Biophysical Journal, Volume 120

## Supplemental information

# Endocytosis against high turgor pressure is made easier by partial coating and freely rotating base

Rui Ma and Julien Berro

# **Supporting Material for "Endocytosis against high turgor pressure is made easier by partial protein coating and a freely rotating base"**

Rui Ma<sup>1,2,3\*</sup> and Julien Berro<sup>2,3,4\*</sup>

<sup>1</sup>Department of Physics, Xiamen University, Xiamen, 361005, China

<sup>2</sup>Department of Molecular Biophysics and Biochemistry, Yale University, New Haven, CT 06520, USA

<sup>3</sup>Nanobiology Institute, Yale University, West Haven, CT 06516, USA

<sup>4</sup>Department of Cell Biology, Yale University School of Medicine, New Haven, CT 06520, USA

\*Correspondence: ruima@xmu.edu.cn

\*Correspondence: julien.berro@yale.edu

### **DERIVATION OF THE ANALYTICAL SOLUTION FOR THE INITIATION FORCE**

The derivation here is based on the analytical solution obtained in the work of [\(1\)](#page-2-0) in the limit of small angles. It assumes that the membrane is almost flat such that the tangential  $\psi \ll 1$ . Keeping only the first order of  $\psi$  and its derivatives and performing the coordinate transformation of  $\psi(s)$  to  $\psi(R)$ , the shape equation can be reduced to

$$
R^{2}\psi'' + R\psi' - (R^{2}\frac{\sigma_{\text{eff}}}{\kappa} + 1)\psi = -\frac{f}{2\pi\kappa}R + \frac{p}{2\kappa}R^{3}
$$
(S1)

where the prime (') indicates the derivative with respect to the radial coordinate R and  $\sigma_{\text{eff}} = \sigma + \frac{1}{2} \kappa c_0^2$ .

The general solution to Eq. [\(S1\)](#page-1-0) that satisfies the boundary condition at the tip  $\psi(R = 0) = 0$  reads

$$
\psi(R) = \frac{f}{2\pi\sigma_{\text{eff}}} \frac{1}{R} - \frac{1}{2} \frac{p}{\sigma_{\text{eff}}} R - \frac{f}{2\pi\sqrt{\kappa\sigma_{\text{eff}}}} K_1(R\sqrt{\sigma_{\text{eff}}/\kappa}) + cI_1(R\sqrt{\sigma_{\text{eff}}/\kappa})
$$
(S2)

where  $I_i(x)$  and  $K_i(x)$  are modified Bessel functions. The constant c is determined by the other boundary condition at  $R = R_b$ . For the free-hinge BC, it reads

<span id="page-1-0"></span>
$$
\psi' + \frac{\psi}{R} = c_0. \tag{S3}
$$

For fixed-hinge BC, it reads

 $\psi = 0.$  (S4)

To calculate the initiation force  $F_{\text{init}}$ , we set the membrane height  $L = 0$ , i.e.,

<span id="page-1-1"></span>
$$
\int_0^{R_\mathrm{b}} \psi(R) = 0 \tag{S5}
$$

For the free-hinge BC, the initiation force in the limit of  $\sigma \to 0$  reads

$$
\frac{F_{\text{init}}}{2\pi} = \frac{4(\kappa c_0^3 + 2p) \left[ 1 - I_0(c_0 R_b / \sqrt{2}) \right] + p c_0^2 R_b^2 I_0(c_0 R_b / \sqrt{2})}{2c_0^2 \left\{ 2K_0(c_0 R_b / \sqrt{2}) + I_0(c_0 R_b / \sqrt{2}) \left[ 2\gamma - \ln(8) + 2\ln(c_0 R_b) \right] \right\}},\tag{S6}
$$

where  $\gamma$  is the Euler constant. As a special case  $c_0 \rightarrow 0$ , Eq. [\(S6\)](#page-1-1) reduces to

$$
F_{\text{init}} = \frac{3}{8}\pi R_{\text{b}}^2 p \tag{S7}
$$

Rui Ma and Julien Berro

For the fixed-hinge BC, the initiation force reads

$$
\frac{F_{\text{init}}}{2\pi} = pR_b^2 \frac{4 - 4I_0(Q) + 2QI_1(Q)}{16 - 8I_0(Q) - 8QK_1(Q) + 4QI_1(Q)(2\ln Q - \ln 4 + 2\gamma)},
$$
\n(S8)

where  $Q = c_0 R_b / \sqrt{2}$ . As a special case  $c_0 \rightarrow 0$ , Eq. [\(S8\)](#page-2-1) reduces to

