimes \mathbf{a}^\alpha) = \varphi_{\alpha;\beta}a^{\alpha\beta}, \tag{27}$$

for any scalar-valued function φ, and $(\nabla\varphi)_{,\alpha}$ is given by

$$(\nabla\varphi)_{,\alpha} = (\varphi_{,\beta}\mathbf{a}^\beta)_{,a} = \varphi_{,\alpha\beta}\mathbf{a}^\beta + \varphi_{,\lambda}(\mathbf{a}^\lambda_{,\alpha} \cdot \mathbf{a}_\beta)\mathbf{a}^\beta = (\varphi_{,\alpha\beta} - \varphi_{,\lambda}\Gamma^\lambda_{\alpha\beta})\mathbf{a}^\beta = \varphi_{\alpha;\beta}\mathbf{a}^\beta. \tag{28}$$

Thus, ΔH can be computed from the above as

$$\begin{aligned}\Delta H = & H_{\alpha;\beta}a^{\alpha\beta} = a^{\alpha\beta}(H_{,\alpha\beta} - H_{,\lambda}\Gamma^\lambda_{\alpha\beta}) \\ = & a^{11}H_{,11} + 2a^{12}H_{,12} + a^{22}H_{,22} - a^{11}(H_{,1}\Gamma^1_{11} + H_{,2}\Gamma^2_{11}) \\ & -2a^{12}(H_{,1}\Gamma^1_{12} + H_{,2}\Gamma^2_{12}) - a^{22}(H_{,1}\Gamma^1_{22} + H_{,2}\Gamma^2_{22}),\end{aligned} \tag{29}$$

where

$$\Gamma^1_{12} = \Gamma^1_{21} = \mathbf{a}_{1,2} \cdot \mathbf{a}^1 = (\mathbf{e}_\theta + z_{,r\theta})\mathbf{k} \cdot \frac{1}{a}[(r^2 + z^2_{,\theta})\mathbf{e}_r - rz_{,r}z_{,\theta}\mathbf{e}_\theta + r^2 z^2_{,r}\mathbf{k}]$$
$$= \frac{rz_{,r}}{a}(-z_{,\theta} + rz_{,r\theta}), \tag{30}$$

and similarly, we have

$$\Gamma^2_{12} = \Gamma^2_{21} = \frac{1}{a}[r(1 + z^2_{,r}) + z_{,r}z_{,\theta}],\ \Gamma^1_{11} = \frac{1}{a}r^2 z_{,r}z_{,rr},\ \Gamma^1_{22} = \frac{1}{a}[-r(r^2 + z^2_{,r}) + r^2 z_{,r}z_{,\theta\theta}],$$
$$\Gamma^2_{11} = \frac{1}{a}z_{,rr}z_{,\theta},\ \Gamma^2_{22} = \frac{1}{a}[rz_{,r}z_{,\theta} + z_{,\theta}z_{,\theta\theta}]. \tag{31}$$

Lastly, from equation (18), the tangential surface gradient of a scalar-valued function is given by

$$\nabla\varphi = \varphi_{,\alpha}\mathbf{a}^\alpha = \varphi_{,1}\mathbf{a}^1 + \varphi_{,2}\mathbf{a}^2 = \varphi_{,r}\frac{1}{a}[(r^2 + z^2_{,\theta})\mathbf{e}_r - rz_{,r}z_{,\theta} + r^2 z_{,r}\mathbf{k}]$$
$$+\varphi_{,\theta}\frac{1}{a}[-rz_{,r}z_{,\theta}\mathbf{e}_r + r(1 + z^2_{,r})\mathbf{e}_\theta + z_{,\theta}\mathbf{k}]. \tag{32}$$

3.2. Superposed incremental deformations in the lipid membrane theory: Polar coordinates

The formulae presented in Sections 1 and 2 can be reduced to more tractable forms under the assumption of superposed incremental deformations (i.e. the product of derivatives can be neglected, e.g. $z_{,r}z_{,\theta} \cong 0$, provided that the induced deformations are reasonably 'small'). Typically, attempts are made to obtained a complete analytic solution. Within this setting, the linearized forms of the covariant and contravariant components of the surface matrix and the induced determinant ($\det|a_{\alpha\beta}| = a \cong 1$) can be obtained as

$$a_{11} = r^2 + z^2_{,r} \cong r^2,\ a_{22} = 1 + z^2_{,\theta} \cong 1,\ \ a_{12} = a_{21}z_{,r}z_{,\theta} \cong 0, \tag{33}$$

$$\det|a_{\alpha\beta}| = a = r^2(1 + z^2_{,r}) + z^2_{,\theta}\ \cong r^2. \tag{34}$$

Thus, equations (17) and (34) yield

$$a^{11} = \frac{r^2 + z^2_{,\theta}}{a} \cong 1,\ a^{22} = \frac{1 + z^2_{,r}}{a} \cong \frac{1}{r^2},\ a^{12} = a^{21} = -\frac{z_{,r}z_{,\theta}}{a} \cong 0. \tag{35}$$

