Elastic theory of low-dimensional continua and its applications in bio- and nano-structures

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This review presents the elastic theory of low-dimensional (one- and two-dimensional) continua and its applications in bio- and nano-structures. First, the curve and surface theory, as the geometric representation of the low-dimensional continua, is briefly described through Cartan moving frame method. The elastic theory of Kirchhoff rod, Helfrich rod, bending-soften rod, fluid membrane, and solid shell is revisited. The free energy density of the continua, is constructed on the basis of the symmetry argument. The fundamental equations can be derived from two kinds of viewpoints: the bottom-up and the top-down standpoints. In the former case, the force and moment balance equations are obtained from Newton’s laws and then some constitute relations are complemented in terms of the free energy density. In the latter case, the fundamental equations are derived directly from the variation of the free energy. Although the fundamental equations have different forms obtained from these two viewpoints, several examples reveal that they are, in fact, equivalent to each other.

Secondly, the application and availability of the elastic theory of low-dimensional continua in bio-structures, including short DNA rings, lipid membranes, and cell membranes, are discussed. The kink stability of short DNA rings is addressed by using the theory of Kirchhoff rod, Helfrich rod, and bending-soften rod. The lipid membranes obey the theory of fluid membrane. The shape equation and the stability of closed lipid vesicles, the shape equation and boundary conditions of open lipid vesicles with free edges as well as vesicles with lipid domains, and the adhesions between a vesicle and a substrate or another vesicle are fully investigated. A cell membrane is simplified as a composite shell of lipid bilayer and membrane skeleton, which is a little similar to the solid shell. The equations to describe the in-plane strains and shapes of cell membranes are obtained. It is found that the membrane skeleton enhances highly the mechanical stability of cell membranes.

Thirdly, the application and availability of the elastic theory of low-dimensional continua in nano-structures, including graphene and carbon nanotubes, are discussed. A revised Lenosky lattice model is proposed based on the local density approximation. Its continuum form up to the second order terms of curvatures and strains is the same as the free energy of 2D solid shells. The intrinsic roughening of graphene and several typical mechanical properties of carbon nanotubes are revisited and investigated based on this continuum form. It is possible to avoid introducing the controversial concepts, the Young’s modulus and thickness of graphene and single-walled carbon nanotubes, with this continuum form.

Keywords: Elastic Theory, DNA Ring, Biomembrane, Graphene, Carbon nanotube, Moving frame method

I. INTRODUCTION

We human beings live in a three-dimensional (3D) space which contains many geometric entities composed of atoms or molecules. The length scale of objects observed with our naked eyes is much larger than the distance between nearest neighbor atoms or molecules in the objects. As a result, the objects can be regarded as continua. If one dimension of an object is much larger than the other two dimensions, such as a rod, we call it a one-dimensional (1D) entity. If one dimension of an object is much smaller than the other two dimensions, such as a thin film, we call it a two-dimensional (2D) entity. In this review, the term “low-dimensional continua” represents 1D and 2D entities.

Elasticity is a property of materials. It means that materials deform under external forces, but return to their original shapes when the forces are removed. Elastic theory, the study on the elasticity of continuum materials, has a long history\textsuperscript{2,3} which records many geniuses such as Hooke (1635–1703), Bernoulli (1700–1782), Euler (1707–1783), Lagrange (1736–1813), Young (1773–1829), Poisson (1781–1840), Navier (1785–1836), Cauchy (1789–1857), Green (1793–1841), Lamé (1795–1870), Saint-Venant (1797–1886), Stokes (1819–1903), Kirchhoff (1824–1887), and so on. Now elastic theory has been a mature branch of physics and summarized in several excellent textbooks.\textsuperscript{4,5,6}

Although the classical elastic theory is applied to macroscopic continuum materials, more and more facts reveal that it can be also available for bio- or nano-structures such as short DNA rings,\textsuperscript{5,6,7,8,9,10,11,12,13} α-helical coiled coils,\textsuperscript{14,15} chiral filaments,\textsuperscript{16,17,18,19,20,21} climbing plants,\textsuperscript{22,23} bacterial flagella,\textsuperscript{24} viral shells,\textsuperscript{25,26,27} bio-membranes,\textsuperscript{28,29,30,31,32,33,34,35,36} zinc oxide nanoribbons,\textsuperscript{37,38,39} and carbon nanotubes,\textsuperscript{40,41,42,43,44,45,46} to some extent.

This review presents the elastic theory of low-dimensional continua and its applications in bio- and nano-structures, which is organized as follows: In Sec. \textsuperscript{II}
we briefly introduce the geometric representation and the elastic theory of low-dimensional continua including 1D rod and 2D fluid membrane or solid shell. The free energy density of the continua is constructed on the basis of the symmetry argument. The fundamental equations can be derived from the bottom-up and the top-down viewpoints. Although they have different forms obtained from these two standpoints, several examples reveal that they are, in fact, equivalent to each other. In Sec. III the application and availability of the elastic theory of low-dimensional continua in bio-structures, including short DNA rings, lipid membranes, and cell membranes, are discussed. We investigate the kink stability of short DNA rings, lipid membranes, and cell membranes, are discussed. We propose a revised Lenosky lattice model and fit four parameters in this model through the local density approximation. We derive its continuum form up to the second order terms of curvatures and strains, which is the same as the free energy of 2D solid sheets. The intrinsic roughening of graphene and several typical mechanical properties of carbon nanotubes are revisited and investigated by using this continuum form. Sec. IV is a brief summary and prospect.

II. FUNDAMENTALS OF GEOMETRIC AND ELASTIC THEORY ON LOW-DIMENSIONAL CONTINUA

In this section, we describe the mathematical basis and the elastic theory of 1D and 2D continua.

A. Geometric representation of low-dimensional continua

The 1D continuum (rod) and 2D continuum (membrane or shell) can be expressed as a smooth curve and a smooth surface, respectively.

1. Curve theory

Fig. 1 depicts a curve \( C \) embedded in the 3D Euclid space. Each point in the curve can be expressed as a vector \( r \) and let \( s \) be the arc length parameter. At point \( r(s) \), one can take \( T, N, \) and \( B \) as the tangent, normal and binormal vectors, respectively. \( \{r, T, N, B\} \) is called the Frenet frame which satisfies the Frenet formula

\[
\begin{align*}
\mathbf{r}' &= \mathbf{T}, \\
\mathbf{T}' &= \kappa \mathbf{N}, \\
\mathbf{N}' &= (\kappa \mathbf{T} + \tau \mathbf{B}), \\
\mathbf{B}' &= -\kappa \mathbf{N},
\end{align*}
\]

where the prime represents the derivative with respect to \( s \), \( \kappa \) and \( \tau \) are the curvature and torsion of the curve, respectively.

The fundamental theory of curve tells us that the bending and twist properties of a smooth curve are uniquely determined by the Frenet formula.

2. Surface theory

Fig. 2 depicts a surface \( M \) embedded in the 3D Euclid space. Imagine that a mass point moves on the surface in the speed of unit and that a right-handed frame, which consists of three unit orthonormal vectors with two vectors always in the tangent plane of the surface, adheres to the mass point. Assume that the mass point is at position expressed as vector \( r \) and the frame superposes three unit orthonormal vectors \( \{e_1, e_2, e_3\} \) with \( e_i \) being the normal vector of surface \( M \) at some time \( s \). When the mass point moves to another position \( r' \) at time \( s + \Delta s \), the frame will superpose three unit orthonormal vectors \( \{e'_1, e'_2, e'_3\} \). Thus we call the frame a moving frame and denote it as \( \{r; e_1, e_2, e_3\} \).

If \( \Delta s \to 0 \), we define

\[
\mathbf{d}r = \lim_{\Delta s \to 0} (r' - r) = \omega_1 \mathbf{e}_1 + \omega_2 \mathbf{e}_2, 
\]

and

\[
\mathbf{d}e_i = \lim_{\Delta s \to 0} (e'_i - e_i) = \omega_{ij} \mathbf{e}_j, \quad (i = 1, 2, 3)
\]

where \( \omega_1, \omega_2 \), and \( \omega_{ij}, (i, j = 1, 2, 3) \) are 1-forms, and \( 'd' \) is the exterior differential operator. Here \( \omega_{12} \) can be understood as the infinite rotation angle of vectors \( e_1 \) and \( e_2 \) around \( e_3 \). Similarly, we can understand the physical meaning of the other \( \omega_{ij} \). It is easy to obtain \( \omega_{ij} = -\omega_{ji} \).
from $e_i \cdot e_j = \delta_{ij}$. Additionally, the structure equations of the surface can be expressed as: \[ d\omega_i = \omega_{12} \wedge \omega_2, \]
\[ d\omega_2 = \omega_{21} \wedge \omega_1, \]
\[ d\omega_{ij} = \omega_{ik} \wedge \omega_{kj} \quad (i, j = 1, 2, 3), \]
and
\[ \left( \begin{array}{c} \omega_{13} \\ \omega_{23} \end{array} \right) = \left( \begin{array}{cc} a & b \\ b & c \end{array} \right) \left( \begin{array}{c} \omega_1 \\ \omega_2 \end{array} \right), \]
where ‘$\wedge$’ represents the wedge product between two differential forms. The matrix $\left( \begin{array}{cc} a & b \\ b & c \end{array} \right)$ is the representation matrix of the curvature tensor $\mathfrak{H}$. Its trace and determinant are two invariants under the coordinate rotation around $e_3$ which are denoted by
\[ 2H = a + c \quad \text{and} \quad K = ac - b^2. \]
They can be expressed as $2H = -(1/R_1 + 1/R_2)$ and $K = 1/R_1 R_2$ by the two principal curvature radii $R_1$ and $R_2$ at each point.

Consider a tangent vector $m$ stemming from $r$. Let $\phi$ be the angle between $m$ and $e_1$. Then the geodesic curvature, the geodesic torsion, and the normal curvature along the direction of $m$ can be expressed:
\[
\begin{align*}
    k_g &= (d\phi + \omega_{12})/ds, \\
    \tau_g &= b \cos 2\phi + (c - a) \cos \phi \sin \phi, \\
    k_n &= a \cos^2 \phi + 2b \cos \phi \sin \phi + c \sin^2 \phi,
\end{align*}
\]
where $ds$ is the arc length element along $m$. If $m$ aligns with $e_1$, then $\phi = 0$, $k_g = \omega_{12}/ds$, $\tau_g = b$, and $k_n = a$.

B. Elastic theory of 1D continua

We will elucidate the elastic theory of rod with inextensible centerline. As shown in Fig. 3, let us simplify a rod as a curve $r(s)$ with $s$ being the arc-length parameter, and cut an infinitesimal element (shown in the magnified box) from the rod. There are forces and moments at the two ends of the element which originating from the interaction of other parts of the rod. $F$ and $M$ represent the force and moment vectors at point $r(s)$, while $F + dF$ and $M + dM$ are the force and moment vectors at point $r(s + ds)$. From Newton’s laws, we can derive the force and moment balance equations:
\[ \sum F = 0 \Rightarrow F' = 0, \]
and
\[ \sum M = 0 \Rightarrow M' + T \times F = 0, \]
where the prime represents the derivative with respect to $s$. One should add the constitutive relation and boundary conditions to make the above two equations closed.

1. Kirchhoff rod theory

A rod with rectangle cross section and centerline $C$ is shown in Fig. 4. Take local coordinates $\{x_1, x_2, x_3\}$ with $x_1$ and $x_2$ paralleling respectively to the two edges of the rectangle, and $x_3$ along the tangent of the centerline. $N$ is the normal of curve $C$. Let $\{x_1, x_2, x_3\}$ denote the basis of the local coordinates and define $\kappa_1 = -x_2 \cdot (dx_3/ds)$, $\kappa_2 = x_1 \cdot (dx_3/ds)$, and $\kappa_3 = x_2 \cdot (dx_1/ds)$. Viewed from geometrical point, $\kappa_1$ and $\kappa_2$ describe the bending of the rod around axes $x_1$ and $x_2$, respectively, and $\kappa_3$ represents the twist of the rod around axis $x_3$. The free energy density $G$ due to the bending and twist can be expressed as a function of $\kappa_1$, $\kappa_2$, and $\kappa_3$. Expanding $G$ up to the second order terms of $\kappa_1$, $\kappa_2$, and $\kappa_3$, we have
\[ G = \gamma + \frac{k_1}{2}(\kappa_1 - \bar{\kappa}_1)^2 + \frac{k_2}{2}(\kappa_2 - \bar{\kappa}_2)^2 + \frac{k_3}{2}(\kappa_3 - \bar{\kappa}_3)^2, \]
where the constant $\gamma$ can be interpreted as the line tension. $\bar{\kappa}_1$ and $\bar{\kappa}_2$ are interpreted as the spontaneous
curvatures while \( \bar{\kappa} \) the spontaneous torsion. Denote \( \mathbf{k} = \kappa_1 \mathbf{x}_1 + \kappa_2 \mathbf{x}_2 + \kappa_3 \mathbf{x}_3 \) and let \( \phi \) be the angle between \( \mathbf{x}_1 \) and \( \mathbf{N} \). Then we have

\[
\begin{align*}
\mathbf{N} &= \cos \phi \mathbf{x}_1 - \sin \phi \mathbf{x}_2, \\
\mathbf{B} &= \sin \phi \mathbf{x}_1 + \cos \phi \mathbf{x}_2,
\end{align*}
\]

(11)

where \( \mathbf{B} \) is the binormal of curve \( C \). From Eqs. (11) and (14), we can derive \( \mathbf{k} = \kappa \sin \phi \mathbf{x}_1 + \kappa \cos \phi \mathbf{x}_2 + (\tau + \phi') \mathbf{x}_3. \)

(12)

Thus \( G \) can be also regarded as the function of \( \kappa, \tau, \phi, \phi' \).

![FIG. 4: Rod with rectangle cross section.](image)

The moment vector is defined as

\[
\mathbf{M} = \frac{\partial G}{\partial \kappa} \mathbf{x}_1 + \frac{\partial G}{\partial \kappa_1} \mathbf{x}_2 + \frac{\partial G}{\partial \kappa_3} \mathbf{x}_3,
\]

(13)

which is called the constitutive relation. Eqs. (8), (9) and (10) with some boundary conditions form a group of closed equations. They are also available for the rod with cross section different from rectangle if only we take \( x_1 \) and \( x_2 \) as the two principal axes of inertia. It should be noted that the equivalent form of these equations can be also obtained from the variational method. This method is called the top-down method while the former one via Newton’s laws called the bottom-up method.

