Vesicle dynamics in external flows

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Experiments:
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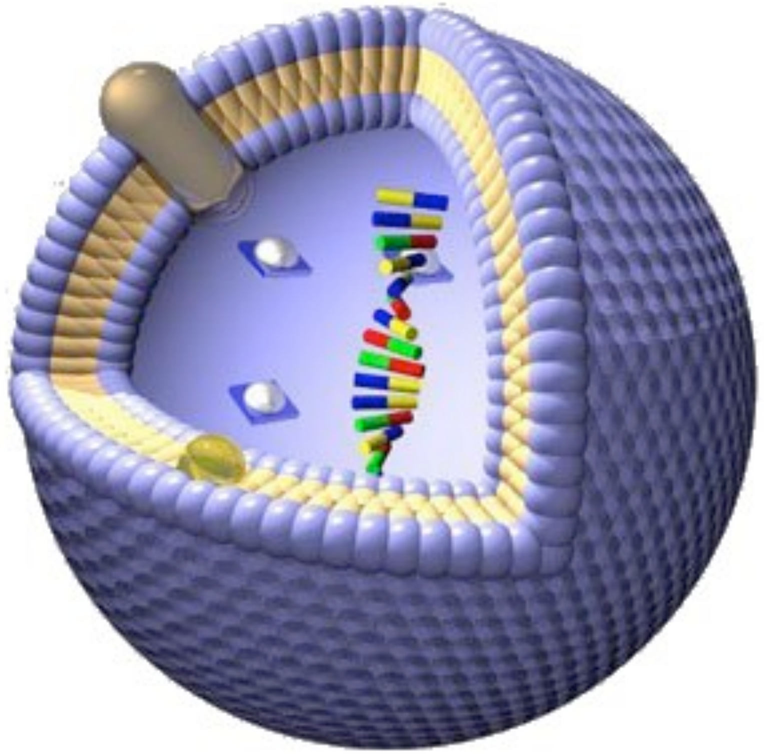
V. Lebedev, K. Turitsyn, S. Vergeles, *New J. Phys.* 10, 043044 (2008)
K. Turitsyn, S. Vergeles, *Phys. Rev. Lett.* 100, 028103 (2008)
V. Lebedev, K. Turitsyn, S. Vergeles, *Phys. Rev. Lett.* 99, 218101 (2007)

Outline

- Introduction: membranes and vesicles
- Experimental observations
- Theoretical models
- Results
- Challenges

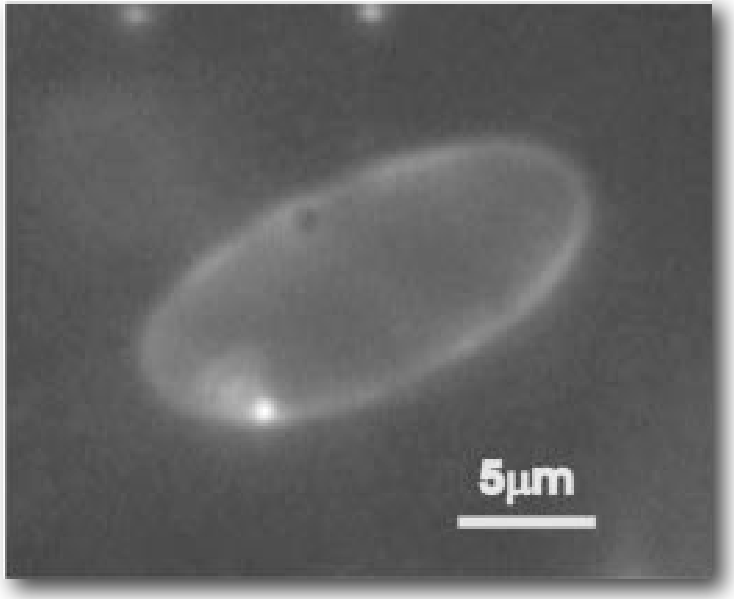
Biological vesicles

Biological vesicles are closed compartments of lipid bilayer. They are a basic tool of the cell for organizing metabolism, transport, enzyme storage, as well as being chemical reaction chambers.



