Supplemental Material: General neck condition for the limit shape of budding vesicles

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Abstract

We present a detailed derivation of the shape equation and linking conditions for lipid vesicles with two-phase domains. We find that the linking conditions are related to the balances of force and moment on the separation curve by using the concepts of stress and moment tensors.

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I. MATHEMATICAL PRELIMINARY

In this section, we introduce the geometry of surfaces and calculus of variation based on the moving frame method. The moving frame method was firstly originated from mechanics. Then this method was carried forward by Cartan in differential geometry. This section may be skipped if the reader is familiar with differential geometry [1], differential forms [2], and calculus of variation by using moving frame method [3, 4].

A. Surface theory based on the moving frame method

The geometric theory of surfaces based on the moving frame method can be found in many elementary textbooks on differential geometry, for example, see [1].

Each point on a 2-dimensional (2D) surface may be represented by a position vector \( \mathbf{r} \). As shown in Fig. 1, at each point we may construct three unit orthonormal vectors \( \mathbf{e}_1, \mathbf{e}_2, \) and \( \mathbf{e}_3 \) with \( \mathbf{e}_3 \) being the normal vector of the surface at point \( \mathbf{r} \). The set of right-handed orthonormal triple-vectors \( \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} \) is called a frame at point \( \mathbf{r} \). The set \( \{\mathbf{r}; \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} \) is called a moving frame.

![FIG. 1. (Color online)The moving frame on a surface.](image)

The differentiation of the frame may be defined as:

\[
\mathrm{d}\mathbf{r} = \omega_1 \mathbf{e}_1 + \omega_2 \mathbf{e}_2, \quad (1)
\]

and

\[
\mathrm{d}\mathbf{e}_i = \omega_{ij} \mathbf{e}_j, \quad (i = 1, 2, 3) \quad (2)
\]
where $\omega_1$, $\omega_2$, and $\omega_{ij} = \omega_{ji}$ ($i, j = 1, 2, 3$) are 1-forms, and 'd' is the exterior differential operator. The repeated subscripts in this paper abide by the Einstein summation convention.

The area element may be expressed as

$$\text{d}A \equiv \omega_1 \wedge \omega_2.$$  \hspace{1cm} (3)

The structure equations of the surface can be expressed as:

$$\begin{cases} 
\text{d}\omega_1 = \omega_{12} \wedge \omega_2, \\
\text{d}\omega_2 = \omega_{21} \wedge \omega_1, \\
\text{d}\omega_{ij} = \omega_{ik} \wedge \omega_{kj} \quad (i, j = 1, 2, 3),
\end{cases}$$  \hspace{1cm} (4)

and

$$\omega_1 \wedge \omega_{13} + \omega_2 \wedge \omega_{23} = 0,$$  \hspace{1cm} (5)

where '\wedge' represents the wedge production between two differential forms. From Eq. (5) we know that $\omega_{13}$ and $\omega_{23}$ may be expressed as

$$\begin{pmatrix} \omega_{13} \\
\omega_{23} \end{pmatrix} = \begin{pmatrix} a & b \\
b & c \end{pmatrix} \begin{pmatrix} \omega_1 \\
\omega_2 \end{pmatrix}.$$  \hspace{1cm} (6)

Then we can define the curvature tensor as

$$\mathcal{C} = ae_1 e_1 + be_1 e_2 + be_2 e_1 + ce_2 e_2,$$  \hspace{1cm} (7)

where $e_i e_j$ ($i, j = 1, 2$) represents the dyad of $e_i$ and $e_j$. The mean curvature is defined as a half of the trace of the curvature tensor, i.e.,

$$H = \text{tr}(\mathcal{C})/2 = (a + c)/2.$$  \hspace{1cm} (8)

The Gaussian curvature is defined as the determinant of the curvature tensor, i.e.,

$$K = \det(\mathcal{C}) = ac - b^2.$$  \hspace{1cm} (9)

For a curve on the surface, at each point on the curve we can construct the tangent vector $t$ and the normal vector $N$ of the curve. The curvature of the curve is defined as

$$\kappa = (\text{d}t/\text{d}s) \cdot N.$$  \hspace{1cm} (10)
where $s$ represents the arc-length parameter of the curve. At the same point, $\mathbf{e}_3$ is the normal vector of the surface. Define vector $\mathbf{N}' = \mathbf{e}_3 \times \mathbf{t}$. Then the normal curvature, the geodesic curvature, and the geodesic torsion of the curve may be defined as

$$\kappa_n = \kappa \mathbf{N} \cdot \mathbf{e}_3, \quad (11)$$
$$\kappa_g = \kappa \mathbf{N} \cdot \mathbf{N}', \quad (12)$$
$$\tau_g = -\mathbf{N}' \cdot (d\mathbf{e}_3/ds), \quad (13)$$

respectively. If we use $\varphi$ to denote the angle between $\mathbf{t}$ and $\mathbf{e}_1$ at the same point, then the normal curvature, the geodesic curvature, and the geodesic torsion of the curve may be further expressed as

$$\kappa_n = a \cos^2 \varphi + 2b \cos \varphi \sin \varphi + c \sin^2 \varphi, \quad (14)$$
$$\tau_g = b \cos 2\varphi + (c - a) \cos \varphi \sin \varphi \quad (15)$$
$$k_g = (d\varphi + \omega_{12})/ds \quad (16)$$

respectively. In particular, if $\mathbf{t}$ aligns with $\mathbf{e}_1$, i.e., $\varphi = 0$, then $\kappa_n, k_g$ and $\tau_g$ may be further simplified as

$$\kappa_n = a, \quad k_g = \omega_{12}/ds, \quad \tau_g = b, \quad (17)$$

respectively. From Eqs.(8), (9) and (17), we may obtain the following identity:

$$\kappa_n(2H - \kappa_n) - \tau_g^2 = K. \quad (18)$$

**B. Hodge star operator and its generalization**

The Hodge star ($\ast$) operator satisfies $\ast \omega_1 = \omega_2$ and $\ast \omega_2 = -\omega_1$ [2]. The generalized Hodge star ($\tilde{\ast}$) operator satisfies $\tilde{\ast} \omega_1 = \omega_2$ and $\tilde{\ast} \omega_2 = -\omega_1$ [3]. The generalized differential operator ($\tilde{\partial}$) satisfies $\tilde{\partial} f = f_1 \omega_1 + f_2 \omega_2$ [3].