The free energy of a rod with length \( L \) can be written as

\[
\mathcal{F} = \int_0^L G(\kappa, \tau; \phi, \phi') \, ds + \mathcal{F}_{bd},
\]

(14)

where \( \mathcal{F}_{bd} \) comes from the contributions of two ends of the rod. The general Euler-Lagrange equations corresponding to Eq. (14) are derived as

\[
\begin{align*}
G_\phi - (G_\phi')' &= 0, \\
G_\kappa'' + 2\tau (G_\tau' / \kappa) + \kappa G_\kappa' + (\kappa^2 - \tau^2) G_\kappa &= \kappa G_\kappa', \\
\tau G_\tau + 2\tau (G_\tau' / \kappa) &= -\kappa G_\kappa, \\
\tau' G_\tau + 2\tau (G_\tau' / \kappa) &= (\kappa^2 / \kappa) G_\tau + (G_\tau'' / \kappa) + (G_\tau'' / \kappa)'' = 0.
\end{align*}
\]

(15–17)

where \( G_\phi, G_\kappa, G_\kappa \) and \( G_\tau \) are the partial derivatives of \( G \) with respect to \( \phi, \kappa, \kappa \) and \( \tau \), respectively. Additionally, \( G_\kappa' \equiv (G_\kappa)' \), \( G_\kappa'' \equiv (G_\kappa)'' \), \( G_\kappa \equiv (G_\kappa)'' \). The brief derivation of Eqs. (15–17) is attached in Appendix A. These equations have been employed to investigate helical and twisted filaments.\(^{12}\) There might be a misprint in Eq. (7) of Ref. 12, corresponding to our above equation (17), because the dimension of its last term is different from that of other terms.

Now we would give a typical example to reveal the equivalence relation between Eqs. (11), (12), (13) and Eqs. (15–17) rather than prove it directly. Let us consider a rod with \( k_1 = k_2 = k_0, k_3 = 0, \) and \( \kappa_1 = \kappa_2 = \kappa_3 = 0 \). The free energy density (10) is simplified as

\[
G = (k_0/2)(\kappa_1^2 + \kappa_2^2) + \gamma = (k_0/2)\kappa^2 + \gamma.
\]

(18)

On the one hand, we have \( M_1 = \kappa_0 k_1 = \kappa_0 k_2 = \kappa_0 \kappa_3 = 0 \) from Eq. (13). The moment balance equation (9) implies \( F_1 = -(\kappa_0 k_1 + k_2) - k_0 k_2 \) and \( F_2 = k_0 k_1 - k_0 k_2 k_3 \). Substituting them into the force balance equation (8), we have \( F_3 = F_{30} - k_0 \kappa^2 / 2 \) and

\[
\begin{align*}
\kappa'' - \kappa \tau^2 + \kappa^3 / 2 - \kappa F_{30} / k_0 &= 0, \\
2 \tau \kappa' + \kappa' &= 0.
\end{align*}
\]

(19–20)

where \( F_{30} \) is an integral constant which represents the line tension of the straight \( (k = 0) \) rod. On the other hand, we have \( G_{\kappa} = k_0 \kappa, G_{\phi} = G_{\phi'} = G_{\tau} = 0 \). Eq. (15) is trivial while Eqs. (16) and (17) \( \phi \) are, respectively, transformed into

\[
\begin{align*}
\kappa'' &= \kappa \tau^2 + \kappa^3 / 2 - \gamma \kappa / k_0 = 0, \\
2 \tau \kappa' + \kappa' &= 0.
\end{align*}
\]

(21–22)

The above equations are the same as Eqs. (19) and (20) obtained from the force and moment balance conditions if only we take \( F_{30} = \gamma \). Thus the equations obtained from the top-down and bottom-up methods are equivalent to each other.

Substituting the free energy density (10) into Eqs. (15–17), we obtain the so called shape equations of Kirchhoff rod as

\[
(k_1 - k_2) \kappa^2 \sin 2 \phi - 2 k_3 (\tau + \phi') + 2 I_{21} \kappa = 0,
\]

(23)

\[
I_1 (2 \kappa'' + \kappa^3 - 2 k_2 \tau^2) + 2 \gamma \kappa + 2 I_{12} (\phi'^2 + \tau^2) + 2 I_{21} \phi'' + 2 (k_1 - k_2) [(\phi' / \kappa \sin 2 \phi) + \phi' / \kappa \sin 2 \phi] - I_\kappa \kappa + 2 k_3 \tau [(\tau' + \phi'') / \kappa] + 2 k_3 (\tau' + \phi'' / \kappa) = 0,
\]

(24)

\[
I_1 (\kappa''(\tau' + 2 \kappa \tau'') - k_3 [\kappa (\tau' + \phi') - \bar{\kappa}_3]) + k_3 (\tau' + \phi'') / \kappa - k_3 [\kappa (\tau' + \phi'') / \kappa] = 0,
\]

(25)

where \( I_1 = k_1 \sin^2 \phi + k_2 \cos^2 \phi, I_\kappa = k_1 \kappa_1 + k_2 \kappa_2 \), \( I_{12} = k_1 \kappa_1 \sin \phi + k_2 \kappa_2 \cos \phi \), and \( I_{21} = k_1 \kappa_1 \sin \phi - k_2 \kappa_2 \cos \phi \). We also suggest that gentle readers consult the work by Zhou et al.\(^{18}\) where the above equations (23–25) and different kinds of boundary conditions are expressed in another representation with the aid of Euler angles.
2. Helfrich rod theory

Helfrich rod theory can be regarded as the fourth order Kirchhoff rod theory with circular cross section to some extent. The free energy density is expressed as \[ G = \frac{1}{2} k_2 \kappa^2 + k_3 \kappa^2 \tau + \frac{1}{4} k_22 \kappa^4 + \frac{1}{2} k_4 (\kappa^2 + \kappa^2 \tau^2) + \gamma, \] (26)
where \( k_2, k_3, k_22 \) and \( k_4 \) are elastic constants while \( \gamma \) is the line tension. It is noted that this free energy density is the simplest stable form including the chirality term but without spontaneous curvature and torsion. It has been employed to investigate the circular DNA in Ref. 20 and the Euler-Lagrange equations corresponding to \( \int G \, ds \) are given as:
\[
k_2 (2 \kappa' \tau + \kappa') + k_22 (\kappa^3 \tau' + 6 \kappa^2 \kappa') + k_3 (6 \kappa^2 \tau' + 6 \kappa' \tau' - 3 \kappa^2 \kappa^2 - 2 \kappa'') + k_4 (4 \kappa^3 \tau' + 3 \kappa^2 \tau^2 - 3 \kappa^2 \kappa' - \kappa^3 \tau') - 4 \kappa' \tau'' - 6 \kappa'' \tau' - 4 \kappa'' \kappa' - 2 \kappa''') = 0, \] (27)
Here we will not go on the more higher order Helfrich rod theory, on which gentle readers can consult Refs. 20 and 21.

3. Theory of bending-soften Rod

There are two kinds of rod theory with bending-induced softening. First, let us assume that the bending moment depends linearly on the curvature for small curvature but not on the curvature for large curvature, which is expressed as
\[
M = \begin{cases} 
    k_1 \kappa, & (\kappa < \kappa_c) \\
    k_1 \kappa_c, & (\kappa > \kappa_c)
\end{cases} \]
(29)
where \( k_1 \) and \( \kappa_c \) are the elastic bending rigidity and the critical curvature, respectively. Eq. (29) describes the bending-induced softening relation of the first kind which is depicted in Fig. 5(a). The corresponding free energy density can be expressed as
\[
G = \gamma + (k_1/2)[\kappa^2 - (\kappa - \kappa_c)^2 \mathcal{H}(\kappa - \kappa_0)], \]
(30)
where \( \mathcal{H}(\cdot) \) is the Heaviside step function. The above form has been employed by Yan et al. to investigate the loop formation mechanism and probability of short DNA rings. We conjecture that this model could solve the paradox in the experiment on the ring closure of single-walled carbon nanotubes with 1,3-dicyclohexylcarbodiimide. Fitting the experiment data with the worm-like chain model, the persistence length is 800 nm for single-walled carbon nanotubes in the diameter of 1 nm which is much smaller than the theoretical value 33 \( \mu \)m estimated in terms of the Young’s modulus and thickness of single-walled carbon nanotubes in Ref. 44.

Consider a rod divided into two parts at \( s = L_c \): one part \((s < L_c)\) has curvatures less than \( \kappa_c \) another one larger than \( \kappa_c \). In terms of the variational method in Appendix A we can derive the equations describing the rod as
\[
k_1 (2 \kappa'' - 2 \kappa \tau^2 + \kappa^3) - 2 \gamma \kappa = 0 \quad (s < L_c), \]
\[
k_1 \kappa_c (\kappa_c - \kappa) = 0 \quad (s < L_c), \]
\[
k_1 \kappa_c (\kappa_c - 2 \tau^2) - 2 \gamma \kappa = 0 \quad (s > L_c), \]
\[
\kappa' = 0 \quad (s > L_c). \]
(33, 34)
At the divided point \( s = L_c \), we have the joint conditions as
\[
\kappa_- = \kappa_+ = \kappa_c, \]
\[
\kappa'_- = 0, \]
\[
\tau_- = \tau_+, \]
(35, 36, 37)
where \((\cdot)_-\) and \((\cdot)_+\) represent the values of \((\cdot)\) at the left and right sides of \( s = L_c \).

Secondly, let us assume that the bending moment depends linearly on the curvature for small curvature but weaker linearly on the curvature for large curvature, which is expressed as
\[
M = \begin{cases} 
    k_1 \kappa, & (\kappa < \kappa_c) \\
    k_2 (\kappa - \kappa_c) + k_1 \kappa_c, & (\kappa > \kappa_c)
\end{cases} \]
(38)
where \( k_1 > k_2 \) are the elastic bending rigidities while \( \kappa_c \) is the critical curvature. Eq. (38) describes the bending-induced softening relation of the second kind which is depicted in Fig. 5(b). The corresponding free energy density can be expressed as
\[
G = \gamma + (k_1/2)\kappa^2 + [(k_2 - k_1)/2](\kappa - \kappa_c)^2 \mathcal{H}(\kappa - \kappa_0), \]
(39)
Consider a rod divided into two parts at \( s = L_c \): one part \((s < L_c)\) has curvatures less than \( \kappa_c \), another one larger than \( \kappa_c \). In terms of the variational method in Appendix A we can derive the equations describing the rod as

\[
\begin{align*}
  k_1(2\kappa'' - 2\kappa\tau^2 + \kappa^3) - 2\gamma\kappa &= 0 \quad (s < L_c), \\
  \kappa' + 2\kappa'\tau &= 0 \quad (s < L_c), \\
  2k_2\kappa'' + [k_2(\kappa - \kappa_c) + k_1\kappa_c](\kappa^2 - 2\tau^2) - 2\gamma\kappa \\
  + (k_2 - k_1)(\kappa - \kappa_c)\kappa c &= 0 \quad (s > L_c), \\
  k_2(\tau' + 2\kappa'\tau) + (k_1 - k_2)\kappa c\tau' &= 0 \quad (s > L_c). 
\end{align*}
\]

At the divided point \( s = L_c \), we have the joint conditions as

\[
\begin{align*}
  k_1(\kappa_+ - \kappa_c) &= k_2(\kappa_+ - \kappa_c) \\
  k_1\kappa_+ &= k_2\kappa'_1 \\
  \tau_- &= \tau_+ \\
  k_1(\kappa_+^2 - \kappa_c^2) &= (k_2 - k_1)(\kappa_+ - \kappa_c)^2. 
\end{align*}
\]

Obviously, the above equations \((40) - (47)\) degenerate into Eqs. \((31) - (37)\) if \( k_2 = 0 \) and into Eqs. \((21) - (22)\) if \( k_2 = k_1 \).

C. Elastic theory of 2D continua

A 2D continuum can be simplified as a surface as shown in Fig. 6. At each point, we can select a frame \( \{e_1, e_2, e_3\} \). A pressure \( p \) is loaded on the surface in the inverse direction of the normal vector \( e_3 \). Let us cut a region enclosed in any curve \( C \) from the surface. \( t \) is the tangent vector at point of curve \( C \). \( b \) is normal to \( t \) and in the tangent plane. The force and moment per length performed by the other region on curve \( C \) are denoted as \( f \) and \( m \), respectively. Through Newton’s laws, the force and moment balance conditions are obtained as

\[
\begin{align*}
  \oint_C f ds - \int p e_3 dA &= 0, \\
  \oint_C m ds + \int r \times f ds - \int r \times p e_3 dA &= 0,
\end{align*}
\]

where \( ds \) and \( dA \) are the arc length element of curve \( C \) and area element of the region enclosed in curve \( C \), respectively.

Define two second order tensors \( \mathcal{S} \) and \( \mathcal{M} \) such that

\[
\mathcal{S} \cdot b = f, \quad \mathcal{M} \cdot b = m.
\]

These two tensors can be called as stress tensor and bending moment tensor, respectively. Using the Stokes’ theorem, we can derive

\[
\begin{align*}
  \int (\text{div} \ \mathcal{S} - p e_3) dA &= 0, \\
  \int (\text{div} \ \mathcal{M} + e_1 \times \mathcal{S}_1 + e_2 \times \mathcal{S}_2) dA &= 0.
\end{align*}
\]

FIG. 6: Force and moment in a 2D continuum.

where \( \mathcal{S}_1 = \mathcal{S} \cdot e_1 \) and \( \mathcal{S}_2 = \mathcal{S} \cdot e_2 \). Since the integral is performed on the region enclosed in an arbitrary curve \( C \), from the above two equations we obtain the force and moment balance conditions of 2D continua as:

\[
\begin{align*}
  \text{div} \ \mathcal{S} &= pe_3, \\
  \text{div} \ \mathcal{M} &= \mathcal{S}_1 \times e_1 + \mathcal{S}_2 \times e_2.
\end{align*}
\]

The above two equations are equivalent to Eq. \((25)\) in Ref. 54 and Eqs. \((28)\) and \((57)\) in Ref. 57. Eqs. \((53)\) and \((54)\) with some complement constitutive relations form the fundamental equations of 2D continua.

1. Fluid membranes

A fluid membrane is a 2D isotropic continuum which cannot withstand in-plane shear strain. Generally, we assume that the fluid is incompressible. The free energy density, \( G \), of fluid membranes should be invariant under the in-plane coordinate transformation. In terms of the surface theory, there are only two fundamental geometric invariants: the mean curvature \( 2H \) and gaussian curvature \( K \). Thus the free energy density should be a function of \( 2H \) and \( K \), that is,

\[
G = G(2H, K).
\]

The free energy of a closed fluid membrane can be expressed as

\[
\mathcal{F} = \int G \ dA + p \int dV,
\]

where \( dA \) is the area element of the membrane and \( dV \) is the volume element enclosed in the membrane. \( p \) is the osmotic pressure, the pressure difference between the outer and inner side of the membrane. The general Euler-Lagrange equation of free energy \((56)\) can be derived
through the variational method shown in Appendix B as

\[ p - 2HG + \frac{(\nabla^2/2 + 2H^2 - K)(\partial G/\partial H)}{\nabla \cdot \nabla + 2KH}(\partial G/\partial K) = 0. \]  

(57)

As we known, the above equation has been derived by several authors such as Ou-Yang et al.\textsuperscript{53,58} and Giaquinta et al.\textsuperscript{59} coming from different research fields. It is recently employed to investigate the modified Korteweg-de Vries surfaces.\textsuperscript{22} Here \( \nabla \cdot \nabla \) can be called as the Laplace operator of the second class which is also fully discussed by Zhang and Xu.\textsuperscript{28}

We emphasize that (54) can be also derived from the bottom-up method, Eqs. (53) and (54) combining a com-plement constitutive relation

\[ \mathfrak{M} = (G_a/2)(e_1 e_1 - e_2 e_2) - G_a e_2 e_1 + G_c e_1 e_2, \]  

(58)

where \( G_a, G_b, \) and \( G_c \) represent the partial derivatives of \( G \) with respect to \( a, b, \) and \( c, \) respectively. Here \( a, b, \) and \( c \) are the components of the curvature tensor \( \mathfrak{R} \) in Eq. (53). To illuminate this point, we consider an example in which the free energy density is taken as \( G = k_c(2H)^2 + \lambda, \) where \( k_c, \lambda \) are the bending modulus and surface tension of the fluid membrane. It follows that \( \mathfrak{M} = 2k_c H(\varepsilon_1 e_2 - e_2 e_1) \) from Eq. (58). Substituting it into Eqs. (53) and (54), we can derive

\[ p - 2\lambda H + 4k_c H(H^2 - K) + 2k_c \nabla^2 H = 0, \]  

(59)

which is the same as the result obtained directly from (57). Simultaneously, we have the stress components

\[ \begin{align*}
\mathfrak{S}_1 &= (2H^2 - 2aH + \lambda)e_1 - 2bHe_2 - 2H_1 e_3, \\
\mathfrak{S}_2 &= -2bHe_1 + (2H^2 - 2cH + \lambda)e_2 - 2H_2 e_3,
\end{align*} \]  

(60)\hspace{1cm}(61)

where \( H_1 \) and \( H_2 \) are the directional derivatives of \( H \) respect to \( e_1 \) and \( e_2. \) These equations have been also derived by Capovilla and Guven.\textsuperscript{57} from which we seem to arrive at a paradox for fluid membranes: we have mentioned that fluid membranes cannot withstand in-plane shear strain, however Eqs. (60) and (61) reveals shear stress still exhibits in non-spherical vesicles.

