

Supplemental Material for: “Flatness and Intrinsic Curvature of Linked-Ring Membranes”

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I. CRITERIA FOR INTERLOCKING RINGS

Consider two 1-D rings, each of radius R , with centers located at positions \vec{r}_1 and \vec{r}_2 and normal vectors \hat{n}_1 and \hat{n}_2 , respectively. Ring #2 is positioned at $\vec{r}_{12} \equiv \vec{r}_2 - \vec{r}_1$ relative to ring #1. These quantities are all illustrated in Fig. S1. Clearly, if $|\vec{r}_{12}| > R$, then it is impossible for the rings to interlock. This is the first condition that should be checked.

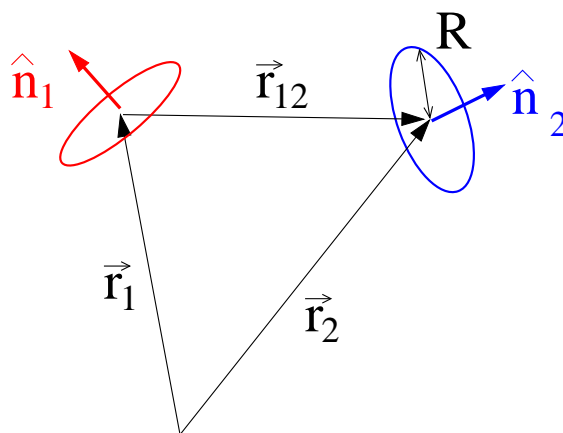


FIG. S1. Illustration of the quantities describing the positions and orientations of two rings.

The rings are each located in planes P_1 and P_2 , as indicated in Fig. S2 below. The planes intersect along a line L , which is drawn with a dashed line in the figure. If the two planes are parallel (or extremely close to being parallel), then the rings cannot overlap. To test this, measure

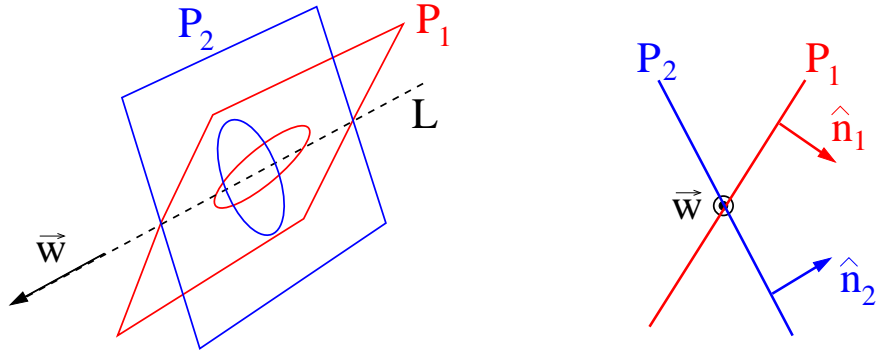


FIG. S2. Illustration of the planes P_1 and P_2 containing each of the two rings. Panel (a) shows the view from an arbitrary perspective. The plain-intersection (PI) line is drawn as a dashed line. Panel (b) views the plane along the PI line.

$\vec{n}_1 \cdot \vec{n}_2$. If this number is equal to (or very, very close to) unity, then the rings do not overlap. This should be the next check.

A vector \vec{w} along the line L is calculated:

$$\vec{w} = \hat{n}_1 \times \hat{n}_2 \quad (\text{S.1})$$

Note: since \vec{n}_1 and \vec{n}_2 are not parallel, this cross product will not vanish. Further note that \vec{w} is perpendicular to both \hat{n}_1 and \hat{n}_2 . For ring #1, define a vector \vec{u} that is perpendicular to \vec{w} and \hat{n}_1

$$\vec{u} = \vec{w} \times \hat{n}_1 \quad (\text{S.2})$$

Note that \vec{u} is tangent to the surface of ring #1. A line that goes through the center of ring #1 is given by:

$$\vec{l}_1 = \vec{r}_1 + s\vec{u} \quad (\text{S.3})$$

Note: This line intersects the PI line and is perpendicular to it. In component form, the this

parametric equation can be written:

$$\begin{aligned}l_{1,x} &= x_1 + su_x, \\l_{1,y} &= y_1 + su_y, \\l_{1,z} &= z_1 + su_z.\end{aligned}\tag{S.4}$$