<span id="page-2-1"></span>
$$
F_{\text{init}} = \frac{1}{4}\pi R_b^2 p \tag{S9}
$$

#### **SPHERICAL CAP APPROXIMATION**

We approximate the dome-shaped membrane with a spherical cap of radius  $R$  (see Figure 7, a and b, inset). The shape of the spherical cap is fully determined by two parameters, the sphere radius  $R$  and the base radius  $R<sub>b</sub>$ . Note that neither the free-hinge BC nor the fixed-hinge BC is satisfied in this case. The membrane height  $L$  of the spherical cap reads

$$
L = R - \sqrt{R^2 - R_b^2},
$$
 (S10)

and the corresponding membrane area  $A = 2\pi R L$  and the volume  $V = \frac{1}{3}\pi L^2 (3R - L)$ . The free energy of the membrane then becomes

$$
E = \left[\frac{1}{2}\kappa\left(\frac{2}{R} - c_0\right)^2 + \sigma\right]A + pV.
$$
\n(S11)

In the case of a fixed base radius, the free energy  $E(R; c_0, R_b)$  is a function of only R. For a barely coated membrane, i.e.,  $c_0R_p = 0$ , the free energy  $E(R; c_0, R_b)$  decreases monotonically with the radius R and the flat shape ( $R = \infty$ ) has the lowest energy (Figure 7 a). However, when  $c_0$  becomes large, e.g.,  $c_0R_p = 1$ , the free energy  $E(R; c_0, R_b)$  has a minimum at a finite radius  $R$  (Figure 7 b). This means the flat shape is no longer stable and the membrane can be bent up by proteins without any external forces.

If the base radius is free to move, i.e.,  $R_b$  being a free parameter, the free energy  $E(R, R_b; c_0)$  becomes a function of both R and  $R_b$ , and always has its trivial minimum  $E = 0$  at  $R_b = 0$ , regardless of the spontaneous curvature  $c_0$  (Figure 7a and b,  $R_b = 0R_p$ ). The corresponding solution at  $R_b = 0$  represents an infinitely small patch of membrane. In the presence of an external force f, the total free energy  $F(R, R_b; c0, f) = E(R, R_b; c0, f) - fL$  can have a nontrivial minimum with a nonzero  $R<sub>b</sub>$ . The minimum force  $f<sub>min</sub>$  to have such a nontrivial minimum, i.e., to lift the membrane up, is given by

$$
f_{\min} = \min_{R,R_b} \frac{E}{L}.
$$
 (S12)

Both the denominator and the numerator are positive numbers, therefore  $f_{\text{min}}$  is always positive. For instance, for  $c_0R_p = 1$ , the minimum force  $f_{\text{min}} = 0.0027 f_p$  is obtained at  $R = 1.998 R_p$  and  $R_b = 0.00057 R_p$ . Therefore an external force is always required to lift the membrane up in this condition. However, the base radius  $R_b = 0.00057 R_p$  is an unrealistically narrow shape given the typical value of  $R_p = 15-30$  nm. Similar problem also exists in the model of [\(2\)](#page-2-2) which used a freely-moving base BC.

#### **REFERENCES**

- <span id="page-2-0"></span>1. Derényi, I., F. Jülicher, and J. Prost, 2002. Formation and Interaction of Membrane Tubes. *Phys. Rev. Lett.* 88:238101. <http://link.aps.org/doi/10.1103/PhysRevLett.88.238101>.
- <span id="page-2-2"></span>2. Dmitrieff, S., and F. Nédélec, 2015. Membrane Mechanics of Endocytosis in Cells with Turgor. *PLoS Comput Biol* 11:1–15. <http://dx.doi.org/10.1371%2Fjournal.pcbi.1004538>.

### **SUPPLEMENTAL FIGURES**



Figure S1: **Free energy of membrane deformations for a fully coated membrane.** (a - d) Free energy of membrane deformations E as a function of membrane height L. The spontaneous curvature is fixed at  $c_0R_p = 0.2$  in (a, b) and  $c_0R_p = 1$  in (c, d). The symbols on the  $E-L$  curve correspond to the same symbols on the  $f-L$  curve shown in Figure 3a-d. In (a - d), the solid line indicates shapes of the lowest free energy and the dashed line indicates shapes of relatively high free energy. The dark color indicates membrane shapes that are all above  $z = 0$ , and the gray color indicates shapes that have parts below  $z = 0$ . In the left column (a, c), the free-hinge BC is imposed at the base points  $R_b = 2R_p$ , while in the right column (b, d), the fixed-hinge BC is imposed. On the left and bottom axes (black), non-dimensionalized quantities are used, while on the right and top axes (blue), quantities are measured in their physical units. The parameters are listed in Table 2.