Giant Unilamellar Vesicles

- Large compared to biological vesicles
- Lipid bilayer:
  - Unilamellar
  - No proteins
  - Liquid phase
  - incompressible
  - Impermeable to surrounding fluids
- Have non-zero excess area
- Different liquids inside and outside



Experimental pictures from
*V. Kantsler, V. Steinberg, PRL **95**, 258101 (2005)*
*V. Kantsler, V. Steinberg, PRL **96**, 036001 (2006)*
*V. Kantsler, E. Segre, V. Steinberg, PRL **99**, 178102 (2007)*
*V. Kantsler, E. Segre, V. Steinberg, PRL **101**, 048101 (2008)*

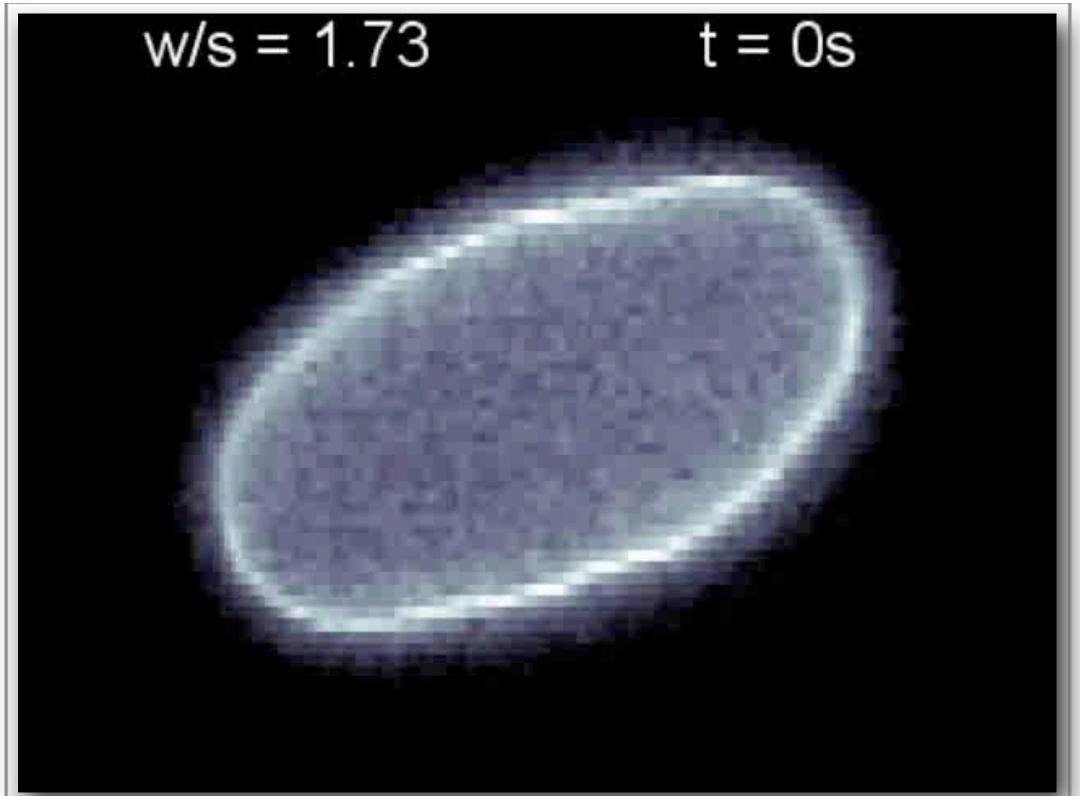
Dynamics in flows

Multiple types of vesicle behavior were observed in external flows:

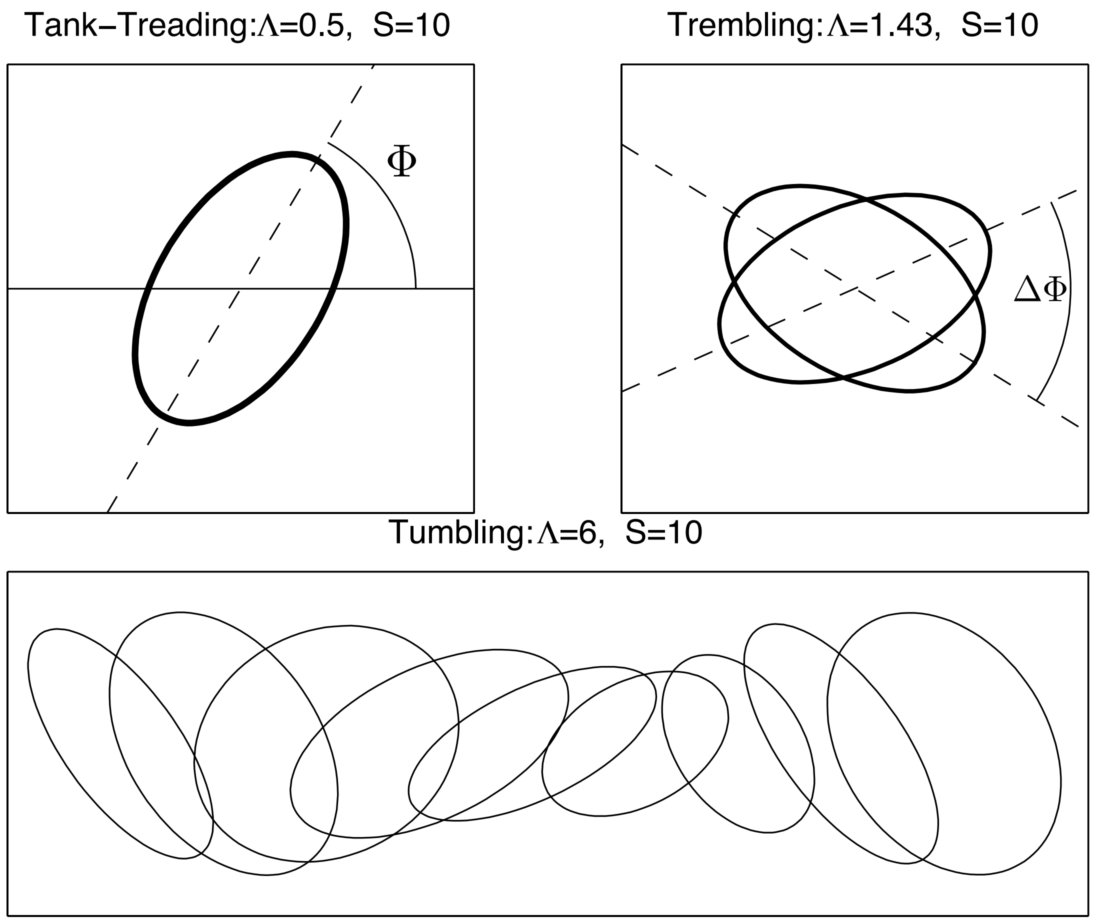
- Tumbling, Trembling, and Tank-Treading motions in stationary shear-type flows
- Membrane wrinkling in time-dependent extensional flows
- Stretching transition in strong extensional flows

Stationary flow experiment

A vesicle placed in planar flow can experience three types of motion (ω - vorticity, s - strain rate):