The variable s is the parameter, whose value determines the location of any point on the line. For ring #2, define a vector \vec{v} that is perpendicular to \vec{w} and \hat{n}_2 :

$$\vec{v} = \vec{w} \times \hat{n}_2\tag{S.5}$$

Note that \vec{v} is tangent to the surface of ring #2. A line which goes through the center of ring #2 (at \vec{r}_2) and is tangent to the ring is given by:

$$\vec{l}_2 = \vec{r}_2 + t\vec{v}\tag{S.6}$$

where t is the parameter that determines the value of any point on the line. Again, this is actually three equations, one for each component, as in Eq. (S.4). **Note:** As for the line defined by Eq. (S.3), the line defined by Eq. (S.6) intersects the PI line and is perpendicular to it. The lines defined by Eqs. (S.3) and (S.6) are illustrated in Fig. S3 (a) . For clarity, the line defined by Eq. (S.6) is shown in panel (b) of the figure. In this case, ring #2 is viewed perpendicular to its plane.

Now determine the closest approach between the two lines. This means finding the two points, one on each line, that have the shortest distance. **Note:** These two points will both be on the PI line. Finding the points of nearest approach between two lines is a standard problem whose solution can be found in numerous places. It can be shown that the two points of nearest approach on each line occur at $s=s_c$ for line #1 and $t = t_c$ for line #2, where

$$s_c = \frac{be - cd}{ac - b^2}\tag{S.7}$$

and

$$t_c = \frac{ae - bd}{ac - b^2},\tag{S.8}$$

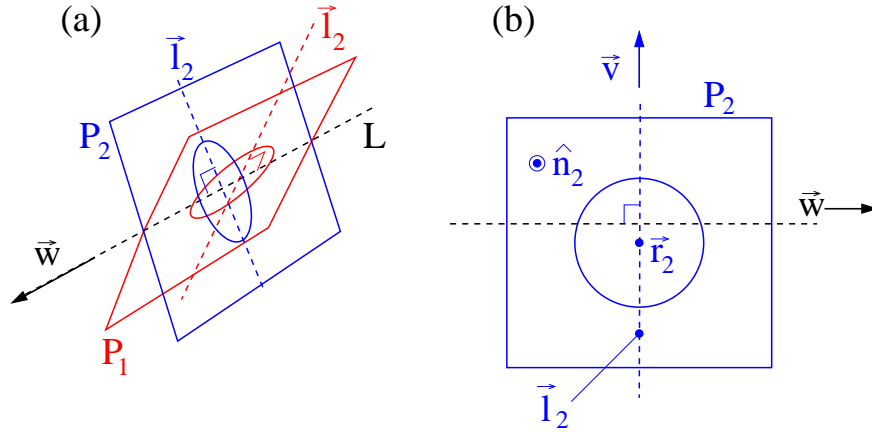


FIG. S3. Illustration of the lines defined by Eqs. (S.3) and (S.6). In panel (a), the line defined by Eq. (S.3) is drawn as a red dashed line, while the line defined by Eq. (S.6) is drawn as a blue dashed line. Note that these lines both intersect the PI line at right angles. In panel (b), the line defined by Eq. (S.6) as well as the vector \vec{v} is illustrated. Here, the perspective is perpendicular to ring #2.