From equations (18) and (35), the linearized form of the dual basis is then given by

$$\mathbf{a}^1 \cong \mathbf{e}_r + z_{,r}\mathbf{k},\ \mathbf{a}^\mathbf{2} \cong \frac{1}{r}\mathbf{e}_\theta + \frac{1}{r^2}\mathbf{k}. \tag{36}$$

In addition, from equations (19) and (34), the local surface orientation can be approximated as

$$\mathbf{n} \cong \mathbf{k} - \frac{1}{r}z_{,\theta}\mathbf{e}_\theta - z_{,r}\mathbf{e}_r = \mathbf{k} - \nabla_p z. \tag{37}$$

Utilizing the results in equations (33) to (37), the components of the curvature now take the following reduced forms:

$$b_{11} = z_{,rr},\ b_{12} = b_{21} = \frac{1}{r}(rz_{,r\theta} - z_{,\theta}),\ b_{22} = \frac{1}{r}(r^2 z_{,r} + rz_{,\theta\theta}). \tag{38}$$

Thus, we obtain the linearized expression of $\mathbf{b}$ as

$$\mathbf{b} \cong z_{,rr}(\mathbf{e}_r \otimes \mathbf{e}_r) + \frac{rz_{,r\theta} - z_{,\theta}}{r^2}[(\mathbf{e}_r \otimes \mathbf{e}_\theta) + (\mathbf{e}_\theta \otimes \mathbf{e}_r)] + \frac{rz_{,r} + z_{,\theta\theta}}{r^2}(\mathbf{e}_\theta \otimes \mathbf{e}_\theta) = \nabla^2_p z, \tag{39}$$

where $\nabla_p^2 z$ is the second gradient on the projected plane (Ω) and the trace of $\nabla_p^2 z$ is the Laplacian on Ω (i.e. $\mathrm{tr}(\nabla_p^2 z) = \Delta_p z$).

Also, from equations (24), (25) and (34), the mean and Gaussian curvatures reduce to

$$H = \frac{1}{2a^{3/2}}[r^3 z_{,rr} + r^2 z_{,r} + r^2 z_{,r}^3 + rz_{,rr} z_{,\theta}^2 - 2rz_{,r\theta} z_{,r} z_{,\theta} + rz_{,\theta\theta} + rz_{,\theta\theta} z_{,r}^2 + 2z_{,r} z_{,\theta}^2]$$
$$\cong \frac{1}{2}[z_{,rr} + \frac{1}{r} z_{,r} + \frac{1}{r^2} z_{,\theta\theta}] = \frac{1}{2}\Delta_p z, \tag{40}$$

$$K = \frac{1}{a^2}[r^3 z_{,r} z_{,rr} + r^2 z_{,rr} z_{,\theta\theta} - r^2 z_{,r\theta}^2 + 2rz_{,r\theta} - z_{,\theta}^2] \cong \mathbf{0}. \tag{41}$$

Consequently, from equations (40) and (41) the corresponding shape equation in equation (26) becomes

$$k[\Delta H + 2H(H^2 - K) - 2\lambda H] \cong \frac{1}{2} k \Delta_p z(\Delta_p z - \lambda \Delta_p z) = P. \tag{42}$$

Now consider the Laplace–Beltrami operator under the assumption of superposed incremental deformations. From equations (30), (31), (35) and (36), the Christoffel symbols reduce to

$$\Gamma_{12}^1 = \Gamma_{21}^1 = \frac{rz_{,r}}{a}(-z_{,\theta} + rz_{,r\theta}) \cong \mathbf{0}, \tag{43}$$

and similarly, we have

$$\Gamma_{12}^2 = \Gamma_{21}^2 = \frac{1}{a}[r(1 + z_{,r}^2) + z_{,r} z_{,\theta}] \cong \frac{\mathbf{1}}{r},$$
$$\Gamma_{11}^1 = \frac{1}{a} r^2 z_{,r} z_{,rr} \cong \mathbf{0}, \ \Gamma_{22}^1 = \frac{1}{a}[-r(r^2 + z_{,r}^2) + r^2 z_{,r} z_{,\theta\theta}] \cong -\mathbf{r},$$
$$\Gamma_{11}^2 = \frac{1}{a} z_{,rr} z_{,\theta} \cong \mathbf{0}, \ \Gamma_{22}^2 = \frac{1}{a}[rz_{,r} z_{,\theta} + z_{,\theta} z_{,\theta\theta}] \cong \mathbf{0}. \tag{44}$$

Therefore, from equation (35) and the above, the leading order form of ΔH is obtained as

$$\Delta H = H_{\alpha;\beta} a^{\alpha\beta} = a^{11} H_{,11} + 2a^{12} H_{,12} + a^{22} H_{,22} - a^{11}(H_{,1}\Gamma_{11}^1 + H_{,2}\Gamma_{11}^2) - 2a^{12}(H_{,1}\Gamma_{12}^1 + H_{,2}\Gamma_{12}^2)$$
$$- a^{22}(H_{,1}\Gamma_{22}^1 + H_{,2}\Gamma_{22}^2)$$
$$\cong H_{,11} + \frac{1}{r^2} H_{,22} + \frac{1}{r} H_{,1} = H_{,rr} + \frac{1}{r} H_{,r} + \frac{1}{r^2} H_{,\theta\theta} = \Delta_p H. \tag{45}$$