2. Solid shells

A solid shell is a 2D isotropic continuum which can endure both bending and in-plane shear strain. The free energy density, \( G, \) of solid shells should be invariant under the in-plane coordinate transformation. There are only two fundamental geometric invariants, \( 2H \) and \( K, \) and two fundamental strain invariants: the trace, \( 2J, \) and the determinate, \( Q, \) of the in-plane strain tensor. Thus free energy density should be a function of \( 2H, K, 2J, \) and \( Q. \) That is, \( G = G(2H, K, 2J, Q). \)

If the solid shell has no initial strains and consists of materials distributing symmetrically with regard to the middle surface of the shell, we can expand \( G \) up to the second order terms of curvatures and strains as

\[ G = (k_c/2)(2H)^2 - \frac{k_c}{2} + (k_d/2)(2J)^2 - kQ, \]  

(62)

where \( k_c \) and \( k_d \) are the bending moduli while \( k_c \) and \( k_d \) are the in-plane rigidity moduli. The theory based on the above free energy density is called Kirchhoff’s linear shell theory.\textsuperscript{3} Especially, if the shell consists of 3D isotropic materials, we have

\[ \begin{align*}
k_c &= Yh^3/12(1 - \nu^2), \\
k_d &= Yh/(1 - \nu^2), \\
k_c/k_c &= k_d/k_d = (1 - \nu),
\end{align*} \]  

(63)\hspace{1cm}(64)\hspace{1cm}(65)

where \( Y \) and \( \nu \) are the Young’s modulus and Poisson ratio while \( h \) is the thickness of the shell.\textsuperscript{3}

For a closed shell, its free energy is expressed as Eq. (59) with \( G \) in Eq. (62). Of course, we can obtain the equations of in-plane strains and shapes through the variational method in Appendix B. The final results are the same as those obtained from Eqs. (53) and (54) with a complement constitutive relations (58) and

\[ \mathfrak{S} = \mathfrak{S}^i + \mathfrak{S}^J \]  

(66)

with

\[ \mathfrak{S}^i = G_{\varepsilon_11} e_1 + (G_{\varepsilon_{12}}/2)(e_1 e_2 + e_2 e_1) + G_{\varepsilon_{22}} e_2, \]  

(67)

where \( G_{\varepsilon_{11}}, G_{\varepsilon_{12}}, \) and \( G_{\varepsilon_{22}} \) represent the partial derivatives of \( G \) with respect to \( \varepsilon_{11}, \varepsilon_{12}, \) and \( \varepsilon_{22} \), the components of the in-plane strain tensor \( \mathfrak{E}. \) Substituting Eq. (66) into Eqs. (53) and (54) and then employing Eqs. (53) and (54), we obtain

\[ d(S_{11}\omega_2 - S_{112}\omega_1) - (S_{212}\omega_2 - S_{212}\omega_1) \land \omega_2 = 0, \]  

(68)\hspace{1cm}(69)

and

\[ \begin{align*}
d(S_{11}\omega_2 - S_{112}\omega_1) - (S_{11}\omega_2 - S_{112}\omega_1) \land \omega_12 = 0,
\end{align*} \]  

(69)\hspace{1cm}(70)

\[ p + 2k_c(2H(H^2 - K) + \nabla^2 H - 4(k_d - \tilde{k})(H - \tilde{K}) / \mathfrak{R} : \mathfrak{E} = 0, \]  

(70)

where \( S_{11} = (2k_d J - \tilde{k} \varepsilon_{22}), \) \( S_{112} = S_{21} = \tilde{k} \varepsilon_{12}, \) \( S_{112} = S_{22} = (k_d J - \tilde{k} \varepsilon_{11}), \) are the components of tensor \( \mathfrak{S}^J. \) \( \mathfrak{R} \) is the curvature tensor related to Eq. (53). The above equations (68)–(70) describe the in-plane strains and shapes of solid shells at equilibrium state. The similar equations and the corresponding dynamics forms have been derived through the variational method in Refs. 49 and 62, respectively, with the aid of moving frame method.

The above equations (68) and (69) can be written as one vector equation by introducing a displacement vector \( \mathbf{u} = u_1 e_1 + u_2 e_2 + u_3 e_3, \) which is related to two invariants \( 2J \) and \( Q \) of the in-plane strain tensor as

\[ \begin{align*}
2J &= \text{div} \mathbf{u} - 2Hu_3, \\
2Q &= (\text{div} \mathbf{u} - 2Hu_3)^2 + (1/2)(\text{curl} \mathbf{u})^2 - (\nabla \mathbf{u})^2,
\end{align*} \]  

(71)\hspace{1cm}(72)
where \( \hat{\mathbf{u}} = \nabla \mathbf{u} - \mathbf{e}_3(\mathbf{e}_1 \cdot \nabla \mathbf{u}) \) is the in-plane part of \( \nabla \mathbf{u} \). Using the new variable \( \mathbf{u} \), Eqs. (68) and (69) can be be written as

\[
(\tilde{\kappa} - 2k_4) \nabla(\text{div} \mathbf{u} - 2Hv_3) - \tilde{\kappa}(\mathbf{u} + K\hat{\mathbf{u}} + \tilde{\nabla}v_3) = 0, \tag{73}
\]

where \( \hat{\mathbf{u}} \) and \( \hat{2}\mathbf{u} \) are the in-plane components of \( \mathbf{u} \) and \( \text{div}(\hat{\mathbf{u}}) \), respectively. \( \nabla \) is the gradient operator of the second class, which is shown in our previous work.84 In particular, \( H, K, \nabla v_3 \) vanish and \( \hat{2}\mathbf{u} \) degenerates into \( \nabla^2 \) for a flat manifold. Then the above equation degenerates into the Cauchy equation3 in 2D plane. Thus Eq. (73) can be regarded as the Cauchy equation in a curved surface.

### III. APPLICATION OF ELASTIC THEORY IN BIO-STRUCTURES

In the above section, we have described fundamentals of geometric and elastic theory on low-dimensional continua. Can this theory be applied to the bio-structures, such as DNA and cell membranes, and so on? DNA is a long chain macromolecule which may be described as an elastic rod. A cell membrane is a thin structure whose thickness and the size of the microscopic components are so much smaller than its lateral dimension that it can be regarded as a 2D continuum phenomenologically. We will discuss the application of the above elastic theory in short DNA rings, lipid membranes and cell membranes in this section.

#### A. Short DNA ring

DNA is a double helical structure whose diameter is about 2.5 nm. Its bending rigidity, described as the persistence length \( l_p \), is about 50 nm (150 bp) at the room temperature. The normal DNA is usually flexible enough because its length is so much larger than \( l_p \) that the fluctuations are quite evident. Thus the rod theory cannot directly be applied to the normal DNA. The statistical theory combining the rod theory is required,63,64 which is out of our topic in this review. However, there is a special kind of short DNA rings,65,66,67 which are in the length scale of \( l_p \) so that the fluctuation effect can be neglected. The diameter is still much smaller than the total length. Thus the rod theory mentioned in Sec. III B is expected to be available for this kind of DNA rings.

Han et al. have used AFM to observe DNA rings consisting of several segments connected by kinks in the presence of Zn\(^{2+} \) ions.65,66,67 Zhao et al. have analyzed the mechanism of this kink instability based on Helfrich rod theory.5 Their main ideas are sketched as follows. First, a circle is a solution to Eqs. (27) and (28). Next, through analyzing the stability of the cycle, it is found that, for the given elastic constants, there exists a critical radius above which DNA circles will be instable. This prediction is in good agreement with the experiments,65,66 where kink deformations were observed in DNA rings of 168 bp but not 126 bp. Above some thresholds of the chiral modulus, \( k_3 \) in Eq. (26), the DNA circles turn into elliptical, triangular, square, or other polygonal shapes, respectively. This fact agrees with the experiments if \( k_3 \) is positively correlated to the condensation of Zn\(^{2+} \) ions.

Interestingly, Zhou and Ou-Yang proposed another interpretation based on the dynamic instability of Kirchhoff rod theory with \( \tilde{\kappa}_2 = \tilde{\kappa}_3 = 0 \) in Eq. (10). Their result is the same as that obtained directly from the first and second order variations of the free energy. We deal with the latter scenario. First, \( \tau = 0, \phi = 0 \), and \( \kappa = 1/R \) satisfy Eqs. (23)–(25) derived from the first order variation of the free energy. That is, a planar circle with radius \( R \) is an equilibrium configuration. Next, through the second order variation of the free energy, we can obtain the characteristic function describing the stability of the circle

\[
g_c(R) = \tilde{\kappa}_1^2 - (1 - \Gamma)\tilde{\kappa}_1/R - \Gamma n^2/R^2 \leq 0 \tag{74}
\]

where \( n > 1 \) is an arbitrary integer and \( \Gamma = k_3/k_1 \). From the above inequality, we obtain the critical radius

\[
R_c = 8\Gamma/\tilde{\kappa}_1[\Gamma - 1 + \sqrt{(\Gamma - 1)^2 + 16\Gamma}], \tag{75}
\]

above which the circle is instable. If only the presence of Zn\(^{2+} \) ions tunes the values of \( \Gamma \) and \( k_3/k_1 \) such that \( R_c \) is in the range between 63/\( \pi \) (bp) and 84/\( \pi \) (bp), the above result is also in agreement with the experiments,65,66 where kink deformations were observed in DNA rings of 168 bp but not 126 bp.

![FIG. 7: A possible configuration of a short DNA ring.](image-url)
Through simple calculations, we find that the fictitious configuration is energetically less favorable than the perfect ring with radius $R$. Therefore, this coarse analysis reveals that the theory of bending-soften rod cannot explain the experiments.

B. Lipid membrane

Lipids are dominant composition of cell membranes. Most of lipid molecules have a polar hydrophilic head group and two hydrophobic hydrocarbon tails. When a quantity of lipid molecules disperse in water, they will assemble themselves into a bilayer vesicle as depicted in Fig. 8 in which the hydrophilic heads shield the hydrophobic tails from the water surroundings because of the hydrophobic forces. This self-assembly process has been numerically investigated by Lipowsky et al. through molecular dynamics simulation based on coarse-grained model or meshless membrane model.

![FIG. 8: A lipid bilayer vesicle.](image)

The thickness of the lipid bilayer and the size of single lipid molecules are much smaller than the scale of the whole lipid bilayer. Additionally, at the physiological temperature, the lipid bilayer is usually at the nematic state where the hydrocarbon chains of the lipid molecules are roughly perpendicular to the bilayer surface. Thus the bilayer can be regarded as a 2D fluid membrane whose free energy density is expressed as Eq. (55). Expanding it up to the second order terms of curvatures, we obtain the Helfrich’s form:

$$G_H = (k_c/2)(2H + c_0)^2 - kK + \lambda, \quad (76)$$

where $k_c$ and $\bar{k}$ are the bending moduli of the lipid bilayer. We emphasize that the minus sign before $\bar{k}$ in Eq. (76) is opposite to Helfrich’s convention. $\lambda$ is the surface tension of the bilayer. $c_0$ is called the spontaneous curvature that reflects asymmetric factors between two sides of the bilayer, including the lipid distribution, the chemical environment, and so on. $k_c$ is about 20 T for lipid bilayers, where the Boltzmann factor is set to 1 and $T$ the room temperature, from which the persistence length of lipid bilayers is estimated about 10 $\mu$m. In this section we only consider the size of lipid bilayers smaller than 10 $\mu$m so that the fluctuation effect on the shape of lipid bilayers can be neglected. The model based on Eq. (76) is called spontaneous curvature model. We still remind gentle readers to note the two similar nonlocal models—the bilayer-coupling model and the area difference model although we will not touch them in the present review.

1. Closed vesicles

The free energy of a lipid vesicle under the osmotic pressure $p$ (the outer pressure minus the inner one) can be written as Eq. (56) with $G = G_H$ being Helfrich’s form (76). Substituting (76) into Eq. (57), we obtain the shape equation of lipid vesicles:

$$p - 2\lambda H + k_c(2H + c_0)(2H^2 - c_0H - 2K) + 2k_c\nabla^2 H = 0. \quad (77)$$

This equation is the fourth order nonlinear equation. It is not easy to find its special solutions. We have known three typical analytical solutions: sphere, torus, and biconcave discoid shape.

For a sphere with radius $R$, we have $H = -1/R$ and $K = 1/R^2$. Substituting them into (77), we arrive at

$$pR^2 + 2\lambda R - k_c c_0(2 - c_0 R) = 0. \quad (78)$$

This equation gives the sphere radius under the osmotic pressure $p$.

A torus is a revolution surface generated by a circle with radius $\rho$ rotating around an axis in the same plane of the circle. The revolution radius $r$ should be larger than $\rho$. A point in the torus can be expressed as a vector $(r, \rho \cos \varphi, \rho \sin \varphi)$. Through simple calculations, we have $2H = -(r + 2\rho \cos \varphi)/\rho (r + \rho \cos \varphi), \quad K = \cos \varphi/\rho (r + \rho \cos \varphi)$. Substituting them into Eq. (77), we derive

$$[2k_c c_0 \rho^2 - 4k_c c_0 \rho + 4\lambda \rho^2 + 2P \rho^3]/\rho^4 \cos^3 \varphi + [(5k_c c_0 \rho^2 - 8k_c c_0 \rho + 10\lambda \rho^2 + 6P \rho^3)/\rho^2] \cos^2 \varphi + [(4k_c c_0 \rho^2 - 4k_c c_0 \rho + 8\lambda \rho^2 + 6P \rho^3)/\rho^2] \cos \varphi + 2k_c/\rho^2 + k_c(c_0^2 \rho^2 - 1) + 2(P + \lambda) \rho^2 = 0, \quad (79)$$

where $\rho = r/\rho$. If $\rho$ is finite, then Eq. (79) holds if and only if the coefficients of $\{1, \cos \varphi, \cos^2 \varphi, \cos^3 \varphi\}$ vanish. It follows $2\lambda \rho^2 = k_c c_0 \rho (4 - c_0 \rho), \quad P \rho^3 = -2k_c c_0 \rho$ and $\rho = \sqrt{2/\lambda}$. That is, there exists a lipid torus with the ratio of its two generated radii being $\sqrt{2}$, which was confirmed in the experiment.