where

$$a = \vec{u} \cdot \vec{u},$$

$$b = \vec{u} \cdot \vec{v},$$

$$c = \vec{v} \cdot \vec{v},$$

$$d = \vec{u} \cdot \vec{w}_0,$$

$$e = \vec{v} \cdot \vec{w}_0,$$

where we have defined

$$\vec{w}_0 = \vec{r}_1 - \vec{r}_2.$$

Label these two points \vec{p}_1 and \vec{p}_2 . They are each defined:

$$\vec{p}_1 = \vec{r}_1 + s_c \vec{u}, \tag{S.9}$$

$$\vec{p}_2 = \vec{r}_2 + t_c \vec{v}, \tag{S.10}$$

where the values of s_c and t_c are given in Eqs. (S.7) and (S.8). Again note that these points lie on the plane-intersection line L . Knowing a point on the line and the direction of the line (\vec{w})

allows us to define the line L . Making the arbitrary choice that this point be \vec{p}_1 , we write:

$$\vec{L} = \vec{p}_1 + \lambda \vec{w} \quad (\text{S.11})$$

where λ is the parameter for the equation. In component form, this equation is:

$$\begin{aligned} L_x &= w_x \lambda + p_{1,x} \equiv a\lambda + b \\ L_y &= w_y \lambda + p_{1,y} \equiv c\lambda + d \\ L_z &= w_z \lambda + p_{1,z} \equiv e\lambda + f \end{aligned} \quad (\text{S.12})$$

where we have defined $a \equiv w_x$, $b \equiv p_{1,x}$, etc., for brevity. The distance of the center of ring #1, located at (x_1, y_1, z_1) , from an arbitrary point along this line is given by:

$$(D(\lambda))^2 = (a\lambda + b - x_1)^2 + (c\lambda + d - y_1)^2 + (e\lambda + f - z_1)^2$$

The minimum distance satisfies

$$\frac{dD^2}{d\lambda} = 0,$$

which can be shown corresponds to a point on the line at $\lambda = \lambda_0$, where

$$\lambda_0 = \frac{ax_1 + cy_1 + ez_1 - ab - cd - ef}{a^2 + c^2 + e^2} \quad (\text{S.13})$$

Thus, the minimum distance from the center of the ring to the line is given by

$$D_0^2 = (a\lambda_0 + b - x_1)^2 + (c\lambda_0 + d - y_1)^2 + (e\lambda_0 + f - z_1)^2 \quad (\text{S.14})$$

Clearly, if $D_0 > R$, then this ring is too far away from the line to be interlocking the other ring. If $D_0 < R$, then it is possible that the rings interlock. Repeat the calculation to find the minimum distance from the center of the other ring to the plane-intersection line. As before, if $D_0 > R$, then this ring is too far away from the line to be interlocking the other ring. If $D_0 < R$, then it is possible that the rings interlock. If both rings satisfy $D_0 < R$, interlocking is possible, and we must now find the points of intersection of one of the rings and the line. The two intersection points of ring #1, $\vec{r}_{\text{int}}^{(1)}$ and $\vec{r}_{\text{int}}^{(2)}$, are illustrated in Fig. S4 below:

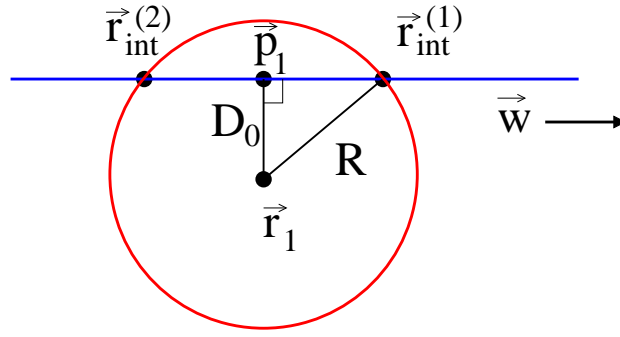


FIG. S4. Illustration showing the intersection points, $\vec{r}_{\text{int}}^{(1)}$ and $\vec{r}_{\text{int}}^{(2)}$, with the plane-intersection line. Note that \vec{p}_1 is defined in Eq. (S.9) and is a point on line defined by Eq. (S.3).