Finally, from equation (32), the surface gradient of a scalar-valued function can be linearized as

$$\nabla\varphi = \varphi_{,\alpha}\mathbf{a}^\alpha = \varphi_{,r}\frac{1}{a}[(r^2 + z_{,\theta}^2)\mathbf{e}_r - rz_{,r} z_{,\theta} + r^2 z_{,r}\mathbf{k}] + \varphi_{,\theta}\frac{1}{a}[-rz_{,r} z_{,\theta}\mathbf{e}_r + r(1 + z_{,r}^2)\mathbf{e}_\theta + z_{,\theta}\mathbf{k}]$$
$$\cong \varphi_{,r}\mathbf{e}_r + \varphi_{,\theta}\frac{1}{r}\mathbf{e}_\theta = \nabla_p\varphi. \tag{46}$$

The results presented above are clearly different from those obtained in the Cartesian coordinate system (equation (12)).

Under the prescription of superposed incremental deformations, the corresponding surface Laplacian (Laplace–Beltrami) and gradient reduce to their conventional counterparts on the projected plane (w_p). In addition, the curvature tensor **b** reduces to the second gradient of $z(r, \theta)$ and its trace is the Laplacian on w_p on which the conventional plate bending theory (the Kirchhoff plate model) is built. The results further suggest that, in the 'small' deformation regime, there is no clear distinction between the surface and the projected plane (similar to the case where the Piola stress and Cauchy stress collapse in linear elasticity). In other words, the linearized model possesses inherent limitations in the deformation analysis of lipid membranes often experiencing 'large' morphological transitions. On the other hand, the analytical expressions obtained from linearized theory can still be an effective means of analysis particularly in field applications and/or experimental environments, since they provide instant feedback of the system (e.g. correlations between parameters, visualizing dominant factors, etc.).

4. Membrane–substrate interaction problems with a circular substrate

Based on the formulae derived in the previous section, we consider a membrane–substrate interaction problem in an annular domain. Utilizing Monge parameterization and under the assumption of superposed incremental deformations, we have

$$\frac{1}{2}k\Delta_p(\Delta_p z) - \lambda\Delta_p z = P,\ \ H = \tfrac{1}{2}\Delta_p z,\ K = 0 \text{ and}$$

$$a = r^2,\ \mathbf{n} = \mathbf{k} - \nabla_p z,\ \mathbf{a}^1 = \mathbf{e}_r + z_{,r}\mathbf{k},\ \mathbf{a}^2 = \frac{1}{r}\mathbf{e}_\theta + \frac{1}{r^2}z_{,r}\mathbf{k},$$
$$\text{and } \mathbf{b} = \nabla_p^2 z \text{ (up to leading order)}, \tag{47}$$

where $z(r,\theta)$ represents the elevation of the membrane, Δ_p and ∇_p are the Laplacian and gradient on the projected field, and H and K are the linearized mean and Gaussian curvatures, respectively.

4.1. Edge conditions for an annular domain

The natural boundary condition for the membrane–substrate interaction is given by [7]

$$F_v\cos\gamma + F_n\sin\gamma - M\mathbf{t}\cdot(\nabla_\Gamma\gamma - \mathbf{Bt}) = \sigma,\ F_\tau - M\tau\cdot(\nabla_\Gamma\gamma - \mathbf{Bt}) = 0, \tag{48}$$

where Γ is the boundaries of the substrate (Γ_i) and the surrounding bounded domain (Γ_o), $\mathbf{B}$ is the curvature tensor of Γ and σ is a wetting constant between the walls and the bulk liquid. F_v, F_n and M are the boundary force components and moment, respectively, on $\partial\omega$ (see Figure 1). The expression of F_n is given by [7]

$$F_n = (\tau W_K)' - (\frac{1}{2}W_H)_{,v} - (W_K)_{,\beta}\tilde{b}^{\alpha\beta}v_\alpha. \tag{49}$$

In addition, for the Helfrich-type membrane (e.g. $W_K = k$ etc.), equation (48) reduces to

$$F_n = \bar{k}\tau'(s) - kH_{,v}. \tag{50}$$

A membrane–substrate interaction is in general energetically unfavorable since the electrically charged Phospholipids are deviated from the orientation of the substrate referenced by the unit normal $\mathbf{N}$ to Γ at a point on $\partial\omega$. The corresponding anchoring condition is defined by [13]

$$\mathbf{n}\cdot\mathbf{N} = \cos\gamma \tag{51}$$

in which γ is assigned and $\mathbf{n}$ is parallel to the director field ($\mathbf{d}$: orientation of phospholipids) of the lipid membranes (i.e. $\mathbf{n}\cdot\mathbf{d} = \mathbf{1}$). In addition, $\mathbf{n}$ is the local orientation of the membrane surface (ω) and is normal to both the tangential (τ) and normal ($\mathbf{v}$) vectors at a point on the parametric curve $\mathbf{r}(s)$ of the membrane. Together, they form a local basis $\mathbf{n} = \mathbf{v}\times\tau$; their projected counterparts on the coordinate plane ω_p are $\mathbf{k} = \mathbf{v}_p\times\tau_p$ (see for example Figure 2 for τ and τ_p). In the present case, $\gamma = \pi/2$ (i.e. $\mathbf{n} = \mathbf{k} = \mathbf{d}$ at the interacting boundary $\partial\omega$) indicating that the hydrophobic tail groups of the bilayer are in contact with the substrate (circular) and, therefore, effectively shielded from the surrounding aqueous phase (see [7]). We also note here that, in the present study, the possibility of lipid tilt is excluded (i.e. in general $\mathbf{n}\cdot\mathbf{d} \neq \mathbf{1}$ in the case of a tilted lipid membrane).