By using the Hodge stars and the differential operators, we may define the gradient operator (of the first kind) and the gradient operator of the second kind as [3]:

$$\nabla f \cdot d\mathbf{r} = df, \quad (19)$$

and

$$\tilde{\nabla} f \cdot *d\mathbf{r} = \tilde{\ast} df, \quad (20)$$
respectively. Simultaneously, we may define the Laplace operator (of the first kind) and the Laplace operator of the second kind as [3]:

\[(\nabla^2 f) \, dA = d \star df,\]  \hspace{1cm} (21)

and

\[(\nabla \cdot \tilde{\nabla} f) \, dA = d\tilde{\star} \tilde{df},\]  \hspace{1cm} (22)

respectively.

For a vector (or tensor) field \( u \) defined on the surface, we may define the 2D curl and divergence of the field as:

\[(\text{curl } u) \, dA = d(u \cdot dr),\]  \hspace{1cm} (23)

and

\[(\text{div } u) \, dA = d(\star u \cdot dr),\]  \hspace{1cm} (24)

respectively.

Some identities are widely used in calculations, we list them as follows:

\[(u \cdot \nabla f) \, dA = u \cdot dr \wedge \star df = df \wedge \star u \cdot dr = (\nabla f \cdot u) \, dA,\]  \hspace{1cm} (25)

\[(u \cdot \tilde{\nabla} f) \, dA = u \cdot dr \wedge \tilde{\star} \tilde{df} = df \wedge \tilde{\star} u \cdot \tilde{dr},\]  \hspace{1cm} (26)

\[dh \wedge \star df = df \wedge \star dh\]

\[dh \wedge \tilde{\star} \tilde{df} = df \wedge \tilde{\star} \tilde{dh}.\]  \hspace{1cm} (27)

C. Stokes theorem and generalized Green identities

The Stokes theorem is a crucial theorem in differential geometry, which reads [1]:

\[\int_{\partial D} \omega = \int_{D} d\omega,\]  \hspace{1cm} (28)

where D is a domain with boundary \( \partial D \). \( \omega \) is a differential form defined on \( \partial D \). Note that the direction of \( \partial D \) is positive if the domain D is always located in its left side when one walks along \( \partial D \). Otherwise, the left-handed side of the above identity takes negative sign.
From the Stokes theorem, we can derive the Green identity and its generalized form as follows [3]:

\[
\int_D (f \, d^* h - h \, d^* f) = \oint_{\partial D} (f \, d h - h \, d f),
\]

\[
\int_D (f \, \hat{d}^* \hat{h} - h \, \hat{d}^* \hat{f}) = \oint_{\partial D} (f \, \hat{d} h - h \, \hat{d} f),
\]

where \( f \) and \( h \) represent smooth functions defined on domain \( D \).

D. Surface variation based on the moving frame

Calculus of variation based on the moving frame method can be found in previous works by the last author and Ou-Yang [3, 4]. Here we only outline the main ideas.

Any infinitesimal deformation of a surface may be achieved by a displacement vector

\[
\delta r \equiv \Omega = \Omega_i e_i,
\]

at each point on the surface, where \( \delta \) can be understood as a variational operator. As shown in Fig. 2, the frame is also changed because of the deformation of the surface, which is denoted as

\[
\delta e_i \equiv \lim_{\delta r \to 0} \delta e_i = \Omega_{ij} e_j \quad (i = 1, 2, 3),
\]

where \( \Omega_{ij} = -\Omega_{ji} \) (\( i, j = 1, 2, 3 \)). We may define an angular vector

\[
\Theta = \Theta_1 e_1 + \Theta_2 e_2 + \Theta_3 e_3
\]

\[
= \Omega_{23} e_1 + \Omega_{31} e_2 + \Omega_{12} e_3,
\]

and rewrite Eq. (32) into

\[
\delta e_i = \Theta \times e_i.
\]

That is, \( \Theta_1 = \Omega_{23}, \Theta_2 = \Omega_{31}, \) and \( \Theta_3 = \Omega_{12} \) correspond to the infinitesimal rotation of the frame around direction \( e_1, e_2, \) and \( e_3 \), respectively.

From \( \delta dr = d\delta r, \delta de_j = d\delta e_j \), we can derive:

\[
\delta \omega_1 + \omega_2 \Omega_{21} = d\Omega \cdot e_1
\]

\[
= d\Omega_1 + \Omega_2 \omega_{21} + \Omega_3 \omega_{31},
\]

\[
\delta \omega_2 + \omega_1 \Omega_{12} = d\Omega \cdot e_2
\]

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FIG. 2. Variation of the moving frame.

\[ \Omega_{12} + \Omega_{23} = d\Omega \cdot e_3 \]

These equations are the basic equations of the variational method based on the moving frame.

With the basic equations (35)-(38), we can derive

\[ \delta dA = (\nabla \cdot \Omega - 2H\Omega_3)dA, \]  
\[ \delta(2H) = [\nabla^2 + (4H^2 - 2K)]\Omega_3 + \nabla(2H) \cdot \Omega, \]  
\[ \delta K = \nabla \cdot \tilde{\nabla} \Omega_3 + 2KH\Omega_3 + \nabla K \cdot \Omega. \]

The derivation of Eqs. (39)-(41) is not a hard task. As an example, we only present the derivation of Eq. (39) in detail. The others may be done in the same way.