Clearly,

$$|\vec{r}_{\text{int}}^{(i)} - \vec{p}_1|^2 = R^2 - D_0^2 \Rightarrow |\vec{r}_{\text{int}}^{(i)} - \vec{p}_1| = \sqrt{R^2 - D_0^2}, \quad \text{for } i = 1 \text{ or } 2$$

It is evident then that

$$\vec{r}_{\text{int}}^{(i)} = \vec{p}_1 \pm \hat{w} \sqrt{R^2 - D_0^2}$$

where

$$\hat{w} \equiv \vec{w}/|\vec{w}|$$

Choose the arbitrary convention for the signs such that the positions of the two intersection points are:

$$\begin{aligned} \vec{r}_{\text{int}}^{(1)} &= \vec{p}_1 + \hat{w} \sqrt{R^2 - D_0^2} \\ \vec{r}_{\text{int}}^{(2)} &= \vec{p}_1 - \hat{w} \sqrt{R^2 - D_0^2}. \end{aligned}$$

Finally, we need to measure the distance between the center of ring #2 from each of these intersection points. If only one of these points lies within a distance of R from \vec{r}_2 , while the other lies outside this range, then the rings overlap. To understand why this is true, note that ring #2 is also in the plane that includes these two intersection points. Thus, the rings overlap

of either one of the two conditions holds:

$$|\vec{r}_2 - \vec{r}_{\text{int}}^{(1)}|^2 < R^2 \quad \underline{\text{and}} \quad |\vec{r}_2 - \vec{r}_{\text{int}}^{(2)}|^2 > R^2$$

OR

$$|\vec{r}_2 - \vec{r}_{\text{int}}^{(1)}|^2 > R^2 \quad \underline{\text{and}} \quad |\vec{r}_2 - \vec{r}_{\text{int}}^{(2)}|^2 < R^2$$

If neither condition holds, then the rings do not overlap.

II. OVERLAP CRITERION FOR TWO TORUSES OF ROTATION

Consider two toruses of rotation. Each torus is characterized by a central ring (i.e. circle) of radius R . The normal vectors for each torus are \hat{n}_a for ring **a** and \hat{n}_b for ring **b**. A cross-section in a plane tangent to the normal vector cuts the torus into two circles, each of radius r . Figure S5 illustrates the two quantities, R and r .

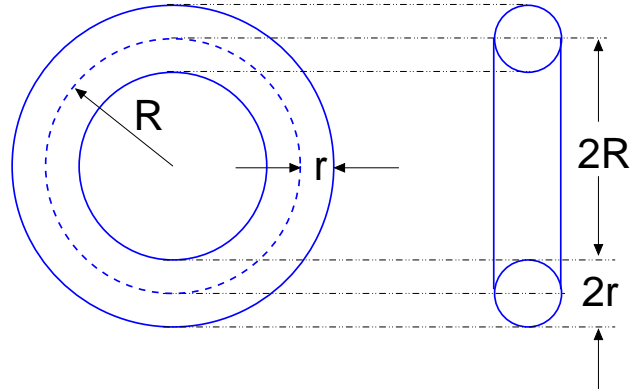


FIG. S5. Illustration showing a torus of rotation from two perspectives to illustrate the two radii, R and r . The dashed blue line on the left is the central ring referred to in the text.

The toruses will overlap if the nearest pair of points on each ring have a distance d that satisfies $d < 2r$. Thus, the overlap calculation reduces to determining this nearest distance between two rings. To calculate this distance, we use the procedure described by Vranek[1]. Consider the two rings in Fig. S5.