To describe the solution of biconcave discoid shape, we write the shape equation (77) under the axisymmetric condition. If a planar curve $z = z(\rho)$ revolves around the $z$-axis, an axisymmetric surface is formed. Each point on the surface is expressed as $r = \{\rho \cos \varphi, \rho \sin \varphi, z(\rho)\}$. 


Denote \( \psi = \arctan(dz/d\rho) \) and \( \Psi = \sin \psi \). Then Eq. (77) is transformed into:

\[
\frac{1}{2} \left[ \frac{\rho \Psi'}{\rho} + c_0 \right] \left\{ \frac{\rho}{\rho} \left[ \frac{\rho \Psi'}{\rho} \right]^2 - c_0 \left( \frac{\rho \Psi'}{\rho} \right) \right\} - \frac{\lambda (\rho \Psi')}{\kappa_c \rho} = \frac{\lambda (\rho \Psi')}{\kappa_c \rho} \]

\[
+ \left\{ \frac{\rho}{\rho} \left[ \frac{\rho \Psi'}{\rho} \right]^2 \right\} \left[ \left[ \frac{\rho \Psi'}{\rho} \right]^2 - \frac{1}{\rho^2} \right] \Psi \Psi' + \frac{\rho}{\kappa_c} = 0, \tag{80} \]

where the prime represents the derivative with respect to \( \rho \). This equation is called the shape equation of axisymmetric lipid vesicles. Its first integral, group structure and corresponding Hamilton’s equations are investigated by Zheng and Liu, Xu and Ou-Yang, and Capovilla et al. respectively.

FIG. 9: A quarter outline of the biconcave surface.

It is easy to verify that \( \Psi = \sin \psi = -c_0 \rho \ln(\rho/\rho_B) \) with a constant \( \rho_B \) is a solution to Eq. (80) if \( p \) and \( \lambda \) are vanishing. For \( 0 < \rho_B \rho < \rho \), the parameter equation

\[
\begin{align*}
\sin \psi &= -c_0 \rho \ln(\rho/\rho_B) \\
z &= z_0 + \int_0^\rho \tan \psi d\rho
\end{align*} \tag{81}
\]

corresponds to a curve shown in Fig. 9. A biconcave discoid surface will be achieved when this curve revolves around z-axis and then reflects concerning the horizontal plane. The above equation (81) can give a good explanation to the shape of human red blood cell under normal physiological conditions. If \( c_0 \rho_B \rho \) is out of the range between 0 and \( \rho \), Eq. (81) corresponds to a prolate ellipsoid or other self-intersecting surfaces.

In the purely mathematical viewpoint, there are also the other solutions to Eq. (77) such as cylinder, constant mean curvature surface, periodic undulation surface, pearling tubule and so on. However, it is a pity that they are open surfaces and do not correspond to truly closed vesicles.

As mentioned above, it is fairly difficult to find the analytical solution to Eq. (77). Thus we appreciate the applications of numerical methods to find the equilibrium shapes of closed vesicles. Two kinds of typical numerical frameworks are usually employed. The first one is to use ‘Surface Evolver’, a software package developed by Brakke, to find the configurations minimizing the free energy under some constraints. The second one is based on the phase field formulation of Helfrich’s free energy density and diffusive interface approximation. The above numerical methods can obtain lipid vesicles with different shapes either axisymmetric or asymmetric. Additionally, the finite element method might be a potential method although very sparse literature treats lipid bilayers by using it.

2. Stability of closed vesicles

When the osmotic pressure is beyond some threshold, a closed vesicle will lose its stability and change its shape abruptly. The threshold is called the critical pressure. To obtain it, one should calculate the second order variation of the free energy with \( G \) being Helfrich’s form, which has been dealt with in the general case as. The volume \( V \) can be negative for the special selection of \( |a_{lm}| \).

\[
\delta^2 F = \int k_c \left[ (\nabla^2 \Omega)_3 \right]^2 + (2H + c_0) \nabla(2H\Omega_3) \cdot \nabla \Omega_3 |dA
\]

\[
+ \int [4k_c(2H^2 - K)^2 + k_c(\rho_0^2 - 4H^2)] + 2\lambda K - 2Hp] \Omega_3^2 |dA
\]

\[
+ \int [k_c(4H^2 + 2c_0H - 4K - \rho_0^2/2) - \lambda \Omega_3 \nabla^2 \Omega_3 |dA
\]

\[
-2k_c \int (2H + c_0) |\nabla \Omega_3 \cdot \nabla \Omega_3 + 2\Omega_3 \nabla \cdot \nabla \Omega_3 |dA, \tag{82}
\]

where \( \Omega_3 \) is a arbitrary small out-of-plane displacement and the operator \( \nabla \) is the gradient operator of the second class.

Here we will mention two results for special configurations.

First, let us consider a lipid sphere that satisfies Eq. (82). On the sphere, the function \( \Omega_3 \) can be expanded by the spherical harmonic functions \( Y_{lm} \) as \( \Omega_3 = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm} Y_{lm} \). Substituting it into Eq. (82), we derive

\[
\delta^2 F = (R/2) \sum_{l,m} |a_{lm}|^2 \{[l(l + 1) - 2](2k_c)[l(l + 1) - c_0 R]/R^3 - p)\}, \tag{83}
\]

From which we can obtain the critical pressure

\[
p_c = 2k_c(6 - c_0 R)/R^3. \tag{83}
\]

If \( p < p_c \), \( \delta^2 F \geq 0 \) for any \( |a_{lm}| \); on the contrary, \( \delta^2 F \) can be negative for the special selection of \( |a_{lm}| \). The above equation depends also on \( c_0 \). If \( c_0 > 6 / R \), then \( p_c \) is negative, which reveals that a sphere vesicle is always instable for large enough \( c_0 \).

Next, let us still regard a long enough lipid tubule as a closed vesicle. Denoted its radius as \( \rho \). From Eq. (77) we have

\[
(\kappa_c/2)(1/\rho^2 - c_0^2) - pp = \lambda. \tag{84}
\]

On the cylindrical surface, \( \Omega_3 \) can be expanded as Fourier series \( \Omega_3 = \sum_{l=-\infty}^{\infty} a_{l} \exp(i\ell \theta) \). Substituting it into Eq. (82) and combining Eq. (84), we derive

\[
\delta^2 F = \sum_{l=-\infty}^{\infty} |a_{l}|^2 \{ [\kappa_c(\ell^2 - 1)/\rho^3] - p \}, \tag{85}
\]

From which we can obtain the critical pressure

\[
p_c = 3\kappa_c/\rho^3. \tag{85}
\]

If \( p < p_c \), \( \delta^2 F \geq 0 \) for any \( |a_{l}| \); on the contrary, \( \delta^2 F \) can be negative for the special selection of \( |a_{l}| \).
3. Open vesicles with free edges

The opening-up process of lipid vesicles by talin, a protein, has recently been observed\textsuperscript{101,102} which pushes us to study the equilibrium equation and boundary conditions of lipid vesicles with free exposed edges. Capovilla \textit{et al.} have addressed this problem and given the equilibrium equation and boundary conditions.\textsuperscript{103} Inspired by the talk “moving frame method” of Chern,\textsuperscript{101} we introduce exterior differential form to deal with the variational problem on open surface and obtain concisely the shape equation and boundary conditions of open lipid vesicles.\textsuperscript{104} Numerical solution to the shape equation and boundary conditions with relaxed method can explain the experimental results very well.\textsuperscript{105} A quantity of open vesicles with free edges have also been obtained numerically by Wang and Du\textsuperscript{106} with the phase field method. Here we will not further discussed the dynamical opening process of the vesicles, which has been recently investigated by Kaga and Ohta.\textsuperscript{107}

![FIG. 10: An open surface with boundary curve C.](image)

We regard an open lipid vesicle with a free edge as a smooth surface with a boundary curve $C$, as shown in Fig. 10. $t$ is the tangent vector of the curve $C$, $b$ in the tangent plane of the surface, is perpendicular to $t$ and points to the opposite side that the surface located in. The free energy of the open lipid vesicle is written as

$$F = \int G_H dA + \gamma \oint_C ds,$$

where $\gamma$ represents the line tension of the edge and $G_H$ has the Helfrich’s form.\textsuperscript{108}

The first order variation of $F$ gives the shape equation

$$k_c(2H+c_0)(2H^2-c_0H-2K)-2\lambda H+2k_c\nabla^2 H = 0,$$\textsuperscript{109} (87)

and the boundary conditions as\textsuperscript{105}

$$[k_c(2H+c_0)-\bar{k}k_n]_C = 0,$$\textsuperscript{107} (88)$$[2k_c\partial H/\partial b + \gamma k_n - \bar{k}\tau'_g]_C = 0,$$\textsuperscript{107} (89)$$[G_H + \gamma k_g]_C = 0,$$\textsuperscript{107} (90)

where $k_n$ and $k_g$ are normal curvature and geodesic curvature of the boundary curve $C$. $\tau'_g$ is the derivative of geodesic torsion $\tau_g$ with respect to the arc length of curve $C$. The mechanical meanings of the above four equations are as follows: Eq. (87) is the normal force balance equation of the membrane; Eq. (88) is the moment balance equation of points in curve $C$ around the direction of $t$; Eq. (89) is the force balance equation of points in curve $C$ along the normal direction of surface; and Eq. (90) is the force balance equation of points in curve $C$ along the direction of $b$. It is necessary to emphasize that the boundary conditions are available for open vesicles with more than one free edge because the edge in our derivation is a general one.

In Ref.\textsuperscript{105}, we have shown two analytical solutions to above equations (87)–(90): One is a cup-like membrane and another is the central part of a torus. Several numerical solutions to these equations are obtained by Umeda \textit{et al.}\textsuperscript{106}. Their results reveal that the line tension $\gamma$ induced by talin correlates negatively with the concentration of talin, which is in agreement with the experimental result that the hole of vesicle is enlarged with the concentration of talin.\textsuperscript{101}

4. Vesicles with lipid domains

The above discussion on open lipid vesicles with free edges can be extended to study a vesicle of several lipid components. The domains usually formed so that each domain contains one or two kinds of lipid molecules. The morphology of axisymmetric vesicles with multi-domains has been theoretically investigated by Jülicher and Lipowsky.\textsuperscript{109} It is found that lipid domains facilitate the budding of vesicles.\textsuperscript{110} The giant vesicles with lipid domains have been observed in recent experiment.\textsuperscript{111} There are two kinds of lipid domains which are at the liquid-ordered state and liquid-disordered state, respectively. It is natural to assume that different kinds of domains have different bending moduli and spontaneous curvatures. The axisymmetric vesicles in the experiment can be explained with Jülicher-Lipowsky theory through numerically method. Baumgart \textit{et al.} have demonstrated that the line tension, the osmotic pressure, the relative bending moduli, and the spontaneous curvature have significant effects on the morphology of a vesicle with two domains being at the liquid-ordered and disordered states, respectively.\textsuperscript{112}

The asymmetric vesicles are also experimentally observed in Ref.\textsuperscript{111}, which enlightens us to investigate the shape equation of each domains and the boundary conditions between domains without any axisymmetric assumptions. Let us consider a vesicle with two domains separated by curve $C$ sketched in Fig. 11. The free energy can be expressed as\textsuperscript{109}

$$F = \int G_H' dA + \int G_H'' dA + \gamma \oint ds + p \oint dV,$$\textsuperscript{109} (91)

where $G_H'$ and $G_H''$ have the Helfrich from with the bending moduli $k'_c$, $\bar{k}'$, $k''_c$, $\bar{k}''$, the spontaneous curvatures $c'_0$, $\bar{c}'_0$, and the surface tensions $\lambda'$, $\lambda''$, respectively. The integrals in the first and second terms of
Eq. (91) are performed on the domain I and II shown in Fig. 11 respectively. \( \gamma \) is the line tension of boundary curve \( C \). \( p \) is the osmotic pressure of the vesicle.

FIG. 11: A vesicle with two domains separated by curve \( C \).

In terms of the physical meanings of Eqs. (87) – (90), we can easily write down the shape equation of domains as:

\[
p - 2\lambda' H + k_c^i(2H + c_0)(2H^2 - c_0^0 H - 2K) + 2k_t^i \nabla^2 H = 0.
\]

(92)

where the superscript \( i = I \) and \( II \) represents the physical quantity of lipid domains I and II, respectively. Additionally, the boundary conditions between domains are as follows:

\[
[k_c^I(2H + c_0) - k_c^{II}(2H + c_0) - (k_t^I - k_t^{II})k_g]_C = 0, \quad (93)
\]

\[
[2(k_c^I + k_c^{II}) \partial H/\partial b - (k_t^I + k_t^{II})r_g + \gamma k_g]_C = 0, \quad (94)
\]

\[
[G^I - G^{II} + \gamma k_g]_C = 0, \quad (95)
\]

where \( \mathbf{b} \) is perpendicular to the boundary curve \( C \) and points to the side of domain \( II \).

As we know, there is still no any numerical result on asymmetric vesicles with domains directly from the above equations in the previous literature. Only in Ref. 107, Wang and Du discussed the morphology of asymmetric vesicles with domains through the phase field model. In the above theory, the detailed architecture of liquid-ordered and disordered phases is neglected. There are special lipid domains at liquid-ordered phase, so called rafts, which are enriched in cholesterol and sphingolipids. Cholesterol is a kind of chiral molecules, which has not been included in the above theory. Recently, a concise theory of chiral lipid membranes developed by Tu and Seifert might be extended to discuss the raft domains.

5. Adhesions of Vesicles

Cell adhesion is a complex biological process which controls many functions of life. It can be understood as a first-order wetting transition, and might be simplified as the adhesion of lipid vesicles. As a model, Seifert and Lipowsky have theoretically investigated a lipid vesicle adhering to a flat rigid substrate and found that the vesicle undergoes a nontrivial adhesion transition from the free state to the bound state, which is governed by the competition between the bending and adhesion energies. Ni et al. have discussed the adhering lipid vesicles with free edges and the adhesion between a lipid tube with a rigid substrate. A big progress on this topic is recently made by Guven and his coworkers, who obtain the general equations to describe the contact line between the vesicle and the rigid substrate or another vesicle.