Using Eqs. (3), (35) and (36), we derive

\[ \delta dA = \delta(\omega_1 \wedge \omega_2) = \delta \omega_1 \wedge \omega_2 + \omega_1 \wedge \delta \omega_2 \]
\[ = (d\Omega_1 - \omega_{12}\Omega_2 - \omega_{13}\Omega_3 - \omega_2\Omega_{21}) \wedge \omega_2 \]
\[ + \omega_1 \wedge (d\Omega_2 - \omega_{21}\Omega_1 - \omega_{23}\Omega_3 - \omega_1\Omega_{12}) \]
\[ = d\Omega_1 \wedge \omega_2 + \Omega_1 d\omega_2 - d\Omega_2 \wedge \omega_1 - \Omega_2 d\omega_1 \]
\[ - \Omega_3 (\omega_{13} \wedge \omega_2 + \omega_1 \wedge \omega_{23}). \]
From Eqs. (1) and (31), we have $\Omega \cdot d\mathbf{r} = \Omega_1 \omega_1 + \Omega_2 \omega_2$, and further

$$*_\Omega \cdot d\mathbf{r} = \Omega_1 \omega_2 - \Omega_2 \omega_1. \tag{43}$$

Then from the definition of divergence (24), we have

$$(\nabla \cdot \Omega) dA = d(*\Omega \cdot d\mathbf{r}) = d(\Omega_1 \omega_2 - \Omega_2 \omega_1)$$

$$= d\Omega_1 \wedge \omega_2 + \Omega_1 d\omega_2 - d\Omega_2 \wedge \omega_1 - \Omega_2 d\omega_1. \tag{44}$$

In addition, Eq. (6) leads to

$$\omega_{13} \wedge \omega_2 + \omega_1 \wedge \omega_2
= (a \omega_1 + b \omega_2) \wedge \omega_2 + \omega_1 \wedge (b \omega_1 + c \omega_2)$$

$$= (a + c) \omega_1 \wedge \omega_2 = 2H dA. \tag{45}$$

Substituting Eqs. (44) and (45) into (42), we arrive at Eq. (39).

II. DERIVATION OF THE SHAPE EQUATION AND THE LINKING CONDITIONS

In this section, we will give a detailed derivation of the shape equation and the linking conditions.

A. Variation of $\int_D G(2H, K) dA$

First, we consider the variation of general bending energy of a lipid domain $D$. The energy per unit area is taken as $G = G(2H, K)$, which is the function of the mean curvature $H$ and the Gaussian curvature $K$. For simplicity, let us denote $G_{2H} = \partial G/\partial (2H)$ and $G_K = \partial G/\partial K$.

Considering Eqs. (39)-(41), we have

$$\delta(GdA)$$

$$= \delta GdA + G\delta dA$$

$$= [G_{2H}\delta(2H) + G_K\delta K]dA + G\delta dA$$

$$= G_{2H}[\nabla^2 \Omega_3 + (4H^2 - 2K)\Omega_3]dA$$
\[ +G_K(\nabla \cdot \tilde{\nabla} \Omega_3 + 2HK \Omega_3) dA \]
\[ +G_K dK \wedge *\Omega \cdot dr + G_{2H}(2H) \wedge *\Omega \cdot dr \]
\[ +G[d(*\Omega \cdot dr - 2H \Omega_3 dA] \]
\[ = G_{2H}d * d\Omega_3 + (4H^2 - 2K)G_{2H} \Omega_3 dA \]
\[ +G_{2H}(2H) \wedge *\Omega \cdot dr + G_K d\tilde{d}\Omega_3 \]
\[ +2HKG_K \Omega_3 dA - 2HG \Omega_3 dA \]
\[ +G_K dK \wedge *\Omega \cdot dr + Gd(*\Omega \cdot dr) \]
\[ = [(4H^2 - 2K)G_{2H} + 2HKG_K - 2HG] \Omega_3 dA \]
\[ +G_{2H}d * d\Omega_3 + G_Kd\tilde{d}\Omega_3 + d(G \ast \Omega \cdot dr). \]  

(46)

Based on the Stokes theorem (28), the Green identities (29)-(30), and the above equation (46), we obtain

\[
\delta \int_D G dA = \int_D \delta(G dA) = \int_D \Omega_3 d \ast dG_{2H} + \oint_{\partial D} (G_{2H} \ast d\Omega_3 - \Omega_3 \ast dG_{2H})
\]
\[ + \int_D \Omega_3 d \tilde{\ast} dG_K + \oint_{\partial D} (G_K \tilde{\ast} d\Omega_3 - \Omega_3 \tilde{\ast} dG_K) + \oint_{\partial D} G \ast \Omega \cdot dr \]
\[ + \int_D [(4H^2 - 2K)G_{2H} + 2HKG_K - 2HG] \Omega_3 dA \]
\[ = \int_D [\nabla^2 G_{2H} + \nabla \cdot \tilde{\nabla} G_K + (4H^2 - 2K)G_{2H} + 2HKG_K - 2HG] \Omega_3 dA \]
\[ + \oint_{\partial D} (G_{2H} \ast d\Omega_3 - \Omega_3 \ast dG_{2H} + G_K \tilde{\ast} d\Omega_3 - \Omega_3 \tilde{\ast} dG_K + G \ast \Omega \cdot dr). \]  

(47)

B. Variation of \( \int_C ds \)

Let us consider a closed curve embedded in a surface. The arc length is denoted as \( s \). For simplicity, we take \( e_1 \) of the moving frame at each point on the curve to be parallel to the tangent vector of the curve. Then we have \( \omega_1 = ds, \omega_2 = 0, a = \kappa_n, b = \tau_g, \) and \( \omega_12 = \kappa_g ds \) [cf. Eq. (17)]. Thus Eq. (35) is transformed into

\[
\delta ds = d\Omega_1 - \Omega_2 \kappa_g ds - \Omega_3 \kappa_n ds. \]  

(48)

Since \( d\Omega_1 \) is a total differential, according to the Stokes theorem (28), we get \( \oint_C d\Omega_1 = 0. \) Thus we obtain

\[
\delta \oint_C ds = \oint_C \delta ds = - \oint_C [\Omega_2 \kappa_g + \Omega_3 \kappa_n] ds. \]  

(49)
C. Variation of volume enclosed by a closed surface

The volume enclosed by a closed surface may be expressed as

\[ V = \int (\frac{1}{3}) r \cdot e_3 dA. \]  (50)

By Eqs. (31)-(39), we obtain

\[ \delta [r \cdot e_3 dA] = d[r \cdot e_3 (\Omega \cdot dr) - \Omega_3 r \cdot *d\mathbf{r}] + 3\Omega_3 dA. \]  (51)

Applying the Stokes theorem (28), we have from the above two equations that

\[ \delta V = \int (\frac{1}{3}) \delta [r \cdot e_3 dA] = \int \Omega_3 dA. \]  (52)