The vector \vec{X} specifies the position of an arbitrary point on ring **b**. It can be shown that the

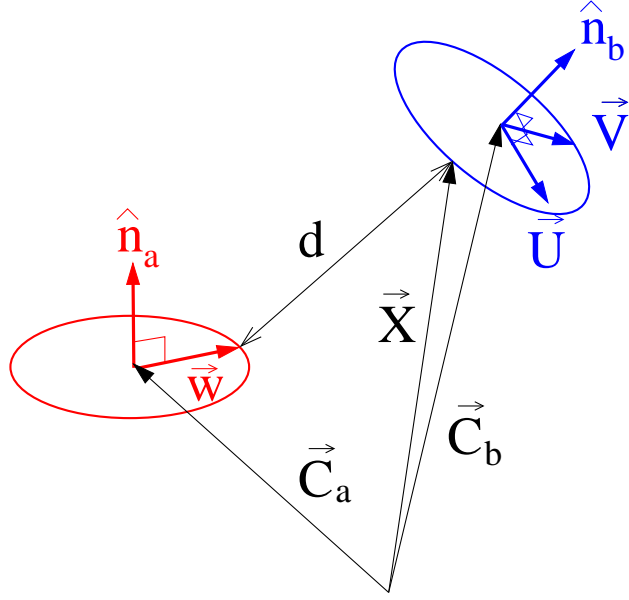


FIG. S6. Illustration showing two rings, **a** and **b**, their normal vectors \hat{n}_a and \hat{n}_b , and the positions of the their centers, \vec{C}_a and \vec{C}_b , respectively. The vectors \vec{U} and \vec{V} lie in the plane of ring **b**, and \vec{W} lies in the plane of ring **a**. In addition, \vec{X} is the position of an arbitrary point on ring **b**, and d is the distance between that point and the nearest point on ring **a**. This figure is based on Fig. 2 of Ref. 1.

distance between this point and the nearest point on ring **a** is:

$$d^2 = R^2 + |\vec{C}_a - \vec{X}|^2 - 2R \left| \vec{X} - \vec{C}_a - \left(\hat{n}_a \cdot (\vec{X} - \vec{C}_a) \right) \hat{n}_a \right| \quad (\text{S.15})$$

The position \vec{X} can be written:

$$\vec{X}(t) = \vec{C}_b + R \left(\vec{U} \cos t + \vec{V} \sin t \right), \quad (\text{S.16})$$

where t is a parameter that ranges from $-\pi$ to π . Substitution of Eq. (S.16) into Eq. (S.15) yields:

$$f(t) \equiv d^2(t) = a_9 \cos t + a_8 \sin t + a_7 + a_6 \sqrt{a_5 \cos^2 t + a_4 \sin^2 t + a_3 \cos t + a_2 \sin t + a_1 \cos t \sin t + a_0} \quad (\text{S.17})$$

The coefficients in Eq. (S.17) are:

$$\begin{aligned}
a_9 &= 2R\vec{C}_b \cdot \vec{U} - 2R\vec{C}_a \cdot \vec{U} \\
a_8 &= 2R\vec{C}_b \cdot \vec{V} - 2R\vec{C}_a \cdot \vec{V} \\
a_7 &= 2R^2 + \vec{C}_a \cdot \vec{C}_a + \vec{C}_b \cdot \vec{C}_b - 2\vec{C}_a \cdot \vec{C}_b \\
a_6 &= -2R \\
a_5 &= -R^2(\vec{n}_a \cdot \vec{U})^2 \\
a_4 &= -R^2(\vec{n}_a \cdot \vec{V})^2 \\
a_3 &= 2R\vec{C}_b \cdot \vec{U} - 2R\vec{C}_a \cdot \vec{U} - 2R(\vec{n}_a \cdot \vec{C}_b - \vec{n}_a \cdot \vec{C}_a)\vec{n}_a \cdot \vec{U} \\
a_2 &= 2R\vec{C}_b \cdot \vec{V} - 2R\vec{C}_a \cdot \vec{V} - 2R(\vec{n}_a \cdot \vec{C}_b - \vec{n}_a \cdot \vec{C}_a)\vec{n}_a \cdot \vec{V} \\
a_1 &= 2R^2\vec{n}_a \cdot \vec{U}\vec{n}_a \cdot \vec{V} \\
a_0 &= R^2 + \vec{C}_b \cdot \vec{C}_b + \vec{C}_a \cdot \vec{C}_a - 2\vec{C}_a \cdot \vec{C}_b - \left(\vec{n}_a \cdot \vec{C}_b - \vec{n}_a \cdot \vec{C}_a\right)^2 \tag{S.18}
\end{aligned}$$