The adhesion between a lipid vesicle and a rigid substrate is depicted in Fig. 12a, where the contact area is denoted by \( A \). The free energy of this system is expressed as:

\[
\mathcal{F} = \int G_H dA + p \int dV - W \bar{A},
\]

(96)

where \( p \) is the osmotic pressure of the vesicle and \( W \) is the strength of the adhesion potential between the vesicle and the substrate. \( G_H \) is the free energy density of Helfrich’s form. For the flat rigid substrate, a characteristic radius and the length scale of the vesicle are defined as \( R_a = \sqrt{2k_c/W} \) and \( R = \sqrt{A/4\pi} \), respectively. If \( R < R_a \), the vesicle is a little stiffer or the attraction is relative weak such that \( A \) approaches to zero. Thus the vesicle is unbound to the substrate and this state is called the free state. On the contrary, the vesicle is at the bound state. At this state, let us take \( \mathbf{t} \) as the tangent vector of the contact line \( C \), and \( \mathbf{b} \) perpendicular to \( \mathbf{t} \) and in the common tangent plane of the lipid vesicle and the substrate. The absolute value of the normal curvature along \( \mathbf{b} \) for the point on the contact line is proven to be \( \sqrt{2W/k_c} \) for an axisymmetric vesicle adhering to the flat substrate. If the rigid substrate is curved, the above conclusion is revised as:

\[
|\kappa_b^V - \kappa_b^S| = \sqrt{2W/k_c},
\]

(97)

where \( \kappa_b^V \) and \( \kappa_b^S \) are the normal curvatures along \( \mathbf{b} \) for the points outside but near the contact line, calculated by using the surfaces of the vesicle and the substrate, respectively.

The adhesion between two lipid vesicles is depicted in Fig. 12b. The free energy of this system is expressed
where \( p^I \) and \( p^{II} \) are the osmotic pressures of the vesicles I and II, respectively. \( A \) and \( W \) are the contact area and adhesion strength, respectively. \( G^I_H \) and \( G^{II}_H \) are the Helfrich’s free energy density of vesicle I and II. The first order variation of (99) gives the same shape equation of two vesicles as (92) and the adhesion boundary conditions. 

\[
(1 + k^I_b/k^I_c)(\kappa^I_b - \kappa^A_b)^2 = 2W/k^I_c, \quad (99)
\]

\[
(1 + k^{II}_b/k^{II}_c)(\kappa^{II}_b - \kappa^A_b)^2 = 2W/k^{II}_c, \quad (100)
\]

\[
\partial(\kappa^I_b + \kappa^{II}_b - \kappa^A_b)/\partial b = 0, \quad (101)
\]

where \( \kappa^I_b \) and \( \kappa^{II}_b \) are the normal curvatures along \( b \) for the points outside the adhesion domain but near the contact line calculated by using the surfaces of vesicles I and II, respectively. \( \kappa^A_b \) is the normal curvature for the points inside the adhesion domain but near the contact line calculated by using the common surface of vesicles I and II. As we know, there is still lack of numerical solutions to the above equations (99)–(101) in the previous literature. Only in the recent work, Ziherl and Svetina have investigated the adhesion between two vesicles by numerically minimizing the free energy (98) with \( k^{III}_c = k^c_b \) and various \( W \).

Is the behavior of vesicle adhesion close to that of cell adhesion? The cell membrane can bear shear strain whose adhesion behavior might be much closer to the adhesion between a polyelectrolyte microcapsule and the substrate. Interestingly, beyond the threshold adhesion strength \( W_c \), the contact length scale increases in proportion to \((W - W_c)^{1/2}\), which is the same as the behavior of vesicle adhesions except the coefficient before \((W - W_c)^{1/2}\).

6. A different viewpoint of surface tension

Although the lipid bilayer cannot withstand the in-plane shear strain, it can still endure the in-plane compression strain. The in-plane compression modulus, \( k_b \), of lipid bilayers is about 0.24 N/m. Considering this point, we may write the free energy of a closed lipid vesicle as

\[
\mathcal{F} = p \int dV + \int G_B dA + \int (k_b/2)(2J_b)^2 dA, \quad (102)
\]

where

\[
G_B = (k_c/2)(2H + c_0)^2 - \bar{k}K, \quad (103)
\]

and \( J_b \) is the in-plane compression or stretch strain. We emphasize that the contribution of chemical potential are omitted when we write the above free energy.

The first order variation of the free energy (102) reveals that \( 2J_b \) is a constant and then

\[
p - 2(2k_bJ_b)H + 2k_c\nabla^2 H + k_c(2H + c_0)(2H^2 - c_0H - 2K) = 0. \quad (104)
\]

Comparing the above equation with the shape equation (77) of lipid vesicles, we deduce that

\[
\lambda = 2k_bJ_b. \quad (105)
\]

In the discussion on the stability of closed lipid vesicles, we have seen that the surface tensor \( \lambda \) has no effect on the critical pressure. The second order variation of the free energy (102) can give the same conclusion. \( \delta^2[p \int dV + \int G_B dA] \) has been shown in Eq. (82) with vanishing \( \lambda \). The additional term is

\[
\delta^2 \int (k_b/2)(2J_b)^2 dA = \int k_b(\text{div} \mathbf{v} - 2H\Omega_3)^2 dA \quad (106)
\]

where \( \mathbf{v} = \Omega_1 \mathbf{e}_1 + \Omega_2 \mathbf{e}_2 + \Omega_3 \mathbf{e}_3 \) represents the infinitesimal displacement vector of the vesicle surface. We can always select the proper deformation modes such that \( \text{div} \mathbf{v} - 2H\Omega_3 = 0 \) and then \( \delta^2[\int (k_b/2)(2J_b)^2 dA] \) vanishes, but \( \delta^2[p \int dV + \int G_B dA] \) is not affected. That is, the critical pressure is determined merely by \( \delta^2[p \int dV + \int G_B dA] \), which is independent on the compression modulus of lipid bilayer \( k_b \).

C. Cell membrane

Cell membrane consists of lipids, proteins, and a small quantity of carbohydrates and so on. A simple but widely accepted model for cell membranes is the fluid mosaic model proposed by Singer and Nicolson in 1972. In this model, the cell membrane is considered as a lipid bilayer where the lipid molecules can move freely in the membrane surface like fluid, while the proteins are embedded in the lipid bilayer. Some proteins, so called integral membrane proteins, traverse entirely in the lipid bilayer and play the role of information and matter communications between the interior of the cell and its outer environment. The others, so called peripheral membrane proteins, are partially embedded in the bilayer and accomplish the other biological functions. Beneath the lipid membrane, the membrane skeleton, a network of proteins, links with the proteins embedded in the lipid membrane. Mature mammalian and human erythrocytes (i.e., red blood cells) are lack of a cell nucleus. Thus they provide a good experimental model for studying the mechanical properties of cell membranes. On the theoretical side, spontaneous curvature model, rubber membrane model, and dual network model have been employed to investigate the mechanical and thermal fluctuation properties of erythrocyte membranes. We will address the elasticity and stability of composite shell model for cell membranes in this section.
1. Composite shell model of cell membranes

A cell membrane can be simplified as a composite shell of lipid bilayer and membrane skeleton. The membrane skeleton, inside of the cell membrane, is a network of protein filaments as shown in Fig. 13. The joint points of the network are bulk proteins embedded in the lipid bilayer. The whole membrane skeleton seems to float the sea of the lipid bilayer. It can have a global movement along the surface of the bilayer but the movement of the joints along the normal direction is totally coupled with the bilayer. In the mechanical point of view, the lipid bilayer can endure the in-plane shear strain but hardly bear the bending deformation. On the contrary, the membrane skeleton can endure the in-plane shear strain but hardly bear the bending deformation. The composite shell overcomes the shortage of the lipid bilayer and the membrane skeleton. It can sustain both bending deformation and in-plane shear strain.

![Inside of cell membrane](Lipid
Bulk protein
Protein filament)

![Outside of cell membrane](Bulk protein)

**FIG. 13:** Local schematic picture of the composite shell model for a cell membrane.

The contour length of protein chain between joints in the membrane skeleton is about 100 nm which is much smaller than the size (~10 μm) of cell membranes. The lipid bilayer is 2D homogenous. The membrane skeleton is roughly a 2D locally hexagonal lattice. As is well known, the mechanical property of a 2D hexagonal lattice is 2D isotropic. Thus the composite shell of the lipid bilayer plus the membrane skeleton can still be regarded as a 2D isotropic continuum. Its free energy density should be invariant under the in-plane coordinate transformation and can be written as

$$G_{cm} = G_{cm}(2H, K; 2J, Q).$$

We can expand $G_{cm}$ up to the second order terms of curvatures and strains as

$$G_{cm} = G_B + (k_b/2)(2J_b)^2 + G_{sk},$$

where $G_B$ results mainly from the bending energy of the lipid bilayer, which has the form as Eq. 103. $(k_b/2)(2J_b)^2$ is the contribution of in-plane compression of the lipid bilayer where $k_b$ and $2J_b$ are the compression modulus and relative area compression of the lipid bilayer. $G_{sk} = (k_d/2)(2J)^2 - kQ$ is the in-plane compression and shear energy density which comes from the entropic elasticity of the membrane skeleton. $k_d$ and $k$ are the compression and shear moduli of the membrane skeleton, respectively. Their values are experimentally determined as $k_d = \tilde{k} = 4.8 \mu \text{N/m.}$ and $Q$ and $J$ are the trace and determinant of the strain tensor of the membrane skeleton. Because there is no in-plane coupling between the lipid bilayer and the membrane skeleton in the composite shell model, thus $J_b$ for the lipid bilayer and $J$ for the membrane skeleton have no local correlation. In the above subsection, we have mentioned that the effect of $(k_b/2)(2J_b)^2$ can be replaced with the surface tension $\lambda = 2k_bJ_b$. Considering a closed cell membrane under osmotic pressure $p$, the free energy can be written as

$$\mathcal{F} = \int G_{cm} \, dA + p \int dV. \quad (108)$$

Similarly to Sec. II C, if we define a displacement vector $u$ satisfying Eqs. (71) and (72), we can derive the Euler-Lagrange equations corresponding to the free energy (108) as

$$\left(\tilde{k} - k_d\right)\nabla(2J) - \tilde{k}(\nabla^2 u + K\tilde{u} + \nabla u_3) = 0, \quad (109)$$

$$p + 2k_c[(2H + c_0)(2H^2 - c_0H - 2K) + 2\nabla^2 H] - 2\lambda H + 2H(\tilde{k} - k_d)(2J) - \tilde{k}\mathcal{R} : \nabla u = 0, \quad (110)$$

where $u$ and $\nabla^2 u$ are the in-plane components of $u$ and $\nabla(\nabla u)$, respectively. $\mathcal{R}$ is the curvature tensor related to Eq. (59). $\nabla$ is called the gradient operator of the second class, which is shown in our previous work.

Generally speaking, it is difficult to find the analytical solutions to Eqs. (109) and (110). But we can verify that a spherical membrane with homogenous in-plane strains satisfy these equations. The radius $R$ and the homogenous in-plane strain $\varepsilon$ should obey the following relation:

$$pR^2 + 2(\lambda + 2k_d\varepsilon - \tilde{k}\varepsilon)R + k_c(c_0R - 2) = 0. \quad (111)$$

2. Stability of cell membranes and the function of membrane skeleton

When the osmotic pressure is beyond some threshold, a closed cell membrane will lose its stability and change its shape abruptly. The threshold is called the critical osmotic pressure $\lambda$.

To obtain it, one should calculate the second order variation of the free energy (108) in terms of Appendix B. The variational result is

$$\delta^2 \mathcal{F} = \int k_c[(\nabla^2 \Omega_3)^2 + (2H + c_0)\nabla(2H\Omega_3) : \nabla \Omega_3]dA + \int [4k_c(2H^2 - K^2) + k_cK(c_0^2 - 4H^2) + 2\lambda K - 2Hp]\Omega_3^2 dA$$

$$+ \int [k_c(14H^2 + 2c_0H - 4K - c_0^2/2) - \lambda]\Omega_3\nabla^2 \Omega_3 dA$$

$$- 2k_0(2H + c_0)\nabla \Omega_3 : \nabla \Omega_3 + 2\Omega_3 \nabla \cdot \nabla \Omega_3 dA$$

$$- k_d \int [v \cdot \nabla + 2H\Omega_3] (\text{div} v - 2H\Omega_3) dA$$

$$+ (k/2) \int (\text{curl} v^2) dA - \tilde{k} \int K\nabla^2 dA + \tilde{k} \int \Omega_3 \nabla \cdot v dA$$

$$+ (\tilde{k}/2) \int (\text{curl} v^2) dA - \tilde{k} \int K\nabla^2 dA + \tilde{k} \int \Omega_3 \nabla \cdot v dA$$
where \( \mathbf{v} = \Omega_1 \mathbf{e}_1 + \Omega_2 \mathbf{e}_2 + \Omega_3 \mathbf{e}_3 \) is the infinitesimal displacement vector of the cell membrane whose in-plane component is denoted as \( \mathbf{v} = \Omega_1 \mathbf{e}_1 + \Omega_2 \mathbf{e}_2 \).

In terms of the Hodge decomposed theorem, \( \mathbf{v} \) can be expressed by two scalar functions \( \Omega \) and \( \chi \) as
\[
\mathbf{v} \cdot d\mathbf{r} = d\Omega + *d\chi,
\]
where \( * \) is the Hodge star. Then we have \( \text{div} \mathbf{v} = \nabla^2 \Omega \) and \( \text{curl} \mathbf{v} = \nabla^2 \chi \). For the spherical cell membrane satisfying Eq. \( (111) \), Eq. \( (112) \) can be divided into two parts: one is
\[
\delta^2 \mathcal{F}_1 = \left( \frac{\tilde{k}}{2} \right) \int \left[ (\nabla^2 \chi)^2 + (2/R^2) \chi \nabla^2 \chi \right] dA;
\]
and another is
\[
\delta^2 \mathcal{F}_2 = \int \Omega_3^2 \left[ 2 c_0 k_c / R^3 + p/R + (4k_d - 2\tilde{k}) / R^2 \right] dA
+ \int \Omega_3 \nabla^2 \Omega_3 \left[ k_c c_0 / R + 2k_c / R^2 + pR/2 \right] dA
+ \int k_c (\nabla^2 \Omega_3)^2 dA + \left( \frac{4k_d - 2\tilde{k}}{R} \right) \int \Omega_3 \nabla^2 \Omega dA
+ k_d \int (\nabla^2 \chi)^2 dA + \left( \frac{\tilde{k}}{R^2} \right) \int \Omega \nabla^2 \Omega dA.
\]

It is easy to verify that \( \delta^2 \mathcal{F}_1 \) is always positive on a spherical surface. Then the stability of the spherical cell membrane is merely determined by \( \delta^2 \mathcal{F}_2 \). By analogy with our previous work, we can prove that \( \delta^2 \mathcal{F}_2 \) is also positive if
\[
p < p_i \equiv \frac{2\tilde{k}(2k_d - \tilde{k})}{k_d(l + 1) - \tilde{k}} + \frac{2k_c}{R^3} \left[ (l + 1) - c_0 R \right],
\]
for any integer \( l \geq 2 \). Thus the critical pressure is
\[
p_c \equiv \min \{ p_i \ (l = 2, 3, 4, \ldots) \}.
\]

Obviously, if \( \tilde{k} = 0 \), i.e., the effect of membrane skeleton vanishes in the cell membrane, \( p_c \) degenerates into the critical pressure \( k^3 \) of a spherical lipid vesicle.