D. General free energy and its variation

Let us consider a vesicle with two-phase domains as shown in Fig. 3. Curve C is the separation boundary between two domains. The tangent vector \( \mathbf{t} \) indicates the positive direction of separation curve C. On the tangent plane of the surface at any point (for example point Q) on the separation curve C, we take a vector \( \mathbf{b}^I (\mathbf{b}^II) \), which is perpendicular to \( \mathbf{t} \) and points to the side that domain I (II) is located in. Assume that the surface is smooth enough such that \( \mathbf{b}^II = -\mathbf{b}^I \), and the moving frame \( \{e_1, e_2, e_3\} \) is continuous across curve C. In addition, we assume that the moving frame \( \{e_1, e_2, e_3\} \) at any point on the curve C happens to satisfy \( e_1 = \mathbf{t}, e_2 = \mathbf{b}^I = -\mathbf{b}^II \). Thus, we have \( \omega_1 = ds, \omega_2 = 0, \omega_1 = \kappa_\sigma ds, \)
\[ a = \kappa_n, \ b = \tau_g, \ c = 2H - a = 2H - \kappa_n \text{ on curve C. Then Eq. (37) on curve C is transformed into} \]

\[-\Theta_2 ds = d\Omega_3 + \kappa_n \Omega_1 ds + \tau g_2 \Omega_2 ds \tag{53}\]

with consideration of Eq. (33). Furthermore, from Eqs. (19) and (20), we obtain

\[ \ast dG_{2H} = - (e_2 \cdot \nabla G_{2H}) ds, \]

\[ \tilde{\ast} dG_K = - (e_2 \cdot \tilde{\nabla} G_K) ds. \tag{54}\]

The free energy of the vesicle with two-phase domains may be expressed as

\[ F = \int_{D_I} G_I dA + \int_{D_{II}} G_{II} dA + \gamma \int_C ds + pV, \tag{55}\]

where \( G^\alpha = G(2H^\alpha, K^\alpha) \) represents general bending energy per unit area of lipid domain \( \alpha (\alpha = I, II) \). \( \gamma \) represents the line tension of separation curve. \( p \) is the osmotic pressure defining the pressure difference between the outside and inside.

With the consideration of Eqs. (47), (49) and (52), the variation of the above free energy may be expressed as

\[ \delta F = \int_{\partial D_I} [\nabla^2 G_{2H}^I + \nabla \cdot \tilde{\nabla} G_K^I + (4H^I_1^2 - 2K^I_1)G_{2H}^I + 2H^I_1 K^I_1 G_K^I - 2H^I_1 G_{II}^I] \Omega_3 dA \\
+ \int_{\partial D_{II}} [G_{2H}^I d\Omega_3 - \Omega_3 \ast dG_{2H}^I + G_K^I \tilde{\ast} d\Omega_3 - \Omega_3 \tilde{\ast} dG_K^I + G^I \ast \Omega \cdot dr] \\
+ \int_{\partial D_{II}} [\nabla^2 G_{2H}^{II} + \nabla \cdot \tilde{\nabla} G_K^{II} + (4H^{II}_1^2 - 2K^{II}_1)G_{2H}^{II} + 2H^{II}_1 K^{II}_1 G_K^{II} - 2H^{II}_1 G_{II}^{II}] \Omega_3 dA \\
+ \int_{\partial D_{II}} [G_{2H}^{II} d\Omega_3 - \Omega_3 \ast dG_{2H}^{II} + G_K^{II} \tilde{\ast} d\Omega_3 - \Omega_3 \tilde{\ast} dG_K^{II} + G^{II} \ast \Omega \cdot dr] \\
- \gamma \int_C [\Omega_2 \kappa_2 + \Omega_3 \kappa_3] ds + p \left[ \int_{D_I} \Omega_3 dA + \int_{D_{II}} \Omega_3 dA \right]. \tag{56}\]

When one walks along the positive direction of C, domain I is located on the left-handed side of C. Thus the boundary of domain I coincides with C, i.e., \( \partial D_I = C \). Then we have

\[ \int_{\partial D_I} [G_{2H}^I d\Omega_3 - \Omega_3 \ast dG_{2H}^I \\
+ G_K^I \tilde{\ast} d\Omega_3 - \Omega_3 \tilde{\ast} dG_K^I + G^I \ast \Omega \cdot dr] \\
eq \int_{D_I} [G_{2H}^I d\Omega_3 - \Omega_3 \ast dG_{2H}^I \\
+ G_K^I \tilde{\ast} d\Omega_3 - \Omega_3 \tilde{\ast} dG_K^I + G^I \ast \Omega \cdot dr]. \tag{57}\]
On curve $C$, from Eqs. (33), (37), (43), (53) and (54), we obtain

\[
G_{2H}^I \ast d\Omega_3 - \Omega_3 \ast dG_{2H}^I + G_{K}^I \hat{\ast} \hat{d}\Omega_3 \\
- \Omega_3 \hat{\ast} \hat{d}G_{K}^I + G^I \ast \Omega \cdot dr \\
= \Omega_2 \left[ G_{2H}^I \left( 2H^I - \kappa_n \right) + G_{K}^I K^I - G^I \right] ds \\
+ \Omega_3 e_2 \cdot \left( \nabla G_{2H}^I + \hat{\nabla} G_{K}^I \right) + G_{K}^I \hat{\tau}_g ds \\
- \Theta_1 \left( G_{2H}^I + G_{K}^I \kappa_n \right) ds + G_{K}^I \hat{\tau}_g^2 \Omega_2 ds \\
+ \left( G_{2H}^I + G_{K}^I \kappa_n \right) \Omega_1 \tau_g ds
\] (58)