To determine the minimum distance, we could simply solve $f'(t) = 0$. This will require solving for the roots of a polynomial of degree 8, which is extremely time consuming. The approach of Vranek[1] provides a much faster alternative. First note that over the range $-\pi \leq t < \pi$, it is possible to show that:

- $f(t) = 0$ has at most four roots
- $f(t)$ has either (1) one minimum and one maximum **or** (2) two minima and two maxima.

We conduct a numerical search for the first minimum using Brent's method.[2] We use the Numerical Recipes function "mnbrack" to first bracket the minimum, and then use the function "brent" to find a minimum. Let t_1 be the location of the minimum and $D_1 \equiv f(t_1)$ be the value of the distance function at the minimum. This minimum is either a local or absolute minimum. We will now determine which it is. Shift the function by $D_1 = f(t_1)$ to create a new function:

$$g(t) = f(t) - D_1 \tag{S.19}$$

We next seek the solution of $g(t) = 0$. This can be obtained by conversion to the polynomial equation of the fourth degree. Using $z \equiv \cos t$, this leads to

$$P_4(z) = 0, \tag{S.20}$$

where

$$P_4(z) \equiv b_4 z^4 + b_3 z^3 + b_2 z^2 + b_1 z + b_0 \quad (\text{S.21})$$

where

$$\begin{aligned} b_4 &= c_6^2 + c_5^2, \\ b_3 &= 2c_1 c_5 + 2c_4 c_6, \\ b_2 &= c_1^2 - c_5^2 + 2c_3 c_6 + c_4^2, \\ b_1 &= -2c_1 c_5 + 2c_3 c_4, \\ b_0 &= c_3^2 - c_1^2, \end{aligned} \quad (\text{S.22})$$

and

$$\begin{aligned} c_1 &= 2a_8(a_7 - D_0) - a_6^2 a_2, \\ c_2 &= a_6^2 a_4, \\ c_3 &= (a_7 - D_0)^2 - a_6^2 a_0 + a_8^2 - a_6^2 a_4, \\ c_4 &= 2a_9(a_7 - D_0) - a_6^2 a_3, \\ c_5 &= 2a_9 a_8 - a_6^2 a_1, \\ c_6 &= -a_8^2 + a_6^2 a_4 + a_9^2 - a_6^2 a_5, \end{aligned} \quad (\text{S.23})$$

and where the a_i coefficients are given in Eqs. (S.18). Since it is simultaneously true that $g(t_1) = 0$ and $g(t_1)$ is a minimum, it follows that $z = z_1 \equiv g(t_1)$ is a double-root, i.e.,

$$P_4(z) = (z - z_1)^2 P_2(z), \quad (\text{S.24})$$

where

$$P_2(z) = d_2 z^2 + d_1 z + d_0 \quad (\text{S.25})$$

is a second-degree polynomial with coefficients d_0 , d_1 and d_2 . Equating the right sides of

Eqs. (S.21) and (S.24), and using Eq. (S.25), it can be shown that:

$$\begin{aligned} d_0 &= b_0/z_1^2, \\ d_1 &= (b_1 + 2b_0/z_1)/z_1^2, \\ d_2 &= b_4. \end{aligned} \tag{S.26}$$

It is possible that there are two other roots of the equation $P_4(z) = 0$. From Eqs. (S.24) and (S.25), these roots must satisfy:

$$P_2(z) = d_2z^2 + d_1z + d_0 = 0 \tag{S.27}$$

Now, if

$$d_1^2 - 4d_2d_0 < 0 \tag{S.28}$$

then the roots do not exist. This means that either:

1. The second minimum is greater than the minimum D_1 the distance function located z_1
2. The second minimum does not exist