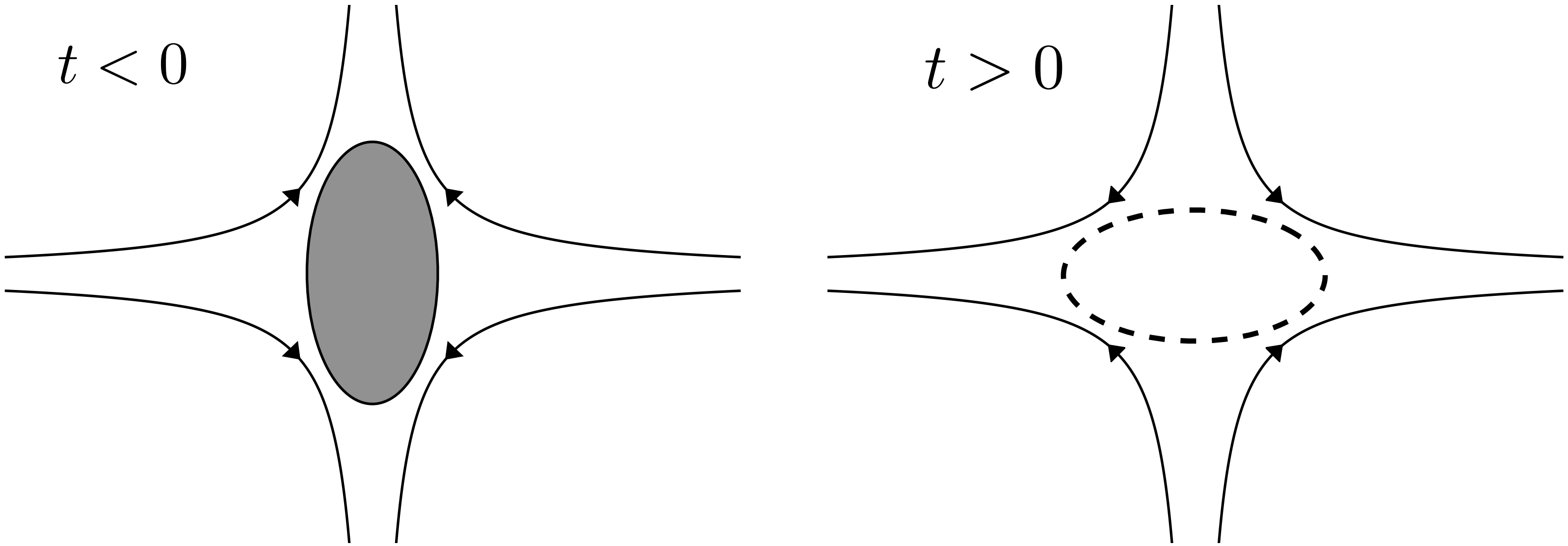
Three different regimes



Wrinkling Experiment 1

Vesicle is immersed in non-stationary extensional flow with

$$\partial_x V_x = -\partial_y V_y = -S\,\mathrm{sign}(t)$$

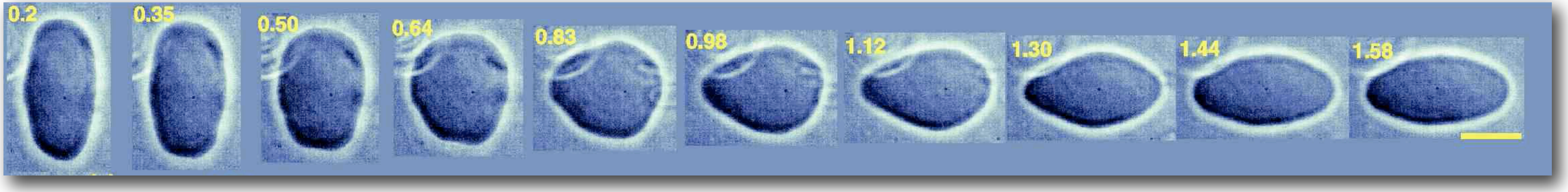


After the switch of the flow direction the vesicle starts its relaxation to a new stationary state

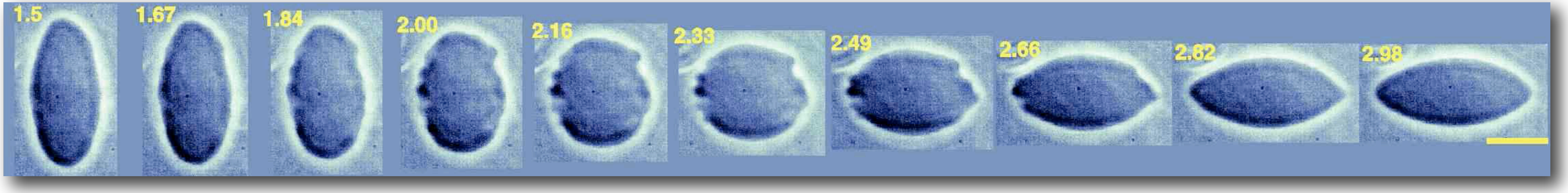
Wrinkling Experiment 2

Transitional dynamics of a vesicle significantly depends on the strength of the flow.