Substituting the above equation and $\tau_g^2 = (2H^I - \kappa_n)\kappa_n - K^I$ [Eq. (18)] into Eq. (57) and then using integration by parts, we may obtain

\[
\oint_{\partial D} \left[ G_{2H}^I \ast d\Omega_3 - \Omega_3 \ast dG_{2H}^I + G_{K}^I \hat{\ast} \hat{d}\Omega_3 \\
- \Omega_3 \hat{\ast} \hat{d}G_{K}^I + G^I \ast \Omega \cdot dr \right] \\
= \int_C \Omega_2 \left[ \left( 2H^I - \kappa_n \right) \left( G_{2H}^I + G_{K}^I \kappa_n \right) - G^I \right] ds \\
+ \int_C \left[ e_2 \cdot \left( \nabla G_{2H}^I + \hat{\nabla} G_{K}^I \right) - \frac{d}{ds} \left( G_{K}^I \hat{\tau}_g \right) \right] \Omega_3 ds \\
- \int_C \Theta_1 \left( G_{2H}^I + G_{K}^I \kappa_n \right) ds \\
+ \int_C \left( G_{2H}^I + G_{K}^I \kappa_n \right) \Omega_1 \tau_g ds
\] (59)

Similarly, when one walks along the positive direction of $C$, domain $II$ is located on the right-hand side of $C$. Thus the boundary of domain $II$ is anti-parallel to $C$, i.e., $\partial D^I = -C$. Following the same procedure mentioned above, we obtain

\[
\oint_{\partial D^II} \left[ G_{2H}^{II} \ast d\Omega_3 - \Omega_3 \ast dG_{2H}^{II} + G_{K}^{II} \hat{\ast} \hat{d}\Omega_3 \\
- \Omega_3 \hat{\ast} \hat{d}G_{K}^{II} + G^{II} \ast \Omega \cdot dr \right] \\
= - \int_C \Omega_2 \left[ \left( 2H^{II} - \kappa_n \right) \left( G_{2H}^{II} + G_{K}^{II} \kappa_n \right) - G^{II} \right] ds \\
- \int_C \left[ e_2 \cdot \left( \nabla G_{2H}^{II} + \hat{\nabla} G_{K}^{II} \right) - \frac{d}{ds} \left( G_{K}^{II} \hat{\tau}_g \right) \right] \Omega_3 ds \\
+ \int_C \Theta_1 \left( G_{2H}^{II} + G_{K}^{II} \kappa_n \right) ds \\
- \int_C \left( G_{2H}^{II} + G_{K}^{II} \kappa_n \right) \Omega_1 \tau_g ds
\] (60)

Now, substituting Eqs. (59) and (60) into (56), we obtain
\[
\delta F = \int_{D_t} \left[ \nabla^2 G_{2H}^I + \nabla \cdot \tilde{\nabla} C_K + (4H^I - 2K^I) G_{2H}^I + 2H^I K^I C_K - 2H^I G^I + p \right] \Omega_3 dA \\
+ \int_{D_H} \left[ \nabla^2 G_{2H}^{II} + \nabla \cdot \tilde{\nabla} G_K^{II} + (4H^{II} - 2K^{II}) G_{2H}^{II} + 2H^{II} K^{II} C_K^{II} - 2H^{II} G^{II} + p \right] \Omega_3 dA \\
+ \int_C \left[ (G_{2H}^I + G_K^I \kappa_n) - (G_{2H}^{II} + G_K^{II} \kappa_n) \right] \Omega_1 \tau_g ds \\
- \int_C \left[ (G_{2H}^I + G_K^I \kappa_n) - (G_{2H}^{II} + G_K^{II} \kappa_n) \right] \Theta_1 ds \\
+ \int_C \left[ 2H^I - \kappa_n \right] \left[ (G_{2H}^I + G_K^I \kappa_n) - (G_{2H}^{II} + G_K^{II} \kappa_n) \right] ds \\
+ \int_C \left[ b^I \cdot (\nabla G_{2H}^I + \tilde{\nabla} G_K^I) + b^{II} \cdot (\nabla G_{2H}^{II} + \tilde{\nabla} G_K^{II}) - \frac{d}{ds} \left( G_K^I \tau_g - G_K^{II} \tau_g \right) - \gamma \kappa_g \right] \Omega_3 ds.
\]

Note that, in the last line, we have used \( e_2 = b^I = -b^{II} \) on the separation curve \( C \).

**E. Shape equation and linking conditions**

The variables \( \Omega_1, \Omega_2, \Omega_3 \), and \( \Theta_1 \) in Eq. (61) are independent of each other. Thus we may derive the following shape equation for two domains

\[
\nabla^2 G_{2H}^\alpha + \nabla \cdot \tilde{\nabla} G_K^\alpha + (4H^\alpha - 2K^\alpha) G_{2H}^\alpha \\
+ 2H^\alpha K^\alpha G_K^\alpha - 2H^\alpha G^\alpha + p = 0, \ (\alpha = I, II)
\]

and three linking conditions for the separation curve \( C \):

\[
G_{2H}^I + G_K^I \kappa_n = G_{2H}^{II} + G_K^{II} \kappa_n, \quad \text{(63)}
\]

\[
b^I \cdot (\nabla G_{2H}^I + \tilde{\nabla} G_K^I) + b^{II} \cdot (\nabla G_{2H}^{II} + \tilde{\nabla} G_K^{II}) \\
= \frac{d}{ds} \left[ (G_K^I - G_K^{II}) \tau_g \right] + \gamma \kappa_n, \quad \text{(64)}
\]

and

\[
\left( 2H^I - \kappa_n \right) \left( G_{2H}^I + G_K^I \kappa_n \right) - \left( 2H^{II} - \kappa_n \right) \left( G_{2H}^{II} + G_K^{II} \kappa_n \right) \\
= G^I - G^{II} + \gamma \kappa_g, \quad \text{(65)}
\]

If we consider Eq. (63), the third linking condition may be simplified as

\[
2H^I \left( G_{2H}^I + G_K^I \kappa_n \right) - 2H^{II} \left( G_{2H}^{II} + G_K^{II} \kappa_n \right) \\
= G^I - G^{II} + \gamma \kappa_g \quad \text{(66)}
\]
Now we consider the Helfrich spontaneous curvature model, \( G^\alpha = \frac{k_c^\alpha}{2} (2H^\alpha + c_0^\alpha)^2 + \bar{k}^\alpha K^\alpha + \lambda^\alpha \) (\( \alpha = I, II \)), where \( k_c^\alpha, \bar{k}^\alpha, \) and \( c_0^\alpha, \lambda^\alpha \) represent the bending rigidity, the Gaussian bending modulus, the spontaneous curvature, and the surface tension of domain \( \alpha \), respectively. In this model, we have \( G_{2H}^\alpha = k_c^\alpha (2H^\alpha + c_0^\alpha) \), \( G_K^\alpha = \bar{k}^\alpha \), \( \tilde{\nabla} G_K^\alpha = 0 \). Then the shape equation may be transformed into

\[
\begin{align*}
{k_c^\alpha (2H^\alpha + c_0^\alpha)} & \left[ 2 (H^\alpha)^2 - c_0^\alpha H^\alpha - 2K^\alpha \right] \\
+ k_c^\alpha \nabla^2 (2H^\alpha) + p - 2\lambda^\alpha H^\alpha &= 0, \quad (\alpha = I, II). \\
\end{align*}
\]