Either way, it implies that D_1 is the global minimum of the distance function of Eq. (S.17). If

$$d_1^2 - 4d_2d_0 > 0 \tag{S.29}$$

then the roots do exist. Call these two roots z_a and z_b . Using the quadratic formula, it follows:

$$z_a = \frac{-d_1 - \sqrt{d_1^2 - 4d_2d_0}}{2d_2}, \tag{S.30}$$

$$z_b = \frac{-d_1 + \sqrt{d_1^2 - 4d_2d_0}}{2d_2}, \tag{S.31}$$

If the roots exist, this implies that there is a second minimum, D_2 , in the range $z_a < z_2 < z_b$. It is also clear that $g(z_2) < g(z_1) = 0$. This therefore implies that D_2 is the global minimum, located at $z = z_2$. To find z_2 , we once again use the numerical routine “mnbrak” to bracket the minimum and the routine “brent” to locate the minimum. We have now determined the global minimum of the distance function of Eq. (S.17). Call this D_{\min} . The minimum distance between

any pair of points, one on each ring, is thus:

$$d_{\min} = \sqrt{D_{\min}} \quad (\text{S.32})$$

The square-root is required since $f(t)$ defined in the distance function of Eq. (S.17) is the square of the distance. Finally, the condition for overlap is:

- $d_{\min} < 2r \Rightarrow$ toruses overlap
- $d_{\min} > 2r \Rightarrow$ toruses do not overlap

III. CLARIFICATION ON THE SIGN OF THE CONCAVITY

Figure 3(a) of the article shows the time dependence of the concavity, ζ , for an HT membrane, which fluctuates between positive and negative values. Determining the sign of ζ requires dealing with an ambiguity in the direction of the eigenvector \hat{n}_3 . As illustrated in Fig. 2 of the article, \hat{n}_3 determines the direction of the axis for the coordinate ξ used in the definition of the concavity in Eq. (2). The components of the vector \hat{n}_3 are calculated by a Numerical Recipes routine that returns the eigenvalues and eigenvectors of the shape tensor, $S_{\alpha\beta}$, defined in Eq. (1). Note however that if \hat{n}_3 is an eigenvector then so is $-\hat{n}_3$, and it is not obvious which of the two vectors will be returned by the algorithm. Failure to address this problem renders the sign of ζ essentially meaningless.

This ambiguity can be addressed by using the fixed connectivity of the rings in the membrane. We used the following simple procedure. Each time the eigenvectors and eigenvalues of $S_{\alpha\beta}$ were calculated for a given set of coordinates, we calculated the vector \vec{U} , defined as

$$\vec{U} \equiv \sum_{i=1}^5 \vec{R}_i \times \vec{R}_{i+1} + \vec{R}_6 \times \vec{R}_1. \quad (\text{S.33})$$

Here, the vectors \vec{R}_i are the displacements between the centers of the nearest 6-valence rings that are closest to the ring at or nearest to the center of the membrane. These are illustrated in Fig. S7 below. The vector \hat{n}_3 is defined such that $\hat{n}_3 \cdot \vec{U} > 0$. If the value of \hat{n}_3 returned by the algorithm is negative, then its direction is inverted. Note that the Eq. (S.33) and the illustration both correspond to HT and ST membranes. The case of SS membranes can be addressed by minor changes to the definition of \vec{U} .

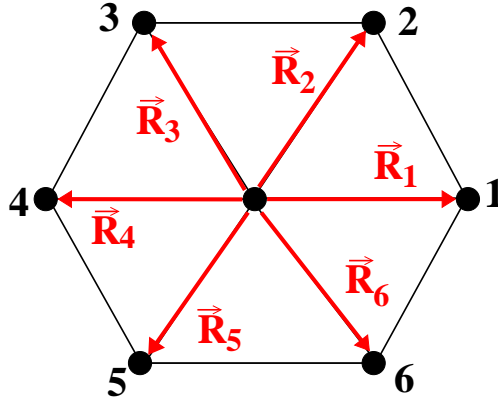


FIG. S7. Illustration of the vectors \vec{R}_i used in Eq. (S.33). The black dots denote the centers of neighbouring rings. The central dot is the central ring in the membrane.