When \( \tilde{k} k_d (2k_d - \tilde{k}) R^2 / k_c (6k_d - \tilde{k}) > 1 \), the critical pressure is derived from Eqs. \( (110) \) and \( (117) \) as
\[
p_c = \frac{4 \sqrt{R^3}}{\sqrt{\left( \frac{\tilde{k}}{k_d} \right) (2k_d - \tilde{k}) k_c}}.
\]

As an example, let us consider a cell membrane with typical values of \( \tilde{k} = k_d = 4.8 \mu N/m \) \( k_c = 10^{-10} \) J, and \( R = 10 \mu m \). Through a simply manipulation, we find that \( k_d (2k_d - \tilde{k}) R^2 / k_c (6k_d - \tilde{k}) > 1 \), and so Eq. \( (113) \) holds, from which we obtain the critical pressure \( p_c = 0.03 \) Pa. However, if the membrane skeleton vanishes, \( k = 0 \), we calculate \( p_c = 0.001 \) Pa from Eqs. \( (110) \) and \( (117) \). This example reveals a mechanical function of membrane skeleton: it highly enhances the stability of cell membranes.

As a byproduct, Eq. \( (113) \) also gives the critical pressure
\[
p_c = \sqrt{4/3(1 - \nu^2)} \ Y (h/R)^2
\]
for a spherical thin solid shell of 3D isotropic materials if we take \( k_c \) and \( k_d \) as Eqs. \( (63) \) and \( (64) \). This formula is the same as the classic strict result obtained by Pogorelov from the other method.

IV. APPLICATION OF ELASTIC THEORY IN NANO-STRUCTURES

In the last section, we have expatiated on the application of Elastic theory in bio-structures. In this section, we will discuss whether and to what extent this theory can be applied to nano-structures, especially the graphitic structures, such as graphene and carbon nanotubes.

A. Graphene

Graphene is a single layer of carbon atoms with a 2D honeycomb lattice as shown in Fig. \( (14a) \). It has been a rapidly rising star in the material science and
condensed-matter physics since it was successfully cleaved from buck graphite. It is found that the free-standing graphene sheet would be a strictly 2D atomic crystal which is stable under ambient conditions. However, Mermin has theoretically proved that the 2D crystalline order could not exist at finite temperature. There are two possible ways to solve this paradox: (i) The graphene might not be a perfect 2D crystal. Recently, Meyer et al. have investigated the structure of suspended graphene sheets and found that the graphene sheets are not genuine flat. They also argue that the graphene sheets could be stabilized by the out-of-plane deformation in the third dimension resulting from the thermal fluctuations. Fasolino et al. have also discussed the height fluctuations by means of Monte Carlo simulations. Their result at room temperature is in good agreement with the experiment mentioned above. (ii) Mermin theorem is valid for power-law potentials of the Lennard-Jones type while the interaction between nearest neighbor atoms (covalent bond) in the graphene might not be of this type.

To fully understand the experimental result and possible stable mechanism in theory, we will address the Lenosky lattice model and its revised form as follows.

1. Revised Lenosky lattice model and its continuum limit

We start from the concise formula proposed by Lenosky et al. in 1992 to describe the deformation energy of a single layer of curved graphite. The first term, \( r_0 \) is the initial bond length of planar graphite, and \( r_{ij} \) is the bond length between atoms \( i \) and \( j \) after the deformations. In the remaining terms, \( u_{ij} \) is a unit vector pointing from atom \( i \) to its neighbor \( j \), and \( n_i \) is the unit vector normal to the plane determined by the three neighbors of atom \( i \). The sum \( \sum_{(ij)} \) is taken over the three nearest neighbor atoms \( j \) to atom \( i \), and \( \sum_{(ij)} \) is taken over all the nearest neighbor atoms.

The parameters \( \epsilon_1, \epsilon_2, \epsilon_3 \) (0.96, 1.29, 0.05) eV were determined by Lenosky et al. through local density approximation. The value of \( \epsilon_0 \) was given by Zhou et al. as \( \epsilon_0 = 57 \) eV/Å^2 through the force-constant method.

In the above energy form, the second term requires that the energy cost due to in-plane bond angle changes is the same as that due to out-of-plane bond angle changes. However, the experiment by inelastic neutron scattering techniques reveals that the energy costs due to in-plane and out-of-plane bond angle changes are quite different from each other. To describe this effect, we revise the Lenosky lattice model as

\[
E_g = \frac{\epsilon_0}{2} \sum_{(ij)} (r_{ij} - r_0)^2 + \epsilon_1 \sum_i (\sum_{(j)} u_{ij})^2 + \epsilon_2 \sum_{(ij)} (1 - n_i \cdot n_j) + \epsilon_3 \sum_{(ij)} (n_i \cdot u_{ij})(n_j \cdot u_{ji}),
\]

(120)

The first two terms are the contributions of bond length and bond angle changes to the energy. The last two terms are the contributions from the \( \pi \)-electron resonance. In the first term, \( r_0 \) is the initial bond length of planar graphite, and \( r_{ij} \) is the bond length between atoms \( i \) and \( j \) after the deformations. In the remaining terms, \( u_{ij} \) is a unit vector pointing from atom \( i \) to its neighbor \( j \), and \( n_i \) is the unit vector normal to the plane determined by the three neighbors of atom \( i \). The summation \( \sum_{(ij)} \) is taken over the three nearest neighbor atoms \( j \) to atom \( i \), and \( \sum_{(ij)} \) is taken over all the nearest neighbor atoms.

The parameters \( \epsilon_1, \epsilon_2, \epsilon_3 \) (0.96, 1.29, 0.05) eV were determined by Lenosky et al. through local density approximation. The value of \( \epsilon_0 \) was given by Zhou et al. as \( \epsilon_0 = 57 \) eV/Å^2 through the force-constant method.

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\[
E_g = \frac{\epsilon_0}{2} \sum_{(ij)} (r_{ij} - r_0)^2 + \epsilon_1 \sum_i \sum_{(j \neq k)} (u_{ij}^t u_{ik}^t + 1/2)^2 + \epsilon_2 \sum_{(ij)} (1 - n_i \cdot n_j),
\]

(121)

where \( u_{ij}^t = u_{ij} - (n_i \cdot u_{ij})n_i \) and \( n_i^t = n_i \cdot u_{ij} \). If the three nearest neighbor atoms to atom \( i \) are labeled as 1, 2, and 3, the summation \( \sum_{(j \neq k)} \) is understood as \( \sum_{1 \leq j < k \leq 3} \). The second and third terms of Eq. (121) represent the energy costs due to in-plane and out-of-plane bond angle changes, respectively. We have omitted the term \( \epsilon_3 \sum_{(ij)} (n_i \cdot u_{ij})(n_j \cdot u_{ji}) \) relative to the original Lenosky model, because its contribution is very small in terms of the results by Lenosky et al.

The parameters in Eq. (121) are determined by fitting the total energy of variously perturbed configurations of \( \sqrt{7} \times \sqrt{7} \) unit cell of graphite (14 atoms). The total energy is obtained through the first-principles calculations (the ABINIT package). The calculations are carried by using Troullier-Martins pseudopotentials, wave-energy cutoff of 50 Hartree, and 4 \times 4 \times 1 Monkhorst-Pack k-points in Brillouin-zone. The exchange-correlation energy are treated within the local-density approximation in the Ceperley-Alder form with the Perdew-Wang parametrization. Our result is \( r_0 = 1.41 \) Å, \( \epsilon_0 = 46.34 \) eV/Å^2, \( \epsilon_1 = 4.88 \) eV, \( \epsilon_2 = 1.04 \) eV, and \( \epsilon_2 = 1.24 \) eV. The value of \( \epsilon_0 \) is a little smaller than that obtained by Zhou et al. from force constant method. The values of \( \epsilon_1 \) and \( \epsilon_2 \) are very close to those of \( \epsilon_1 \) and \( \epsilon_2 \) obtained by Lenosky et al. from local density approximation. The key reason is that the main energy contribution in the configurations discussed by Lenosky et al. comes from the third and fourth term in Eq. (121).

Now let us derive the continuum limit form of the revised Lenosky lattice model by analogy with the method in our previous work. Now consider a curved graphene and take a fictitious smooth surface such that all carbon atoms are on that surface. The in-plane stain can be expressed as \( \mathbf{E}_i = \left( \begin{array}{c} \epsilon_{11} \\ \epsilon_{12} \\ \epsilon_{22} \end{array} \right) \) in the local frame \{\( \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \)\} at atom \( i \). The bond vector \( \mathbf{r}_{ij} \) from atom \( i \) to its neighbor \( j \) after the deformations and the initial bond vector \( \mathbf{r}_{ij}^0 \) before the deformations satisfy

\[
\mathbf{r}_{ij} = (\mathbf{I} + \mathbf{E}_i) \cdot \mathbf{r}_{ij}^0,
\]

where \( \mathbf{I} \) is the unit matrix. The initial bond vectors \( \mathbf{r}_{ij}^0 \) can be expanded to the order of \( r_0^2 \kappa^2 \) as

\[
\mathbf{r}_{ij}^0 = (1 - r_0^2 \kappa_j^2/6)\mathbf{T}_j + (\kappa_j \tau_j \mathbf{r}_{ij}^0/6)\mathbf{B}_j + [r_0 \kappa_j/2 + (r_0^2/6)dk_j]/ds]n_j,
\]

(122)

where \( j = 1, 2, 3 \) denote three sp^2-bond curves from atom \( i \) to one of its three neighbor atoms \( j \) on the graphene surface. The symbols \( \mathbf{T}_j \), \( \mathbf{N}_j \), and \( \mathbf{B}_j \) represent the unit tangential, normal, and binormal vectors of the bond curve
from $i$-atom to $j$-atom, which satisfy the Frenet theorem Eq. \( \Pi \). $\kappa$, $\tau$ refer to the curvature and torsion while $s$ is the arc-length parameter along the bond curve. Assume the $sp^2$-bond along the geodesic curve of the graphene surface. The vectors $\mathbf{T}_i$ and $\mathbf{B}_j$ can be expressed by $\mathbf{T}_i = \cos \theta_i \mathbf{e}_1 + \sin \theta_i \mathbf{e}_2$ and $\mathbf{B}_j = -\sin \theta_j \mathbf{e}_1 + \cos \theta_j \mathbf{e}_2$, where $\theta_i$ is the rotating angle from $\mathbf{e}_1$ to $\mathbf{T}_j$. We have the expressions of $\mathbf{u}_{ij} = r_{ij}/r_{ij}$ and $\mathbf{n}_i = \mathbf{N}_i$ with $r_{ij} = |r_{ij}|$ for the deformed graphene. Then Eq. (121) is transformed into the continuum limit up to the second-order magnitudes of $\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{12}$ and $r_0 K$ as

\[
E_g = \int \left[ \frac{k_c}{2} (2H)^2 - \tilde{k} K + \frac{k_d}{2} (2J)^2 - \tilde{k} Q \right] dA, \quad (123)
\]

with four parameters

\[
k_c = (9\varepsilon_{1n} + 6\varepsilon_2) r_0^2/8\Omega_0, \quad (124)
\]

\[
\tilde{k} = 3c_0 r_0^2/4\Omega_0, \quad (125)
\]

\[
k_d = 9(\varepsilon_0 r_0^2 + 3\varepsilon_{12})/16\Omega_0, \quad (126)
\]

\[
\tilde{k} = (3c_0 r_0^2 + 9\varepsilon_{12})/8\Omega_0, \quad (127)
\]

where $\Omega_0 = 3\sqrt{5} r_0^2/4$ is the occupied area per atom. The continuum form (123) has first derived in our previous work \[44\] which is, in fact, the natural conclusion of the theory of 2D isotropic materials mentioned in Sec. IIC. The curved graphene comprises a lot of hexagons which has approximately local hexagonal symmetry. In fact, 2D structures with hexagonal symmetry are 2D isotropic.\[144\] Thus the elasticity of the graphene can be reasonably described by the shell theory of 2D isotropic materials mentioned in Sec. IIC and so its energy has the form of Eq. (123). We also notice that a flaw in the coefficient before $\varepsilon_1$ in the expression of $k_c$ in our previous work \[44\] is transformed into

\[
E_g = (k_c/2) \int (\nabla^2 w)^2 d^2 \mathbf{x}, \quad (128)
\]

where $w \equiv (x_1, x_2)$ represents the point on the graphene plane before deformations.

Adopting the Fourier series

\[
w(\mathbf{x}) = (1/L) \sum \tilde{w}_q \exp (i\mathbf{q} \cdot \mathbf{x}), \quad (129)
\]

with $q \equiv (2\pi/L, 2n\pi/L)$, we transform Eq. (128) into

\[
E_g = (k_c/2) \sum_q q^4 |\tilde{w}_q|^2, \quad (130)
\]

and then the corresponding partition function is derived as

\[
Z = \prod_q d\tilde{w}_q \exp (-E_g/T) = \prod_q \sqrt{2\pi T/k_c q^4}, \quad (131)
\]

where the Boltzmann constant has been set to 1. It follows that the equipartition theorem:

\[
\langle (k_c/2) \tilde{w}_q^2 \rangle = -T \partial \ln Z / \partial \ln q^4 = T/2, \quad (132)
\]

where $\langle . \rangle$ represents the ensemble average. The above equation is equivalent to

\[
\langle |\tilde{w}_q|^2 \rangle = T/k_c q^4. \quad (133)
\]

Similarly, $\langle w^2 \rangle$ is derived as

\[
\langle w^2 \rangle = \sum_q \langle |\tilde{w}_q|^2 \rangle = \frac{T L^2}{16\pi^2 k_c} \sum_{mn} \frac{1}{(l^2 + n^2)^2}. \quad (134)
\]

Through simply numerical manipulations, we have \[159\]

\[
\langle w^2 \rangle \approx \frac{T L^2}{150 k_c}. \quad (135)
\]

for the graphene contains more than 100 atoms.

In terms of Ref. \[157\], we estimate $k_c \approx 0.46$ eV at $T = 300$ K. Substituting it into Eq. (135) and taking $L = 25$ nm as the experiment \[143\], we have $\sqrt{\langle w^2 \rangle} \approx 0.5$ nm. This value is a little smaller than the largest out-of-plane deformation 1 nm in the experiment. However, they are consistent with each other because 0.5 nm is the mean square value which should be smaller than the largest out-of-plane deformation in the experiment.

**B. Carbon nanotube**

There are two kinds of carbon nanotubes: single- and multi-walled carbon nanotubes, which are synthesized in the last decade of 20 century.\[160,161\] Simply speaking, a single-walled carbon nanotube (SWNT) can be regarded

2. **Intrinsic roughening in graphene at temperature $T$**

Let us consider the freely suspended graphene which is almost a flat layer with the area $L^2$. The small out-of-plane displacement is denoted by $w$. The energy (123) is
as a seamless cylinder wrapped up from a graphitic sheet, as shown in Fig. [11], whose diameter is in nanometer scale and length from tens of nanometers to several micrometers if we ignore its two end caps. A multi-walled carbon nanotube (MWNT) consists of a series of coaxial SWNTs with layer distance about 3.4 Å.