The linking conditions may be simplified as

\[
\begin{align*}
k_c^I (2H^I + c_0^I) + \bar{k}^I \kappa_n &= k_c^{II} (2H^{II} + c_0^{II}) + \bar{k}^{II} \kappa_n, \\
\frac{\partial}{\partial b^I} \left[ k_c^I (2H^I + c_0^I) \right] + \frac{\partial}{\partial b^{II}} \left[ k_c^{II} (2H^{II} + c_0^{II}) \right] &= (\bar{k}^I - \bar{k}^{II}) \frac{d\tau_g}{ds} + \gamma \kappa_n, \\
\end{align*}
\]

and

\[
\begin{align*}
\frac{k_c^I}{2} [4 (H^I)^2 - (c_0^I)^2] - \frac{k_c^{II}}{2} [4 (H^{II})^2 - (c_0^{II})^2] \\
+ (\bar{k}^I - \bar{k}^{II}) \left( \kappa_n^2 + \tau_g^2 \right) &= \lambda^I - \lambda^{II} + \gamma \kappa_g. \\
\end{align*}
\]

Note that, when writing Eq. (69) we have used the definition of directional derivative:

\[
\frac{\partial f}{\partial u} \equiv u \cdot \nabla f, \\
\]

where \( f \) represents a function and \( u \) represents a unit vector.

In the special case of \( \bar{k}^I = \bar{k}^{II} \), the above linking conditions may be further simplified as:

\[
k_c^I (2H^I + c_0^I) = k_c^{II} (2H^{II} + c_0^{II}), \\
\frac{\partial}{\partial b^I} \left[ k_c^I (2H^I + c_0^I) \right] + \frac{\partial}{\partial b^{II}} \left[ k_c^{II} (2H^{II} + c_0^{II}) \right] = \gamma \kappa_n, \\
\]

and

\[
\begin{align*}
\frac{k_c^I}{2} [4 (H^I)^2 - (c_0^I)^2] - \frac{k_c^{II}}{2} [4 (H^{II})^2 - (c_0^{II})^2] \\
= \lambda^I - \lambda^{II} + \gamma \kappa_g. \\
\end{align*}
\]
III. RELATION BETWEEN THE LINKING CONDITIONS AND THE BALANCES OF FORCE AND MOMENT

The linking conditions (63)-(66) are related to the balances of force and moment on the separation curve. Roughly speaking, Eq. (63) represents the balance of moment around the tangent vector of the separation curve. Eqs. (64) and (65) represent the balance of forces in the directions of $e_3$ and $e_2$, respectively. In this section, we will make these more clear by the concepts of stress and moment tensors [5–8] in lipid membranes.

A. Definition of stress tensor and moment tensor

The concept of stress comes from the force balance and the moment balance for any domain on a lipid membrane. As shown in Fig. 4, we cut a domain bounded by a curve $C$ from the lipid membrane. At each point, we construct a right-handed orthogonal frame \{\(e_1, e_2, n\)\} with $n = e_3$ being the unit normal vector. A pressure $p$ is loaded on the surface against the normal direction. $t$ is the unit tangent vector of curve $C$. Unit vector $b$ is located in the tangent plane and it is normal to $t$. Vectors $f$ and $m$ represent the force and the moment per unit length applied on curve $C$ by lipids out of the domain, respectively.

![FIG. 4. (Color online) Force and moment balances of a domain cut from a fluid membrane.](image)

According to Newtonian mechanics, a physical object is in equilibrium when the force
balance and the moment balance are simultaneously satisfied. It follows that
\[ \int_C \mathbf{f} ds - \int p \mathbf{n} dA = 0, \]  
(75)
\[ \int_C \mathbf{m} ds + \int_C \mathbf{r} \times \mathbf{f} ds - \int (\mathbf{r} \times p) \mathbf{n} dA = 0, \]  
(76)
where ds and dA are the arc length element of curve C and the area element of the domain, respectively. \( \mathbf{r} \) represents the position vector of a point on the surface.

We can mathematically define two second order tensors \( \mathbf{S} \) and \( \mathbf{M} \) such that
\[ \mathbf{S} \cdot \mathbf{b} = \mathbf{f}, \quad \text{and} \quad \mathbf{M} \cdot \mathbf{b} = \mathbf{m}. \]  
(77)
These two tensors are called stress tensor and bending moment tensor, respectively. Since \( \mathbf{b} ds = \star d\mathbf{r} \), using the Stokes theorem and considering the arbitrariness of the domain, we can derive the equilibrium equations:
\[ \text{div} \mathbf{S} = p \mathbf{n}, \]  
(78)
\[ \text{div} \mathbf{M} = \mathbf{S}_1 \times \mathbf{e}_1 + \mathbf{S}_2 \times \mathbf{e}_2, \]  
(79)
with \( \mathbf{S}_1 \equiv \mathbf{S} \cdot \mathbf{e}_1 \) and \( \mathbf{S}_2 \equiv \mathbf{S} \cdot \mathbf{e}_2 \).