Note that the sign of ζ is unimportant in most of the calculations in the study. Since the probability distribution satisfies $\mathcal{P}(\zeta) = \mathcal{P}(-\zeta)$, only $|\zeta|$ was needed to determine the free energy functions shown in Fig. 7 and 10 of the article. The calculation procedure was only used to generate the results shown Fig. 6(a) and (b) for the purpose of illustrating free-energy barrier jumping.

IV. CALCULATION OF GAUSSIAN CURVATURE

In the article we calculate the Gaussian curvature, κ_G , for the hexagonal-shaped membrane with triangular linking topology (i.e. an HT membrane) illustrated in Fig. 1(a) of the manuscript. To do this, we employ the method described by Meyer *et al.* in Ref. [3], which is suitable for calculating κ_G at nodes of a triangular mesh. Here, we briefly outline the implementation of the procedure to HT membranes.

We consider the centers of the 6-valence rings of the HT membranes as nodes in a triangular mesh. In the vicinity of the i th node, the Gaussian curvature is approximately given by:

$$\int_{\mathcal{A}_i} \kappa_G(i) dA = 2\pi - \sum_{j=1}^{n_f} \theta_j \quad (\text{S.34})$$

Each node is characterized by a set of $n_f = 6$ angles, θ_j , which are illustrated in Fig. S8. The area \mathcal{A}_i is the sum of contributions to the Voronoi area for the central node (i.e. the i th node)

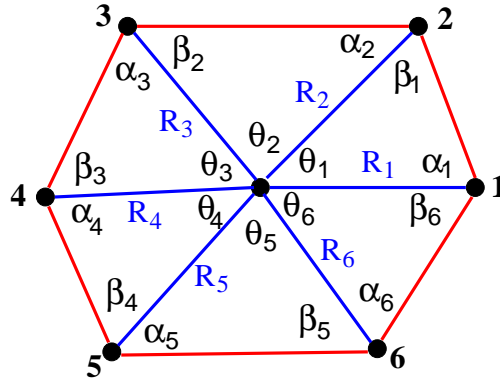


FIG. S8. Illustration of the quantities used in the equations used to calculate the Gaussian curvature. Each black dot denotes a center of a 6-valence ring. The six rings that surround the central ring are connected via one 2-valence ring.

from each of the six triangles surrounding it. This contribution for the j th triangle is given by

$$\mathcal{A}_{\text{vor},j} = \frac{1}{8} (R_j^2 \cot \beta_j + R_{j+1} \cot \alpha_j), \quad (\text{S.35})$$

where the angles α_i and β_i as well as the distances R_i are labeled in the figure. (Note that for the triangle with $j = 6$, the index $j + 1$ should be replaced with 1.) As noted by Meyer *et al.*, [3] the Voronoi area is inappropriate for the case of an obtuse triangle. They use instead the following choice in place of the Voronoi area for such triangles: If the θ_j is obtuse, then the area contribution is $A_T/2$, where A_T is the triangle area; otherwise, either α_j or β_j is obtuse, in which case the area contribution is $A_T/4$.

In the simulation, the Gaussian curvature is measured at every 6-valence ring during sampling and averaged as follows:

$$\kappa_G = \frac{\sum_i \int_{\mathcal{A}_i} \kappa_G(i) dA}{\sum_i \int_{\mathcal{A}_i} dA}, \quad (\text{S.36})$$

where $\kappa_G(i)$ is the Gaussian curvature at node i .

[1] D. Vranek, *J. Graph. Tools* **7**, 23 (2002).

[2] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes in C* (Cambridge University Press, Cambridge, 1988) Chap. 10.

- [3] M. Meyer, M. Desbrun, P. Schröder, and A. H. Barr, in *Visualization and Mathematics III* (Springer, 2003) pp. 35–57.