The arc length derivative of $\mathbf{r}(S)$ (under the Monge representation) on the projected curve can be evaluated as (see Figure 2)

$$\mathbf{r}(S)' = \frac{d\mathbf{r}}{dS} = \frac{d(\theta + z(\theta)\mathbf{k})}{dS} = \frac{d\theta}{dS} + \left(\frac{z(\theta)}{d\theta}\cdot\frac{d\theta}{dS}\right)\mathbf{k} = \tau_p + (\nabla_p z\cdot\tau_p)\mathbf{k}; \frac{d\theta}{dS} \equiv \tau_p. \tag{52}$$

Equation (52) is also equivalent to

$$\mathbf{r}(S)' = \frac{d\mathbf{r}(s)}{ds}\frac{ds}{dS} = \tau|\mathbf{r}(s)'|, \quad \frac{d\mathbf{r}(s)}{ds} \equiv \tau, \quad \frac{ds}{dS} \equiv |\mathbf{r}(s)'|. \tag{53}$$

Thus, from equations (52) and (53) we obtain

$$\mathbf{r}(S)' = \tau|\mathbf{r}(s)'|,\ \tau_p + (\nabla_p z \cdot \tau_p)\mathbf{k}, \text{ and} \tag{54}$$

$$|\mathbf{r}(s)'| = |\tau_p + (\nabla_p z \cdot \tau_p)\mathbf{k}| = \sqrt{1 + (\nabla_p z \cdot \tau_p)^2} \cong 1. \tag{55}$$

Comparing the right-hand sides of equations (54) and (55) yields

$$\tau \cong \tau_p + (\nabla_p z \cdot \tau_p)\mathbf{k}. \tag{56}$$

Utilizing the results in (47), the above further gives

$$\mathbf{v} = \tau \times \mathbf{n} \cong [\tau_p + (\nabla_p z \cdot \tau_p)\mathbf{k}] \times (\mathbf{k} - \nabla_\mathbf{p}\mathbf{z}) = \mathbf{v}_p + \nabla_p z \times \tau_p. \tag{57}$$

Now, $H_{,\,v}$ can be rewritten as

$$H_{,\,v} = \left(\frac{\partial H}{\partial \theta^\alpha}\right)\left(\frac{\partial \theta^\alpha}{\partial \mathbf{r}}\right) \cdot \frac{\partial \mathbf{r}}{\partial v} = \mathbf{a}^\alpha H_{,\,\alpha} \cdot \left(\frac{\partial \mathbf{r}}{\partial \theta^\alpha}\right)\left(\frac{\partial \theta^\alpha}{\partial v}\right) = \mathbf{a}^\alpha H_{,\,\alpha} \cdot \mathbf{a}_\beta v^\beta = \mathbf{v} \cdot \mathbf{a}^\alpha H_{,\,\alpha}. \tag{58}$$

By substituting equations (47) and (57) into equation (58), the leading-order expression of $H_{,\,\alpha}$ can be evaluated on the projected plane as

$$\begin{aligned} H_{,\,v} &= \mathbf{v} \cdot \mathbf{a}^\alpha H_{,\,\alpha} = [\mathbf{v}_p + \nabla_p z \times \tau_p + \ldots] \cdot [\mathbf{e}_\alpha + z_{,\,\alpha}\mathbf{k} + \ldots]H_{,\,\alpha} \\ &\cong \mathbf{v}_p \cdot (\mathbf{e}_\alpha H_{,\,\alpha}) = \mathbf{v}_p \cdot \nabla_p H. \end{aligned} \tag{59}$$

Also, the arc length derivative of $\tau(S)$ on the projected curve is defined by

$$\tau'(S) = \frac{d\tau}{dS} = \frac{d\tau}{d\theta} \cdot \frac{d\theta}{dS} = \nabla_p \tau \cdot \tau_p. \tag{60}$$

In view of equations (59) and (60), equation (50) becomes

$$F_n \cong \bar{k} \nabla_p \tau \cdot \tau_p - k \mathbf{v}_p \cdot \nabla_p H. \tag{61}$$

