# Vesicle formation induced by thermal fluctuations

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## Supporting Information Available

## Appendix

### Obtaining the phase field model

To write the Canham-Helfrich free energy equation in terms of a phase field order parameter $\phi$ we will have to first define the total and Gaussian curvatures. Having the surface normal vector $\hat{n}$ one can define then the curvature tensor

$$Q_{ij} = \nabla_i n_j, \tag{1}$$

as the normal vector $n$ changes along the surface are directly related to the curvature of a surface.

Now, using the curvature tensor $Q$ we can write the curvature $C$ and the Gaussian curvature $K$. The determinant of the curvature tensor $Q$ is always zero, but using its trace we can write the curvature[1]

$$C = \mathrm{tr}[Q]. \tag{2}$$

The Gaussian curvature is a bit more complex being

$$K = \sum_{i,j} \left[ \Big( Q_{ii}Q_{jj} - Q_{ij}^2 \Big) \frac{1-\delta_{ij}}{2} \right]. \tag{3}$$

The expression is focused on the non-diagonal elements of the tensor because it is related to the overall shape that the surface takes around a point and whether is plane, curved, or presents a saddle-splay shape.

To compute the simulations with a simple model that avoid the need of tracking the interface position we will use a phase field model. Therefore, we define an order parameter $\phi(\mathbf{x})$ that represents if the volume of fluid at the point $\mathbf{x}$ corresponds to either external or internal fluid to the vesicle. In this article, we choose the values $\phi(\mathbf{x}) = +1$ for the internal fluid of the vesicle and $\phi(\mathbf{x}) = -1$ for the external fluid. With this order parameter, we can write the curvature parameters as[2]

$$C[\phi] = \frac{\sqrt{2}}{\epsilon(1-\phi^2)} \Big( -\phi + \phi^3 - \epsilon^2 \nabla^2 \phi \Big), \tag{4}$$

and, to compute $K$, we will be using the curvature tensor written for a phase field

$$Q_{ij} = \frac{\sqrt{2}\epsilon}{1-\phi^2} \left[ \partial_i \partial_j \phi + \frac{2\phi}{1-\phi^2} \partial_i \phi \partial_j \phi \right], \tag{5}$$

where $\partial_i$ refers to a derivative and $i, j$ can be any of our cartesian coordinates $(x, y, z)$. We will be computing the Canham-Helfrich free energy as a phase field which we will split into two different contributions $F = F_{C_0} + F_G$, which consists of the Curvature energy term and the Gaussian curvature term.

The minimisation of the Canham-Helfrich free energy is computed numerically in this scheme. In this methodology the main goal is to change from a surface energy to a volumetric energy by defining an order parameter. For this we use a surface differential expressed like

$$dS = \frac{3}{4\sqrt{2}\epsilon}\left(1-\phi^2\right)^2 dV. \tag{6}$$

**Obtain $\mathbf{T_1}$ and $\mathbf{T_2}$**

The Gaussian energy term written as a phase field model involve many derivatives of the order parameter $\phi$. For simplicity, we have called them $T_1$ and $T_2$, here we have written explicitly as introduced in.[3] The various derivatives of $\phi$ are written for simplicity as $\phi_i$ where $i$ is either $x$ $y$ $z$

$$T_1 = \phi_{xx}\phi_{yy} + \phi_{xx}\phi_{zz} + \phi_{yy}\phi_{zz} - (\phi_{xy})^2 - (\phi_{xz})^2 - (\phi_{yz})^2, \tag{7}$$

and

$$\begin{aligned} T_2 = \phi_{xx}(\phi_y)^2 + &\phi_{xx}(\phi_z)^2 + \phi_{yy}(\phi_x)^2 + \phi_{yy}(\phi_z)^2 + \phi_{zz}(\phi_x)^2 + \phi_{zz}(\phi_y)^2 \\ &- 2\phi_x\phi_y\phi_{xy} - 2\phi_x\phi_z\phi_{xz} - 2\phi_y\phi_z\phi_{yz}. \end{aligned} \tag{8}$$

## References


(1) Campelo, F. *Shapes in cells. Dynamic instabilities, morphology, and curvature in biological membranes.*; Universitat de Barcelona: Spain, 2008.

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(3) Rueda-Contreras, M. D.; Gallen, A. F.; Romero-Arias, J. R.; Hernandez-Machado, A.;

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