Figure S2: **Free energy of membrane deformations for a partially coated membrane**.(a - d) Free energy of membrane deformations E as a function of membrane height L. The coating area is fixed at  $a_0/(2\pi R_p^2) = 1$  in (a, b) and  $a_0/(2\pi R_p^2) = 2$  in (c, d). The symbols on the  $E-L$  curve correspond to the same symbols on the  $f-L$  curve shown in Figure 4a-d. In (a - d), the solid line indicates shapes of the lowest free energy and the dashed line indicates shapes of relatively high free energy. The dark color indicates membrane shapes that are all above  $z = 0$ , and the gray color indicates shapes that have parts below  $z = 0$ . In the left column (a, c), the free-hinge BC is imposed at the base points  $R_b = 2R_p$ , while in the right column (b, d), the fixed-hinge BC is imposed. On the left and bottom axes (black), non-dimensionalized quantities are used, while on the right and top axes (blue), quantities are measured in their physical units. The parameters are listed in Table 2.



Figure S3: **Free energy of membrane deformations for a partially coated membrane**.(a - d) Free energy of membrane deformations E as a function of membrane height L. The coating area is fixed at  $a_0/(2\pi R_p^2) = 1$  in (a, b) and  $a_0/(2\pi R_p^2) = 2$  in (c, d). The symbols on the  $E-L$  curve correspond to the same symbols on the  $f-L$  curve shown in Figure 5a-d. In (a - d), the solid line indicates shapes of the lowest free energy and the dashed line indicates shapes of relatively high free energy. The dark color indicates membrane shapes that are all above  $z = 0$ , and the gray color indicates shapes that have parts below  $z = 0$ . In the left column (a, c), the free-hinge BC is imposed at the base points  $R_b = 2R_p$ , while in the right column (b, d), the fixed-hinge BC is imposed. On the left and bottom axes (black), non-dimensionalized quantities are used, while on the right and top axes (blue), quantities are measured in their physical units. The parameters are listed in Table 2.



Figure S4: **Fitting error as a function of the fitting parameter**  $R_p$  for the two BCs. The first row shows the fitting error for the dataset of  $R_t$  v.s. L, and the second row for the dataset of  $D_t$  v.s. L and the third row for the sum. In the left column, the free-hinge BC is imposed, while in the right column, the fixed-hinge BC is imposed.



Figure S5: **Free energy of membrane deformations in the presence of external force under spherical cap approximation.** Free energy of the membrane as a function of the sphere radius R for  $c_0R_p = 0$  in (a) and  $c_0R_p = 1$  in (b). The external force  $f = f_p$ . For different base radii  $R_b$ , the range of R is  $[R_b, \infty]$ , where  $R = R_b$  corresponds to a hemi-spherical cap and  $R = \infty$ corresponds to a flat shape.



Figure S6:  $F-L$  curves for the fixed-hinge BC with different values of the angle  $\psi$  at the base for a fully uncoated **membrane.** The parameters are the same as in Figure 2d except that the angle at the base is varied.



Figure S7:  $F-L$  curves for a partially coated membrane with different values of  $\alpha$  that controls the sharpness of the **coating edge.** The parameters are the same as in Figure 4a and b except that the parameter  $\alpha$  that controls the sharpness of the coating edge is varied. In the left column, the free-hinge BC is imposed at the base points  $R_b = 2R_p$ , while in the right column, the fixed-hinge BC is imposed.



Figure S8: F-L curves for a bare membrane with distributed forces. The forces are assumed to be distributed in an area of  $a_f$  near the membrane tip and pointing in the normal direction. The y-axis in (a, b) indicates the magnitude of the total force, while in  $(c,d)$  indicates the vertical component of the total force. The black curve represents the  $f$ - $L$  curve under the point force assumption. The parameters are the same as in Figure 2c and d with an additional parameter  $\alpha_f = 10/(2\pi R_p^2)$ . In the left column (a,c), the free-hinge BC is imposed at the base points  $R_b = 2R_p$ , while in the right column (b,d), the fixed-hinge BC is imposed.