Here the expression of τ can be obtained via the curvature tensor $\mathbf{b}$ as

$$\mathbf{b}\mathbf{v} \cdot \tau = \tau\tau \cdot \tau = \tau, \tag{62}$$

and

$$\mathbf{b} = k_v(\mathbf{v} \otimes \mathbf{v}) + k_\tau(\tau \otimes \tau) + \tau(\tau \otimes v + \mathbf{v} \otimes \tau), \tag{63}$$

where $\mathbf{b}$ is expressed in local coordinates ($\mathbf{n} = \mathbf{v} \times \tau$), k_v and k_τ are the normal curvatures of ω in the directions of $\mathbf{v}$ and τ, respectively, and τ is the twist of the surface ω. Consequently, from equations (47), (56), and (57), together with equation (62), we find that

$$\tau = \mathbf{b}\mathbf{v} \cdot \tau \cong [\nabla_p^2 z(\mathbf{v}_\mathbf{p} + \nabla_p z \times \tau_\mathbf{p})] \cdot [\tau_\mathbf{p} + (\nabla_\mathbf{p}\mathbf{z} \cdot \tau_\mathbf{p})\mathbf{k}] \cong \tau_\mathbf{p} \cdot (\nabla_p^2 z)\mathbf{v}_\mathbf{p}. \tag{64}$$

Finally, the curvatures of the inner and outer boundaries of an annular domain are found to be

$$\mathbf{B}_i = -r_\mathrm{i}^{-1}\mathbf{e}_\theta \otimes \mathbf{e}_\theta \text{ (inner boundary: } \partial\omega_i),\ \mathbf{B}_i = -r_\mathrm{o}^{-1}\mathbf{e}_\theta \otimes \mathbf{e}_\theta \text{ (outer boundary: } \partial\omega_o), \tag{65}$$

where r_i and r_o are the radii of the inner and outer boundaries of the annular domain, respectively. Hence, by noticing the lipid anchoring condition ($\gamma = \pi/2$) and $\mathbf{t} = \mathbf{n} = \mathbf{k}$ at the boundaries, we find from equation (48) that

$$\begin{aligned} F_v \cos\frac{\pi}{2} + F_n \sin\frac{\pi}{2} - M\mathbf{t} \cdot \left(\nabla_\Gamma\left(\frac{\pi}{2}\right) - (-\mathbf{r}_\mathrm{i}^{-1}\mathbf{e}_\theta \otimes \mathbf{e}_\theta)\mathbf{t}\right) &= F_n = \sigma, \\ F_\tau - M\tau \cdot \left(\nabla_\Gamma\left(\frac{\pi}{2}\right) - (-\mathbf{r}_\mathrm{i}^{-1}\mathbf{e}_\theta \otimes \mathbf{e}_\theta)\mathbf{t}\right) &= F_\tau = 0 \text{ (on } \partial\omega_i), \end{aligned} \tag{66}$$

and similarly for the outer boundary:

$$F_n = \sigma,\ F_\tau = 0 \text{ (on } \partial\omega_o). \tag{67}$$

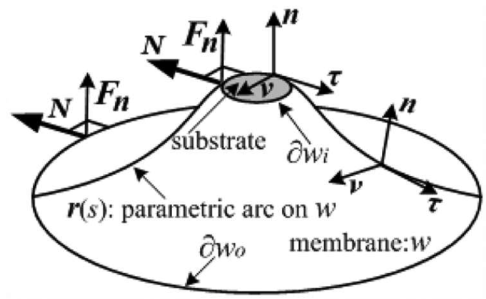

Figure 1. Schematic of the substrate–membrane structure.

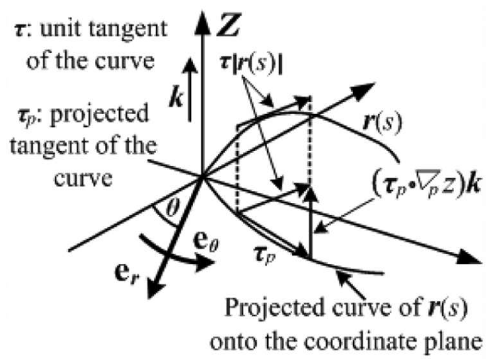

Figure 2. Schematic of projected vector of Γ: Example(τ).

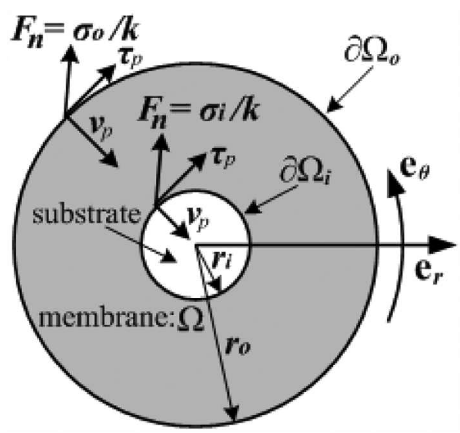

Figure 3. Schematic of the substrate–membrane interaction problem.

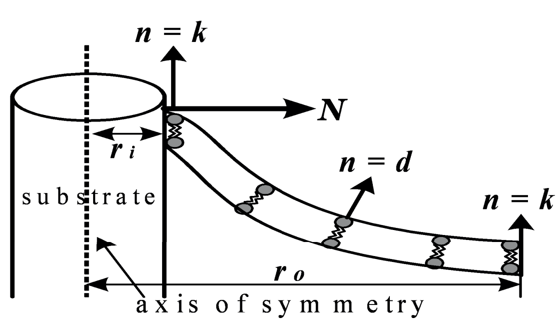

Figure 4. Anchoring and edge conditions on the inner and outer boundaries.