SWNTs can be expressed as a pair of integers (n,m), so called index, in terms of the wrapping rule. They are divided into two classes: achiral tubes if \( n = m \) or \( nm = 0 \) and chiral tubes for others. The electronic properties of SWNTs depend sensitively on the index; they are metallic if \( n - m \) is multiple of 3, else semiconductor. SWNTs also possess many novel mechanical properties in particular high stiffness and axial strength, which are not sensitive to the tube diameters and chirality. MWNTs have the similar mechanical properties to SWNTs. In this section, we will review the theoretical and numerical results on the elastic properties of carbon nanotubes, and then discuss how the low-dimensional elastic theory mentioned in Sec. [11] can be applied in carbon nanotubes.

1. General review on the elasticity of carbon nanotubes

The early researches on the elasticity of carbon nanotubes are focused on their Young’s modulus \( Y \) and Poisson ratio \( \nu \). A SWNT is a single layer of carbon atoms. What is the thickness \( h \) of the atomic layer? It is a widely controversial question. Three typical values of the thickness listed in Table I are adopted or obtained in the previous literature Refs. [40, 41, 44] and [167–180]. The first one is about 0.7 Å obtained from fitting the atomic scale model with the elastic shell theory of 3D isotropic materials. [167, 168, 169, 170, 171, 172, 173] The second one is about 1.4 Å derived from molecular dynamics or finite element method. [174, 175] The third one is about 3.4 Å adopting the layer distance of bulk graphite. [176, 177, 178, 179] Recently, Huang et al. have investigated the effective thickness of SWNTs and found it depends on the type of loadings.

The size- or chirality-dependent elastic properties of SWNTs have also been discussed by molecular mechanics model and \textit{ab initio} calculations. The common conclusion is that the Young’s modulus and Poisson ratio depend weakly on the diameter and chirality of SWNTs if the diameter is larger than 1 nm. Only for very small SWNTs, the size and chirality effect is evident. The SWNTs synthesized in the laboratory have usually the diameters larger than 1 nm; thus the size and chirality effect can be neglected safely.

The axial tension properties of MWNTs depend on the layer number of MWNTs for the small layer number and approach quickly to the properties similar to the bulk graphite. [44, 186, 187]

The buckling and stability of carbon nanotubes under pressure or bending is a hot topic in the recent researches, where the critical pressure, moment or the equivalent quantity, critical strain, are highly concerned. A long enough carbon nanotube under an axial loading might be regarded as a Euler rod and the axially critical strain is

\[
\varepsilon_{\text{rod}}^c = \alpha \pi^2 I / A L^2 \propto (\rho / L)^2,
\]

where \( L \), \( \rho \) and \( A \) are the length, radius and cross-sectional area of the carbon nanotube, respectively. \( I \) is the moment of inertia of the nanotube. The value of \( \alpha \) depends on the boundary conditions of the carbon nanotube. This relation has been investigated by atomistic finite element method and molecular dynamics method or \textit{ab initio} calculations.

The basic numerical result is that the tube exhibits rod-like buckling behavior as the right-handed side of Eq. (136) if \( L \gg \rho \). The Timoshenko beam theory, a more complicated theory than Euler rod theory, is also employed to discuss the buckling of MWNTs. The difference between the results of both theories vanishes for large value of \( L / \rho \).

For a short carbon nanotube under axial loading, the continuous shell model of 3D isotropic materials are widely used. The axially critical strain of a short SWNT is

\[
\varepsilon_{\text{zc}}^{\text{shell}} = \alpha \rho / (h^2 / 3(1 - \nu^2))(h / \rho) \propto \rho^{-1},
\]

where \( \rho \) and \( h \) are the radius and effective thickness of the SWNT, respectively. \( \nu \) is the Poisson ratio of the SWNT. The value of \( \alpha \) depends on the boundary condition of the carbon nanotube. For a short MWNT, the above relation is applicable for the outmost layer of the tube because the inter-layer interaction of

| Authors          | \( Y \) | \( \nu \) | \( h \) | Method         | Refs.   |
|------------------|--------|--------|------|---------------|--------|
| Yakobson et al.  | 5.5    | 0.19   | 0.66 | MD            | 40     |
| Tu & Ou-Yang     | 4.7    | 0.34   | 0.75 | LDA           | 44     |
| Kudin et al.     | 3.9    | 0.15   | 0.89 | \textit{ab initio} | 167   |
| Zhou et al.      | 5.1    | 0.24   | 0.74 | TB            | 168    |
| Vodenitcharova et al. | 4.9  | –      | 0.62 | ring theory   | 169    |
| Pantano et al.   | 4.8    | 0.19   | 0.75 | SM & FEM      | 170, 171 |
| Chen and Cao     | 6.8    | –      | 0.80 | SM            | 172    |
| Wang et al.      | 5.1    | 0.16   | 0.67 | \textit{ab initio} | 173    |
| Sears & Batra    | 2.5    | 0.21   | 1.34 | MD            | 174    |
| Tserpes et al.   | 2.4    | –      | 1.47 | FEM           | 175    |
| Lu               | 1.0    | 0.28   | 3.4  | MD            | 41     |
| Hernandez et al. | 1.2    | 0.18   | 3.4  | TB            | 176    |
| Shen & Li        | 1.1    | 0.16   | 3.4  | force-field   | 177    |
| Li & Chou        | 1.0    | –      | 3.4  | SM            | 178    |
| Bao et al.       | 0.9    | –      | 3.4  | MD            | 179    |
| Zhou et al.      | 0.8    | 0.32   | 3.4  | LDA           | 180    |
MWNTs is very small. It has also been investigated by atomic-scale finite element method and molecular dynamics methods and nanoindent experiments. It is found that the tube displays in- deed the shell-like buckling behavior as the right-handed pressure might also be described by the continuous shell model of 3D isotropic materials, and the critical pressure is

$$p_{cr}^{shell} \propto \rho^{-3}, \quad (138)$$

where $\rho$ is the radius of the SWNT. This relation has recently been confirmed by Hasegawa and Nishidate through ab initio calculations. The stability of a MWNT under radial hydrostatic pressure might also have the similar relation as Eq. (138) if only we take $\rho$ as the outmost radius of the MWNT, because the transverse elasticity of MWNT is much weaker than the in-plane elasticity of the outmost single layer of tube.

Bending can also result in the buckling of SWNTs. The kink phenomenon in a SWNT under pure bending has been investigated through molecular dynamics simulations and finite element method. The critical curvature can be described as

$$k_{cr} = \epsilon_{zc}/\rho \propto \rho^{-2}, \quad (139)$$

where $\rho$ is the radius of the SWNT. For the kink phenomenon in a MWNT under pure bending satisfies the similar relation to Eq. (139) with small correction due to inter-layer van der Waals interactions if only we take $\rho$ as the outmost radius of the MWNT.

Here we would not further discuss the problems on the buckling of MWNTs embedded in an elastic medium, the post-buckling behavior and the plastic properties of carbon nanotubes as well as the mechanical properties of nanotube composites, rather than recommend gentle readers to consult the corresponding literature.

2. What are the fundamental quantities for SWNTs?

As mentioned above, different thickness leads to different Young’s modulus (see Table I), which implies that the Young’s modulus and thickness of SWNTs are not well-defined physical quantities. However, the in-plane Young’s modulus $Y_s = Yh$ has the similar value 22 eV/Å$^2$. Thus it is a more well-defined quantity than the Young’s modulus and the thickness. Here we may ask: what are the fundamental quantities for SWNTs?

A SWNT is also a single layer of graphite, whose deformation energy can be also described as the revised Lenosky model. The corresponding continuum limit is Eq. (123) which contains four elastic constants $k_c, \tilde{k}, k_d$, and $\tilde{k}$. These four quantities avoid the controversial thickness of SWNTs. We suggest to use them as the fundamental quantities for SWNTs from which we can obtain some reduced quantities as follows.

Let us consider a cylinder under an axial loading with line density $f$ along the circumference. The corresponding axial and circumferential strains are denoted as $\varepsilon_{11}$ and $\varepsilon_{22}$. With Eq. (129), the free energy of this system is written as

$$F \approx 2\pi \rho L[(k_d/2)(\varepsilon_{11} + \varepsilon_{22})^2 - \tilde{k}\varepsilon_{11}\varepsilon_{22} - f\varepsilon_{11}] \quad (140)$$

where $L$ and $\rho$ are the length and radius of the SWNT. The in-plane Young’s modulus and Poisson ratio can be defined as $Y_s = f/\varepsilon_{11}$ and $\nu_s = -\varepsilon_{22}/\varepsilon_{11}$. From $\partial F/\varepsilon_{11} = 0$ and $\partial F/\varepsilon_{22} = 0$, we derive

$$Y_s = \tilde{k}(2 - \tilde{k}/k_d) = 22.35 \text{ eV/Å}^2, \quad (141)$$
$$\nu_s = 1 - \tilde{k}/k_d = 0.165, \quad (142)$$

where the value of $Y_s$ is close to the in-plane Young’s modulus derived from Table I. It is in between 20–23 eV/Å$^2$ obtained by Sánchez-Portal et al. It is much larger than the value 15 eV/Å$^2$ obtained by Arroyo et al. and Zhang et al. and 17 eV/Å$^2$ by Caillerie et al. but smaller than 34.6 eV/Å$^2$ for armchair tube by Wang. The value of $\nu_s$ is close to the value 0.160–0.19 obtained by Yakobson et al., Kudin et al., Pantano et al., Wang et al., Hernandez et al. and Shen et al.

The other quantity, the bending rigidity $D_s$, is also widely discussed in literature. In terms of Eq. (128), the energy per area of a SWNT without the in-plane strains can be expressed as

$$G_g = k_c/2\rho^2 \equiv D/2\rho^2. \quad (143)$$

Thus the bending rigidity

$$D = k_c = 1.62 \text{ eV}, \quad (144)$$

which is close to the value 1.49–1.72 eV obtained by Kudin et al. and Sánchez-Portal et al. through ab initio calculations. It is a little larger than the values 0.85–1.22 eV obtained Yakobson et al., Pantano et al. and Wang.

In terms of Eqs. (111)–(114), we can infer the values of $k_d, \tilde{k}, k_c$ from the previous literature, which are listed in Table II. There is still lack of literature on $\tilde{k}$ except our previous work 124,125 and the present review. More work on $\tilde{k}$ would be highly appreciated in the future.

We should emphasize that our formula (123) holds up to the order of $(r_0/\rho)^2$ for SWNTs, where $r_0$ is the C-C length and $\rho$ the radius of the SWNT. The omitted terms is in the order of $(r_0/\rho)^4$. This is the main reason for the size effect on the elastic constants in the very small SWNTs found in Refs. 173–183. Additionally, we have not considered the effect of Stone-Wales defects on the local properties of carbon nanotubes. In terms of Refs. 233 and 234, we can deduce that the defects reduce the the elastic constants of carbon nanotubes.
TABLE II: The values of $Y_s$, $\nu_s$, $k_d$, $\tilde{k}$, $k_c$ and $\bar{k}$. (MD = molecular dynamics; TB = tight-binding; SM = structure mechanics; FEM = finite element method; LDA = local density approach; CTIP = continuum theory of interatomic potential)

| Authors          | $Y_s$ (eV/Å$^2$) | $\nu_s$ | $k_d$ (eV/Å$^2$) | $\tilde{k}$ (eV/Å$^2$) | $k_c$ (eV) | $\bar{k}$ (eV) | Method | Refs. |
|------------------|-----------------|---------|-----------------|--------------------|----------|-------------|--------|-------|
| Yakobson et al.  | 22.69           | 0.19    | 23.54           | 19.06              | 0.85     | -           | MD     | 40    |
| Tu & Ou-Yang     | 22.03           | 0.34    | 24.88           | 16.44              | 1.17     | 0.75        | LDA    | 44    |
| Tu & Ou-Yang     | 21.63           | 0.18    | 22.35           | 18.33              | 1.30     | 0.88        | LDA    | 154   |
| Kudin et al.     | 21.69           | 0.15    | 22.19           | 18.86              | 1.49–1.53| -           | ab initio | 167   |
| Zhou et al.      | 23.59           | 0.24    | 25.03           | 19.02              | 1.14     | -           | TB     | 168   |
| Pantano et al.   | 22.25           | 0.19    | 23.34           | 18.91              | 1.09     | -           | SM & FEM | 170,171|
| Chen and Cao     | 34.38           | -       | -               | -                  | -        | -           | SM     | 172   |
| Wang et al.      | 21.36           | 0.16    | 21.92           | 18.41              | 0.82     | -           | ab initio | 173   |
| Sears & Batra    | 20.94           | 0.21    | 21.90           | 17.30              | 3.28     | -           | MD     | 174   |
| Tserpes et al.   | 22.05           | -       | -               | -                  | -        | -           | FEM    | 175   |
| Lu               | 21.25           | 0.28    | 23.06           | 16.60              | -        | -           | MD     | 41    |
| Hernandez et al. | 25.50           | 0.18    | 26.35           | 21.61              | -        | -           | TB     | 176   |
| Shen & Li        | 23.38           | 0.16    | 23.99           | 20.16              | -        | -           | force-field | 177   |
| Li & Chou        | 21.25           | -       | -               | -                  | -        | -           | SM     | 178   |
| Bao et al.       | 19.13           | -       | -               | -                  | -        | -           | MD     | 179   |
| Zhou et al.      | 17.00           | 0.32    | 18.94           | 12.88              | -        | -           | LDA    | 180   |
| Sánchez-Portal   | 19.41–22.40     | 0.12–0.19| 19.92–23.00    | 16.73–19.31        | 1.49–1.72| -           | ab initio | 230   |
| Arroyo et al.    | 15.19           | 0.40    | 18.08           | 10.85              | 0.69     | -           | FEM    | 231   |
| Zhang et al.     | 14.75           | -       | -               | -                  | -        | -           | CTIP   | 232   |
| Caillerie et al. | 17.31           | 0.26    | 18.57           | 13.74              | -        | -           | CTIP   | 233   |
| Wang             | 34.63 or 17.31  | -       | -               | 1.12 or 1.21       | -        | -           | CTIP   | 234   |
| Present work     | 22.35           | 0.16    | 22.97           | 19.19              | 1.62     | 0.72        | LDA    | -     |

3. Revisit the stability of SWNTs

Now we will revisit the stability of SWNTs with the four fundamental quantities $k_c$, $\bar{k}$, $k_d$, and $\tilde{k}$ or the corresponding reduced quantities.