**B. Derivation of expressions of stress tensor and moment tensor from variational principle**

The bending energy of the domain may be expressed as \( \int_D G(2H, K) dA \). The external pressure \( p \) is applied on the domain. The external force \( \mathbf{f} \) and moment \( \mathbf{m} \) are loaded on the boundary of the domain. Since the variables \( \Omega \) in Eq. (31) and \( \Theta \) in Eq. (33) could be regarded as the virtual displacements. In the equilibrium state, the configuration of the domain satisfies the following generalized variational principle:
\[ \delta \int_D G(2H, K) dA + \int_D p \mathbf{n} \cdot \mathbf{\Omega} dA \]
\[ - \int_C \mathbf{f} \cdot \mathbf{\Omega} ds - \int_C \mathbf{m} \cdot \mathbf{\Theta} ds \]
\[ + \int_C \mu [\Theta_1 \omega_2 - \Theta_2 \omega_1 - \Omega_1 \omega_{13} - \Omega_2 \omega_{23} - d\Omega_3] = 0. \]  
(80)
In the second line of the above equation, \( \mu \) is a Lagrange multiplier due to the geometric constraint of Eq. (37).

Since \( \delta \int_D G(2H, K) dA \) has already been calculated in Eq. (47), we substitute it into the above generalized variational principle to get
\[
\begin{align*}
&\int_D \Omega_3 \left[ \nabla^2 G_{2H} + \nabla \cdot \tilde{\nabla} G_K + (4H^2 - 2K)G_{2H} + 2HKG_K - 2HG + p \right] \, dA \\
&\quad + \int_C \frac{\Omega_1}{[G_{2H} (b\omega_1 - a\omega_2) - G_K K\omega_2 + G\omega_2 - \mu(a\omega_1 + b\omega_2) - f_1] \, ds} \\
&\quad + \int_C \frac{\Omega_2}{[G_{2H} (c\omega_1 - b\omega_2) + G_K K\omega_1 - G\omega_1 - \mu(b\omega_1 + c\omega_2) - f_2] \, ds} \\
&\quad + \int_C \frac{\Omega_3}{[-(dG_{2H} + \hat{d}G_K) + d\mu - f_3] \, ds} \\
&\quad + \int_C \frac{\Theta_1}{[-G_{2H}\omega_1 - G_K (a\omega_1 + b\omega_2) + \mu\omega_2 - m_1] \, ds} \\
&\quad + \int_C \frac{\Theta_2}{[-G_{2H}\omega_2 - G_K (b\omega_1 + c\omega_2) - \mu\omega_1 - m_2] \, ds} \\
&\quad - \int_C \frac{\Theta_3 m_3}{m} \, ds = 0.
\end{align*}
\]

After we introduce the Lagrange multiplier \( \mu \) in Eq. (80), the virtual displacements \( \Omega_i \) and \( \Theta_i \) \((i = 1, 2, 3)\) could be regarded as independent variables and from the above equation we obtain the shape equation of the domain

\[
\nabla^2 G_{2H} + \nabla \cdot \tilde{\nabla} G_K + (4H^2 - 2K)G_{2H}
\]

\[
+ 2HKG_K - 2HG + p = 0,
\]

\[\text{Eq. (82)}\]

as well as the components of force and moment vectors:

\[
\begin{align*}
&f_1 = \left( G - aG_{2H} - G_K K - b\mu \right) \frac{\omega_2}{ds} \\
&\quad + (bG_{2H} - a\mu) \frac{\omega_1}{ds} \tag{83} \\
&f_2 = \left( cG_{2H} + G_K K - G - b\mu \right) \frac{\omega_1}{ds} \\
&\quad + (-bG_{2H} - c\mu) \frac{\omega_2}{ds} \tag{84} \\
&f_3 = \left( G_{2H}^2 - bG_{2H}^1 + aG_K^2 + \mu_1 \right) \frac{\omega_1}{ds} \\
&\quad - (G_{2H}^1 + cG_K^1 - bG_K^2) \frac{\omega_2}{ds} \tag{85} \\
&m_1 = \left( G_{2H}^1 - aG_K^1 \right) \frac{\omega_1}{ds} + (\mu - bG_K) \frac{\omega_2}{ds} \tag{86} \\
&m_2 = \left( G_{2H}^2 - cG_K^2 \right) \frac{\omega_2}{ds} - (\mu + bG_K) \frac{\omega_1}{ds} \tag{87} \\
&m_3 = 0, \tag{88}
\end{align*}
\]

where \( G_{2H}^1 \equiv \nabla G_{2H} \cdot e_1, \ G_K^i \equiv \nabla G_K \cdot e_i \) and \( \mu_i = \nabla \mu \cdot e_i \) \((i = 1, 2)\).

Considering \( \mathbf{b} ds = *d\mathbf{r} \) and the definition \( \mathbf{S} \cdot \mathbf{b} = \mathbf{f} = f_1 e_1 + f_2 e_2 + f_3 e_3 \) and \( \mathbf{M} \cdot \mathbf{b} = \mathbf{m} = m_1 e_1 + m_2 e_2 + m e_3 \), we obtain the components of the stress tensor and the moment.
The vanishing components are not displayed here.

Considering the curvature tensor (7) and introduce the unit tensor 

$$I = e_1 e_1 + e_2 e_2,$$

we may expressed the stress tensor and the moment tensor as:

$$S = S_{ij} e_i e_j$$

$$= (G - G_K K) I - n (\nabla G_{2H} + \tilde{\nabla} G_K)$$

$$- (\mu C - n \nabla \mu) \times n - G_{2H} C,$$

and

$$M = M_{ij} e_i e_j$$

$$= \mu I - (G_{2H} I + G_K C) \times n,$$

where \(n \equiv e_3\) represents the normal direction of the surface. It is not hard to check that Eqs. (75) and (76) hold by using the above two equations. In particular, Eq. (75) is equivalent to the shape equation (82).

Considering \(t ds = dr\) and \(b ds = *dr\) for the point on the domain boundary shown in Fig. 4, we may rewrite the force vector and moment vector at that point as

$$f = S \cdot b$$

$$= [G - G_K K - (2H - \kappa_n)G_{2H} + \mu \tau_g] b$$

$$+ [\nabla \mu \cdot t - (\nabla G_{2H} + \tilde{\nabla} G_K) \cdot b] n$$

$$+ (G_{2H} \tau_g - \mu \kappa_n) t,$$

18
and

\[ m = \mathcal{M} \cdot \mathbf{b} \]

\[ = -(G_{2H} + \kappa_n G_K)t + (\mu + \tau_g G_K)b, \]

(100)

where \( \kappa_n \) and \( \tau_g \) represent the normal curvature and the geodesic torsion of the boundary, respectively.