4.2. Substrate–membrane interaction problem on an annular domain

We now consider a substrate–membrane problem under the prescription of a superposed incremental deformation and Monge representation as illustrated in Figure 3. From equation (47), we have that

$$2H = \Delta_p z. \tag{68}$$

Here, we further limit our analysis to the axisymmetric case considering the uniformity of the lipid distribution over the domain of interest and geometrical characteristics of an annular membrane. From the result in equation (68), the membrane shape equation in equation (47) becomes

$$\Delta_p H - \mu^2 H = 0;\ \mu^2 = 2\lambda/k. \tag{69}$$

Hence, from equations (68) and (69), $z(r, \theta) = z(r)$ now takes the form

$$z = \left(\frac{2}{\mu^2}\right) H + \varphi;\ \Delta_p z = 2H = \left(\frac{2}{\mu^2}\right) \Delta_p H \text{ and } \left(\frac{1}{\mu^2}\right) \Delta_p H = H, \tag{70}$$

where φ is a harmonic function satisfying $\Delta\varphi = 0$. In the case of axisymmetry, equation (69) further reduces to

$$rH_{,rr} + H_{,r} - r\mu^2 H = 0;\ \mu^2 = 2\lambda/k. \tag{71}$$

Accordingly, the general solution of $H(r)$ is then given by

$$H(r) = C_1 J_o((-i)\mu^3 r) + C_2 Y_o((-i)\mu^3 r), \tag{72}$$

where J_o and Y_o are the Bessel functions of the first and second kind, respectively. Thus, from equations (70) and (72), the complete analytical solution of $z(r)$ is given by

$$z(r) = \left(\frac{2}{\mu^2}\right) [C_1 J_o((-i)\mu^3 r) + C_2 Y_o((-i)\mu^3 r)] + C_3 I_o((-i)\mu^3 r) + C_4 K_o((-i)\mu^3 r), \tag{73}$$

where φ is the solution of the Laplace equations (i.e. $\Delta_p p = 0$) expressed in terms of Bessel functions as

$$\varphi = C_3 I_o((-i)\mu^3 r) + C_4 K_o((-i)\mu^3 r). \tag{74}$$

Here, I_o and K_o are the modified Bessel functions of the first and second kind. We note here that, again, the emphasis is placed on seeking an analytical solution valid on a 'finite' domain rather than an 'infinite' unbounded domain. The latter case is the consequence of utilizing asymptotic decay conditions on the remote boundary which is physically 'less' significant and therefore may not be suitable for direct field applications and/or experiments.

From equations (61) and (66), on $\partial\Omega_i$ ($r_\mathrm{i} = a$, $\tau_p = -\mathbf{e}_\theta$, $\mathbf{v}_p = -\mathbf{e}_\mathbf{r}$; see Figure 3), we require

$$F_n = \bar{k}\left(\frac{\partial \tau}{\partial r}\mathbf{e}_\mathbf{r} + \frac{1}{r}\frac{\partial \tau}{\partial \theta}\mathbf{e}_\theta\right) \cdot (-\mathbf{e}_\theta) - k(-\mathbf{e}_\mathbf{r}) \cdot \left(\frac{\partial H}{\partial r}\mathbf{e}_\mathbf{r} + \frac{1}{r}\frac{\partial H}{\partial \theta}\mathbf{e}_\theta\right) \tag{75}$$

Since $\tau \cong \tau_\mathbf{p} \cdot (\nabla_p^2 z)\mathbf{v}_\mathbf{p} = -\, \mathbf{e}_\theta \cdot (-\mathbf{e}_\mathbf{r})\nabla_p^2 z = 0$ (equation (64)) and $\mathbf{e}_\theta \cdot \mathbf{e}_\theta = \mathbf{1}$, the above further reduces to

$$F_n = \frac{\partial H}{\partial r} = \frac{\sigma_i}{k} \text{ on } \partial\Omega_i\ (r_\mathrm{i} = a), \tag{76}$$

and similarly on $\partial\Omega_o$ ($r_\mathrm{o} = b$, $\tau_p = -\mathbf{e}_\theta$, $\mathbf{v}_p = -\mathbf{e}_\mathbf{r}$; see Figure 3) we obtain

$$F_n = \frac{\partial H}{\partial r} = \frac{\sigma_o}{k} \text{ on } \partial\Omega_o\ (r_\mathrm{o} = a). \tag{77}$$

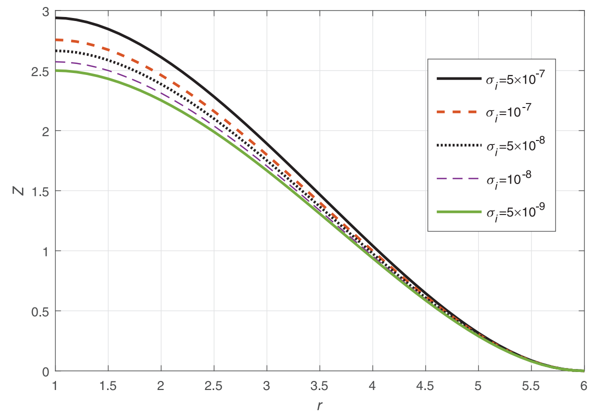

Figure 5. Membrane–substrate interaction $z(r)$ with respect to σ_i/k when $\sigma_0/k = 0.12$.