![Bent SWNT](image)

**FIG. 15:** Bent SWNT. $\rho$ and $1/\kappa$ are the radii of the SWNT and the centerline of the SWNT, respectively.

First, let us consider a bent SWNT as shown in Fig. 15 where $\rho$ and $1/\kappa$ are the radii of the SWNT and the centerline of the SWNT, respectively. Assume that the centerline of the SWNT is not extended and the cross section of the SWNT is still flat after bending under the condition $\rho \ll L \ll 1/\kappa$, where $L$ is the total length of the centerline. In terms of Eq. (139), we can derive the deformation energy due to bending as

$$\Delta F \approx \int_0^L (k_{rod}/2)\kappa^2 ds,$$

where $ds$ is the arc length element of the centerline. The bending modulus of the rod is $k_{rod} = \pi \rho \sqrt{(2 - \tilde{k}/k_d)\bar{k}\rho^2 + k_c}$. For the SWNT with diameter in the order of 1 nm, we can estimate $k_c \ll (2 - \tilde{k}/k_d)\bar{k}\rho^2$. Considering Eq. (141), we have

$$k_{rod} \approx \pi Y_s \rho^3.$$

If an axial compression force $F$ is loaded on the both ends of the SWNT, following Euler rod theory, we can easily derive the critical force, above which the SWNT is instable, as

$$F_{rod}^{c} = 2\alpha \pi k_{rod}/L^2,$$

where $\alpha$ depends on the boundary conditions in two ends of the SWNT. Defining the critical strain as $\varepsilon_{zc}^{rod} = F_{rod}^{c}/2\pi \rho Y_s$ and considering the above two equations, we can derive

$$\varepsilon_{zc}^{rod} = \alpha (\rho/L)^2.$$

This relation has the same asymptotic behavior as Eq. (130), which, as mentioned above, has been confirmed by a lot of theoretical and numerical researches.
Secondly, let us consider a short SWNT with radius \( \rho \) and an axial compression force loaded on its two ends. The force per length along the circumference is denoted as \( f \). Following Ru’s work, considering Eq. (129) we have the critical axial force density as

\[
f_{c}^{shell} = \alpha \sqrt{k_c/Y_s}/\rho,
\]

and the corresponding critical strain

\[
\varepsilon_{zc}^{shell} \equiv f_c/Y_s = (\alpha/\rho)\sqrt{k_c/Y_s},
\]

where \( \alpha \) depends on the boundary conditions in two ends of the SWNT. \( Y_s \) is the in-plane Young’s modulus as shown in Eq. (111). The above relation (150) has the same asymptotic behavior as Eq. (137), which, as mentioned in above, has been confirmed by several theoretical and numerical researches.

Thirdly, let us consider a long enough SWNT with radius \( \rho \) and a radial compression pressure \( p \) loaded on its surface. In terms of the similar method on the stability of cell membranes, we can derive the critical pressure

\[
p_{cr}^{shell} = 3k_c/\rho^3,
\]

above which the SWNT will lose its stability. This relation has the same asymptotic behavior as Eq. (138). The corresponding critical circumferential strain is

\[
\varepsilon_{cr}^{c} = 2p_{cr}^{shell}/Y_s = 6k_c/Y_s \rho^2.
\]

Comparing Eq. (151) with (85), one can find that the critical pressures for carbon nanotubes and lipid tubules are in the same form. Yin et al. have noticed this similarity in the recent work 237. However, the profound mechanism is different: nanotubes can endure the shear strain while lipid tubules cannot.

It seems that no literature discusses the possible instability of a SWNT under axial tension. Here we will give a qualitative analysis. Assume the tension density (i.e., force per length) to be \( f \). The axial strain under the tension is \( f/Y_s \) and the corresponding circumferential strain is \( \nu_s f/Y_s \). When it is beyond the critical value (152), the SWNT will be instable. Thus we obtain the critical tension density

\[
f_{c}^{tsn} = 6k_c/\nu_s \rho^2.
\]

Only if \( f_{c}^{tsn} \) is below the strength of the SWNT, the buckling phenomenon under tension can be observed.

Till now, we have not found that \( \tilde{k} \) exists explicitly in the above equations (148)–(152) for nanotubes. Because the term related to \( \tilde{k} \) in the free energy (123) can be transformed into the boundary term with the aid of Gauss-Bonnet formula, \( \tilde{k} \) should be implicitly contained by \( \alpha \) in these equations, which need the further investigations in the future.

V. CONCLUSION AND PROSPECT

In summary, we present the elastic theory of low-dimensional (one- and two-dimensional) continua and its applications in bio- and nano-structures. The elastic theory of Kirchhoff rod, Helfrich rod, bending-soften rod, fluid membrane, and solid shell is revisited. We construct the free energy density of the continua on the basis of the symmetry argument. The fundamental equations can be derived from the bottom-up and the top-down viewpoints. Although they have different forms obtained from these two viewpoints, several examples reveal that they are, in fact, equivalent to each other. We investigate the kink stability of short DNA rings, the elasticity of lipid membranes, and the adhesions between a vesicle and a substrate or another vesicle. A cell membrane is simplified as a composite shell of lipid bilayer and membrane skeleton. The membrane skeleton is shown to enhance highly the mechanical stability of cell membranes. We propose a revised Lenosky lattice model based on the local density approximation and derive its continuum form up to the second order terms of curvatures and strains, which is the same as the free energy of 2D solid shells. The intrinsic roughening of graphene and several typical mechanical properties of carbon nanotubes are addressed by using this continuum form. We can abandon the controversial thickness and Young’s modulus of graphene and SWNTs if we adopt this continuum form to describe the mechanical properties of graphene and SWNTs.

Finally, we would like to list a few open problems which need to be addressed in the future work.

(i) The vesicles with lipid domains have been investigated in Sec. IIIIB. There is a special lipid domain at liquid-ordered phase, so called the raft, which is enriched in cholesterol and sphingolipids. Cholesterol is a kind of chiral lipid molecules, which has not been included in the previous and present theory of lipid domains. A new theory with the chirality on the raft domain should be developed.

(ii) The composite shell, as a model of cell membranes, has been investigated in Sec. IIIIC where the constraint between the area of the lipid bilayer and membrane skeleton is totally neglected. Additionally, only the small deformation of cell membranes are addressed in this review. The large deformation behavior of cell membranes has recently discussed through numerical simulations. It is necessary to reconsider the composite shell model with the constraint \( \int JdA = \int J_0 dA \) and its behavior under large deformation theoretically.

(iii) We suggest adopting four parameters \( k_c, \bar{k}, k_d, \) and \( \bar{k} \) to describe the mechanics of graphitic structures in Sec. IV. However, there are sparse studies on \( \bar{k} \) in previous literature. It is highly expected to theoretical and experimental work on this quantity.

(iv) We only talk about the thermal fluctuation on the discussion of graphene. The fluctuations of DNA, lipid
membranes, and cell membranes are not in the range of our topics, on which we suggest that gentle readers consult Refs. [10, 33, 62, 64].

(v) The elastic theory presented in this review is a static theory. Thus we are very regretted that we have to omit several important subjects such as the vesicles in shear flows [241, 242, 243, 244, 245] and dynamic response of carbon nanotubes or nanotube networks [246, 247] and so on. These topics will be quickly developed in the future.

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Note added in proof

After this review was in press, we noticed that recent researches [248, 249] on the mechanical properties of nanosprings [248] and amorphous straight nanowires [249] within the framework of Kirchhoff rod. We were also informed of the researches [250, 251] by Arroyo and Belytschko on discussing the buckling pattern of multi-walled carbon nanotubes under pure bending. Additionally, we emphasize that the similar equations to (114) and (115) without p first obtained by Zhang et al. [252]

APPENDIX A: CURVE VARIATIONAL THEORY

Here we sketch merely the derivation of Eqs. (16) and (17) because the derivation of Eq. (15) is trivial.

For convenience, we denote e_1 = N, e_2 = B, e_3 = T. Then we have d\mathbf{r} = \omega_3 e_3 and d\mathbf{e}_i = \omega_i e_j where

\[ \omega_3 = ds, \quad \omega_{12} = \tau \omega_3, \quad \omega_{13} = -\kappa \omega_3, \quad \omega_{23} = 0. \]  

(A1)

Following the spirit of Ref. [44], any infinitesimal deformation of a curve can be achieved by a displacement vector at each point on the curve as

\[ \delta \mathbf{r} \equiv \mathbf{v} = \Omega_1 e_1 + \Omega_2 e_2 + \Omega_3 e_3, \]  

(A2)

where \delta can be understood a variational operator. The frame is also changed because of the deformation of the curve, which is denoted as

\[ \delta \mathbf{e}_i = \Omega_{ij} e_j, \quad (i = 1, 2, 3), \]  

(A3)

where \Omega_{ij} = -\Omega_{ji}, \quad (i, j = 1, 2, 3)\] corresponds to the rotation of the frame due to the deformation of the curve. From \[ \delta \mathbf{d}\mathbf{r} = \delta \mathbf{v}, \delta \mathbf{d}\mathbf{e}_j = \delta \mathbf{d} e_j, \] and \[ \delta \mathbf{d} \phi = \delta \phi = 0, \] we can derive

\[ \delta \omega_3 = \Omega_1 \omega_3 + \Omega_2 \omega_{23} + d\Omega_3, \]  

(A4)

\[ \omega_3 \Omega_{31} = d\Omega_1 + \Omega_2 \omega_{23} + \Omega_3 \omega_{31}, \]  

(A5)

\[ \omega_3 \Omega_{32} = \Omega_1 \omega_2 + d\Omega_2 + \Omega_3 \omega_{32}, \]  

(A6)

\[ \delta \omega_{ij} = d\Omega_{ij} + \Omega_{il} \omega_{lj} - \omega_{il} \Omega_{lj}, \]  

(A7)

\[ \delta \phi' ds = -\phi' \omega_3. \]  

(A8)

Considering the above equations [A1], [A4]–[A8] and integral by parts as well as Stokes’ theorem, we can derive Eqs. (16) and (17) from the free energy (14).

APPENDIX B: SURFACE VARIATIONAL THEORY

Following the spirit of Ref. [49], any infinitesimal deformation of a surface can be achieved by a displacement vector at each point on the surface as

\[ \delta \mathbf{r} \equiv \mathbf{v} = \Omega_1 e_1 + \Omega_2 e_2 + \Omega_3 e_3, \]  

(B1)

where \delta can be understood a variational operator. The frame is also changed because of the deformation of the surface, which is still denoted as

\[ \delta \mathbf{e}_i = \Omega_{ij} e_j, \quad (i = 1, 2, 3), \]  

(B2)

where \Omega_{ij} = -\Omega_{ji}, \quad (i, j = 1, 2, 3)\] corresponds to the rotation of the frame due to the deformation of the surface. From \[ \delta \mathbf{d}\mathbf{r} = \delta \mathbf{v}, \delta \mathbf{d}\mathbf{e}_j = \delta \mathbf{d} e_j, \] and Eqs. (2)–(5), we can derive

\[ \delta \omega_1 = d\mathbf{v} \cdot e_1 - \omega_2 \Omega_{21}, \]  

(B3)

\[ \delta \omega_2 = d\mathbf{v} \cdot e_2 - \omega_1 \Omega_{12}, \]  

(B4)

\[ \Omega_{13} = \Omega_{3,1} + a \Omega_1 + b \Omega_2, \]  

(B5)

\[ \Omega_{23} = \Omega_{3,2} + b \Omega_1 + c \Omega_2, \]  

(B6)

\[ \delta \omega_{ij} = d\Omega_{ij} + \Omega_{il} \omega_{lj} - \omega_{il} \Omega_{lj}. \]  

(B7)

These equations are the essential equations of the surface variational theory based on the moving frame method. With them as well as Eqs. (5) and (6), we can easily derive

\[ \delta dA = (\text{div} \mathbf{v} - 2H \Omega_{3}) dA, \]  

(B8)

\[ \delta (2H) = [\nabla^2 + (4H^2 - 2K)] \Omega_3 + \nabla (2H) \cdot \mathbf{v}. \]  

(B9)

\[ \delta K = \nabla \cdot \nabla \Omega_3 + 2K \nabla H \Omega_3 + \nabla K \cdot \mathbf{v}. \]  

(B10)

Using the above three equations and the Stokes’ theorem, we can easily derive Eq. (57) from the free energy (56), or Eqs. (57)–(60) from the free energy (56), and so on.
APPENDIX C: STOKES' THEOREM AND THE OTHER IMPORTANT GEOMETRIC RELATIONS

The Stokes’ theorem is a crucial theorem in differential geometry. Let us denote the boundary of domain $\mathcal{D}$ as $\partial \mathcal{D}$. The Stokes’ theorem states as: If $\omega$ is a differential form on $\partial \mathcal{D}$, then

$$\int_{\partial \mathcal{D}} \omega = \int_{\mathcal{D}} d\omega. \quad (C1)$$

In particular, $\int_{\mathcal{D}} d\omega = 0$ for a closed domain $\mathcal{D}$.

It contains a lot of geometric relations, which are listed as follows.

(i) For any smooth functions $f$ and $h$ on 2D domain $\mathcal{D}$, we have

$$\int_{\mathcal{D}} (f d\ast h - h d\ast df) = \int_{\partial \mathcal{D}} (f \ast dh - h \ast df), \quad (C2)$$

$$\int_{\mathcal{D}} (f \ast dh - h \ast df) = \int_{\partial \mathcal{D}} (f \ast \bar{d}h - \bar{d}h \ast \bar{df}), \quad (C3)$$

$$\int_{\mathcal{D}} (f \ast \bar{d}h - \bar{d}h \ast \bar{df}) = \int_{\partial \mathcal{D}} (f \ast \bar{d}h - \bar{d}h \ast \bar{df}). \quad (C4)$$

where $d$ and $\bar{d}$ are generalized differential operator and Hodge star which satisfy $\bar{d}f = f_1 \omega_{12} + f_2 \omega_{23}$ and $d\ast f = f_1 \omega_{12} - f_2 \omega_{23}$ if $df = f_1 \omega_1 + f_2 \omega_2$.

(ii) If $u$ is a vector defined on a closed surface, then

$$\int_{\mathcal{D}} du \cdot \ast du = - \int_{\mathcal{D}} u \cdot d * du, \quad (C5)$$

where the dot represents the inner product of vectors.

(iii) For the tensors $\mathcal{S}$ and $\mathcal{M}$ defined in Sec. [11] we have

$$\int_{\partial \mathcal{D}} \mathcal{S} \cdot b \, ds = \int_{\mathcal{D}} \text{div} \mathcal{S} \, dA, \quad (C6)$$

$$\int_{\partial \mathcal{D}} \mathcal{M} \cdot b \, ds = \int_{\mathcal{D}} \text{div} \mathcal{M} \, dA, \quad (C7)$$

where $\mathcal{D}$ is a 2D domain with boundary $\partial \mathcal{D}$ and $b$ is the normal vector of $\partial \mathcal{D}$ in the tangent plane.

The above three items are also called the Stokes’ theorem in this review, which are widely used in the variational process.

The other geometric identities linking the vector form and differential form on a smooth surface used in this review are summarized as follows without additional proof.

$$\text{curl} u \, dA = d(u \cdot dr), \quad (C8)$$

$$\text{div} u \, dA = d(*u \cdot dr), \quad (C9)$$

$$\nabla \cdot u \, dA = d(*u \cdot dr), \quad (C10)$$

$$\nabla f \cdot dr = df, \quad (C12)$$

$$\nabla f \cdot dr = \bar{df}, \quad (C13)$$

$$\nabla^2 f \, dA = d \ast df, \quad (C14)$$

$$\nabla \cdot \nabla f \, dA = d \ast \bar{df}, \quad (C15)$$

$$\nabla \cdot \nabla f \, dA = d \ast \bar{df}, \quad (C16)$$

$$\nabla f \cdot u \, dA = df \wedge \ast u \cdot dr, \quad (C17)$$

$$\nabla^2 u \, dA = d \ast du, \quad (C18)$$

$$\nabla u \cdot dr = du. \quad (C19)$$

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