C. Balances of force and moment for a string with uniform tension

Let us consider a stretching string with line tension \( \gamma \) as shown in Fig. 5, the force and moment per unit length applied on the string are denoted as \( f \) and \( m \). The string is parameterized by the its arc length. Let us cut an infinitesimal element with arc length \( \Delta s \) situated in between points \( \mathbf{r}(s) \) and \( \mathbf{r}(s+\Delta s) \) from the string. The forces \( -\gamma t(s), \gamma t(s+\Delta s), f\Delta s \) and the moment \( m\Delta s \) are loaded on the element. Here \( t(s) \) and \( t(s+\Delta s) \) represent the tangent vectors of string at points \( \mathbf{r}(s) \) and \( \mathbf{r}(s+\Delta s) \), respectively.

From the balance of force \( \gamma t(s+\Delta s) - \gamma t(s) + f(s)\Delta s = 0 \), we obtain

\[ \gamma \kappa(s)N + f(s) = 0 \]

(101)

by considering Eq.(10) and \( \Delta s \to 0 \). Here \( \kappa(s) \) represents the curvature of string. Similarly, from the balance of moment \( \mathbf{r}(s) \times f(s)\Delta s + \mathbf{r}(s+\Delta s) \times \gamma t(s+\Delta s) - \mathbf{r}(s) \times \gamma t(s) + m(s)\Delta s = 0 \), we may derive

\[ m(s) = 0. \]

(102)
D. Linking conditions for the separation boundary of a vesicle with two-phase domains

Let us consider a vesicle with two-phase domains shown on the left-hand side of Fig. 6. We cut an infinitesimally thin ribbon along the separation boundary C, which is shown on the right-hand side of Fig. 6. Consider a point Q on curve C. The tangent vector of C at point Q is denoted by \( \mathbf{t} \). The normal vector of surface at point Q is denoted as \( \mathbf{n} \). The infinitesimally thin ribbon may be regarded as a domain cut from a surface. The tangent vector of its left-hand edge and that of its right-hand edge should be taken as \( \mathbf{t}^I = -\mathbf{t} \) and \( \mathbf{t}^II = \mathbf{t} \), respectively, which is compatible with the positive orientation of domain boundary shown in Fig. 4. In addition, the normal vectors of surface for the point on the left-hand edge and that on the left-hand edge satisfy \( \mathbf{n}^I = \mathbf{n}^II = \mathbf{n} \). Define \( \mathbf{b}^I \equiv \mathbf{t}^I \times \mathbf{n} \) and \( \mathbf{b}^II \equiv \mathbf{t}^II \times \mathbf{n} \). Obviously, \( \mathbf{b}^I = -\mathbf{b}^II \).

\[
G_{2H} + \kappa_n G_K^I \mathbf{t}^I + (\mu^I + \tau_g G_K^I) \mathbf{b}^I
- (G_{2H}^II + \kappa_n G_K^II) \mathbf{t}^II + (\mu^II + \tau_g G_K^II) \mathbf{b}^II. \tag{103}
\]

Since \( \mathbf{t}^I = -\mathbf{t}^II = -\mathbf{t} \) and \( \mathbf{b}^I = -\mathbf{b}^II \), substituting Eq. (103) into Eq. (102), we obtain

\[
G_{2H}^I + \kappa_n G_K^I = G_{2H}^II + \kappa_n G_K^II, \tag{104}
\]

and

\[
\mu^II - \mu^I = \tau_g (G_K^I - G_K^II). \tag{105}
\]
Eq. (104) is exactly the linking condition (63). From Eq. (103) we see that this linking condition represents the moment balance along the tangent direction of curve C.

Similarly, using Eq. (99), we may express the force per unit length along C as

\[
f = f^I + f^H \\
= (G^I_{2H} \tau^I_g - \mu^I_\kappa n) t^I + (G^H_{2H} \tau^I_g - \mu^H_\kappa n) t^H \\
+ [G^I - G^I_K K^I - (2H^I - \kappa_n) G^I_{2H} + \mu^I_\tau g] b^I \\
+ [G^H - G^H_K K^H - (2H^H - \kappa_n) G^H_{2H} + \mu^H_\tau g] b^H \\
+ [\nabla ^I \mu \cdot t^I - (\nabla G^I_{2H} + \tilde{\nabla} G^I_K) \cdot b^I + \nabla ^H \mu \cdot t^H \\
- (\nabla G^H_{2H} + \tilde{\nabla} G^H_K) \cdot b^H] n.
\]

With the consideration of \( t^I = -t^H = -t, \ b^I = -b^H, \) Eqs. (18), (104), and (105), the force per unit length may be further simplified as

\[
f = [G^I - 2H^I (G^I_{2H} + \kappa_n G^I_K) - G^H] \\
+ 2H^H (G^H_{2H} + \kappa_n G^H_K)] b^I \\
+ \left[ \frac{d(\tau^I_g G^I_K - \tau^H_g G^H_K)}{ds} - (\nabla G^I_{2H} + \tilde{\nabla} G^I_K) \cdot b^I \\
- (\nabla G^H_{2H} + \tilde{\nabla} G^H_K) \cdot b^H \right] n.
\]

Substituting the above equation into Eq. (101), and using definitions \( \kappa_n \equiv \kappa N \cdot n \) and \( \kappa_g \equiv \kappa N \cdot b^I \), we may obtain

\[
(\nabla G^I_{2H} + \tilde{\nabla} G^I_K) \cdot b^I + (\nabla G^H_{2H} + \tilde{\nabla} G^H_K) \cdot b^H \\
= \gamma \kappa_n + \frac{d[(G^I_K - G^H_K) \tau^I_g]}{ds}, \tag{108}
\]

and

\[
2H^I (G^I_{2H} + \kappa_n G^I_K) - 2H^H (G^H_{2H} + \kappa_n G^H_K) \\
= \gamma \kappa_g + G^I - G^H. \tag{109}
\]

Eq. (108) exactly coincides with the linking condition (64). From Eqs. (101) and (107) we see that this linking condition represents the force balance along the normal direction of surface for the point on curve C. Similarly, Eq. (109) can be exactly identified with the
linking condition (66), which represents the force balance along the $b^I$ direction for the point on curve C.