Accordingly, from equations (72), (76), and (77), the unknown constants C_1 and C_2 can be determined to be

$$C_1 = \frac{(\frac{\sigma_i}{k})Y_1((-i)\mu^3 a) - (\frac{\sigma_o}{k})Y_1((-i)\mu^3 b)}{(-i)\mu^3[J_1((-i)\mu^3 a)Y_1((-i)\mu^3 b) - Y_1((-i)\mu^3 a)J_1((-i)\mu^3 b)]} \text{ and}$$
$$C_2 = \frac{(\frac{\sigma_i}{k})J_1((-i)\mu^3 a) - (\frac{\sigma_o}{k})J_1((-i)\mu^3 b)}{(-i)\mu^3[J_1((-i)\mu^3 a)Y_1((-i)\mu^3 b) - Y_1((-i)\mu^3 a)J_1((-i)\mu^3 b)]}. \quad (78)$$

Since $\mathbf{n} = \mathbf{k}$ on the boundaries (see Figure 4), equation (47) yields

$$\mathbf{n} = \mathbf{k} - \nabla_p z \rightarrow \nabla_p z(r) = \frac{\partial z}{\partial r}\mathbf{e_r} + \frac{1}{r}\frac{\partial z}{\partial \theta}\mathbf{e}_\theta = \frac{\partial z}{\partial r}\mathbf{e_r} = 0 \text{ on both } \partial\Omega_i \text{ and } \partial\Omega_o. \quad (79)$$

Therefore, C_3 and C_4 can be found from equations (73) and (79):

$$C_3 = -\frac{2[(\frac{\sigma_i}{k})K_1((-i)\mu^3 a) - (\frac{\sigma_o}{k})K_1((-i)\mu^3 b)]}{(-i)\mu^5[I_1((-i)\mu^3 a)K_1((-i)\mu^3 b) - K_1((-i)\mu^3 a)J_1((-i)\mu^3 b)]} \text{ and}$$
$$C_4 = -\frac{2[(\frac{\sigma_i}{k})I_1((-i)\mu^3 a) - (\frac{\sigma_o}{k})I_1((-i)\mu^3 b)]}{(-i)\mu^5[I_1((-i)\mu^3 a)K_1((-i)\mu^3 b) - K_1((-i)\mu^3 a)J_1((-i)\mu^3 b)]}. \quad (80)$$

Consequently, the solution of $z(r)$ is given by

$$z(r) = \left(\frac{2}{\mu^2}\right)[C_1 J_o((-i)\mu^3 r) + C_2 Y_o((-i)\mu^3 r)] + C_3 I_o((-i)\mu^3 r) + C_4 K_o((-i)\mu^3 r), \quad (81)$$

where the unknown constants C_1, C_2, C_3 and C_4 are completely determined in equations (78) and (80). The corresponding results are presented in Figures 5 to 10. We also note here that parameters (e.g. λ, k and σ) in the simulations are normalized unless otherwise mentioned and the adopted material properties of a membrane are consistent with the experimental results given in [14, 15] for a lipid membrane of thickness 10 nm in a relaxed state (i.e. $k = 82 \times 10^{-9}$ N·mm, $\bar{k} = 0$). Figures 5 to 8 demonstrate that solutions for both $z(r)$ and $H(r)$ are bounded and smooth within a finite domain of interest (annulus). In particular, the results in Figures 9 and 10 illustrate that the solution is smooth and stable as r_i converges to a few nanometers which further indicates that the proposed solution can be employed in membrane tethering experiments knowing the typical length scale of a phospholipid (see, for example, [16]).

5. Conclusions

In this manuscript, we consider the superposed incremental deformations of lipid membranes interacting with a circular substrate. Instead of employing asymptotic decay conditions on a 'remote' boundary, we imposed physically more realistic conditions (i.e. traction and lipid orientations) on the deterministic boundary (outer rim of an

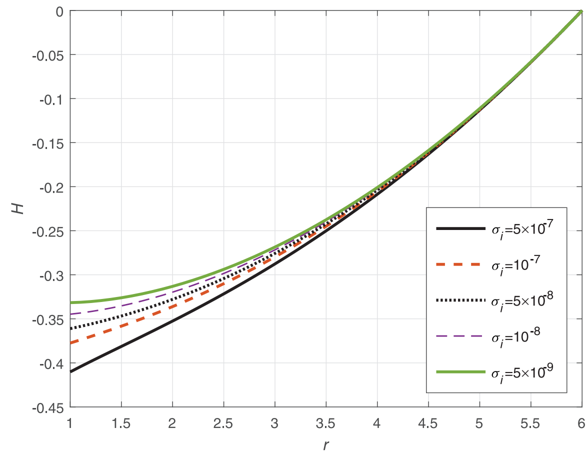

Figure 6. Solution of $H(r)$ with respect to σ_i/k when $\sigma_0/k = 0.12$.

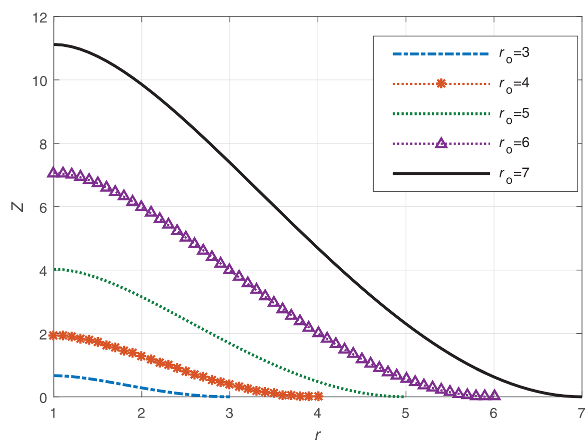

Figure 7. Membrane–substrate interaction with respect to r_o when $\sigma_0/k = 0.12$, $\sigma_i/k = 0.61$.

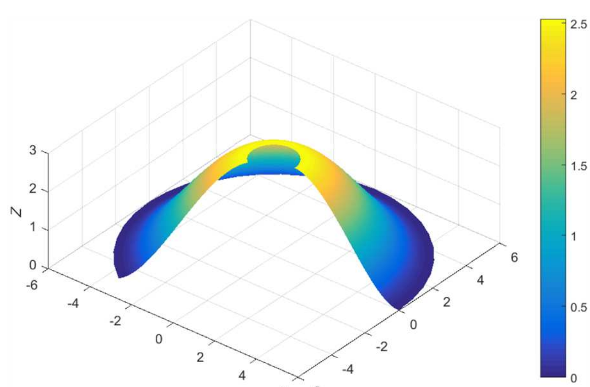

Figure 8. Membrane–substrate interaction when $\sigma_0/k = 0.12$, $\sigma_i/k = 0.61$.

annular domain) and obtained a complete analytical solution via the superposed incremental deformations and Monge surface parameterization. The resulting solution is smooth/stable within the finite annular domain and, more importantly, demonstrates excellent stability as the radius of the inner boundary (substrate) approaches a few nanometers. This further promotes practical implications of the model in various field exercises such as membrane tethering tests and bending experiments. Within the description of the superposed incremental deformations, we conduct a complete examination of the necessary boundary conditions and other geometrical

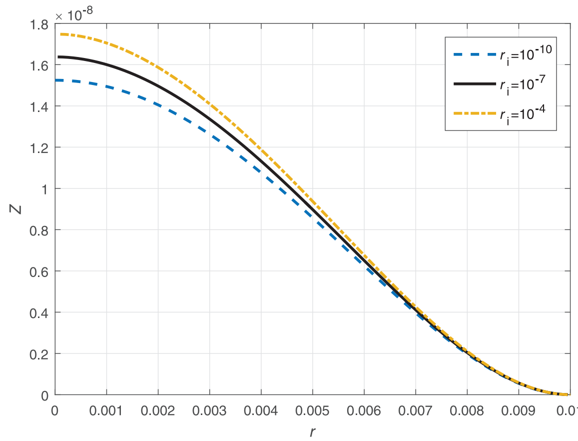

Figure 9. Deformations of a lipid membrane with respect to r_i when $r_o = 0.01$ m, $\sigma_0/k = 0.12$, $\sigma_i/k =$ 0.61.

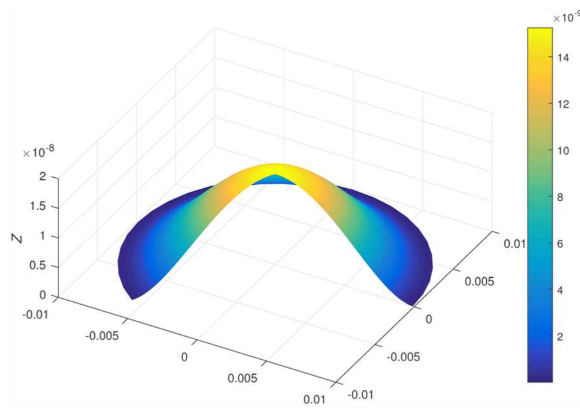

Figure 10. Simulation result of tethered lipid membrane when $\sigma_0/k = 0.12$, $\sigma_i/k = 0.61$.

quantities of membranes and illustrate that the surface deformed configuration and the projected plane (reference frame) collapses in the 'small' deformation regime. As such, the surface Laplacian (Laplace–Beltrami) and gradient reduce to their conventional counterparts on the projected plane (ω_p) and the corresponding curvature tensor **b** deduces into the second gradient of $z(r, \theta)$. Its trace is found to be the Laplacian on ω_p (i.e. $\Delta_p z = \text{tr}(\nabla_p^2 z)$). In addition, the final deformed configuration is energetically favorable/stable within the adopted energy functional (Helfrich) and unique by virtue of the virtual work statement [6]. A complete analysis of the membrane anchoring condition on the boundaries (including lipid orientations) is also presented in an effort to enhance the applicability of the presented model.

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