In weak flows the shape of vesicle remains smooth:

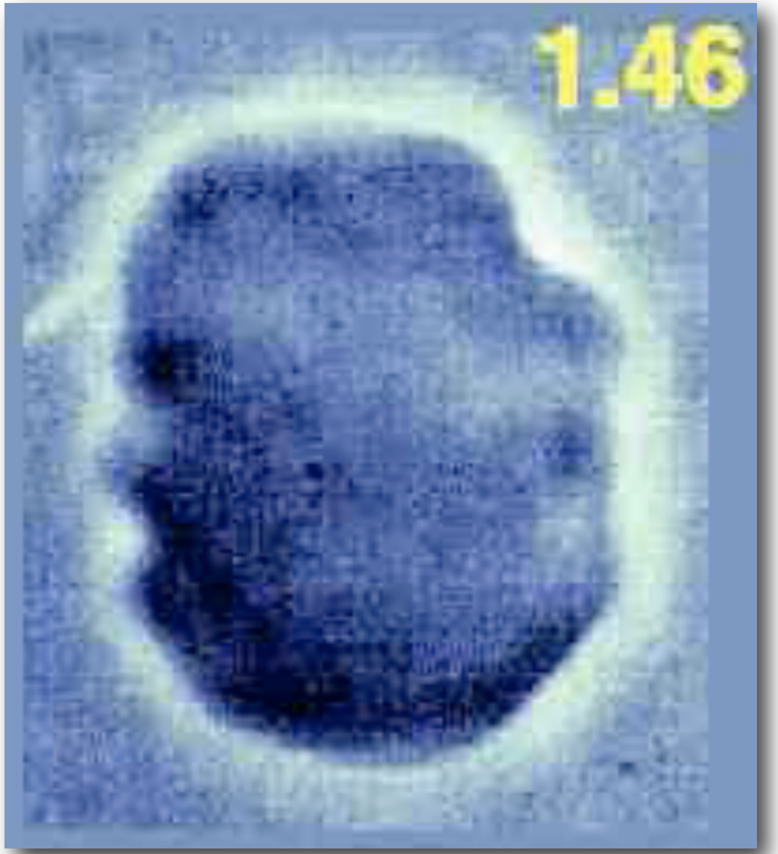


In strong flows wrinkles are formed on the membrane:



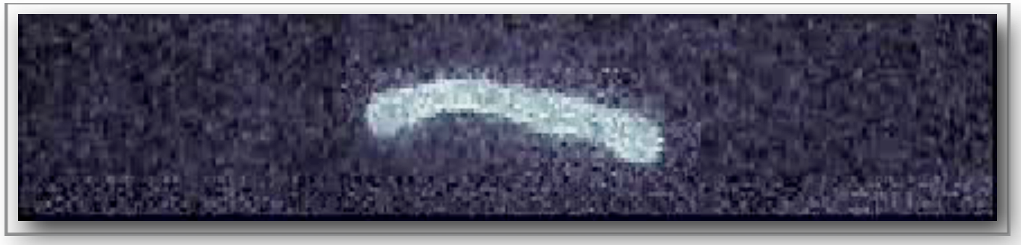
Wrinkles

- Wrinkles appear only in strong flows
- Their wavelength is much smaller than the vesicle size, and depends on the flow strength
- Wrinkles disappear when the vesicle reaches its new stationary state
- Similar membrane deformations have been observed in budding-fission experiments (*Solon et.al., PRL, 06*)



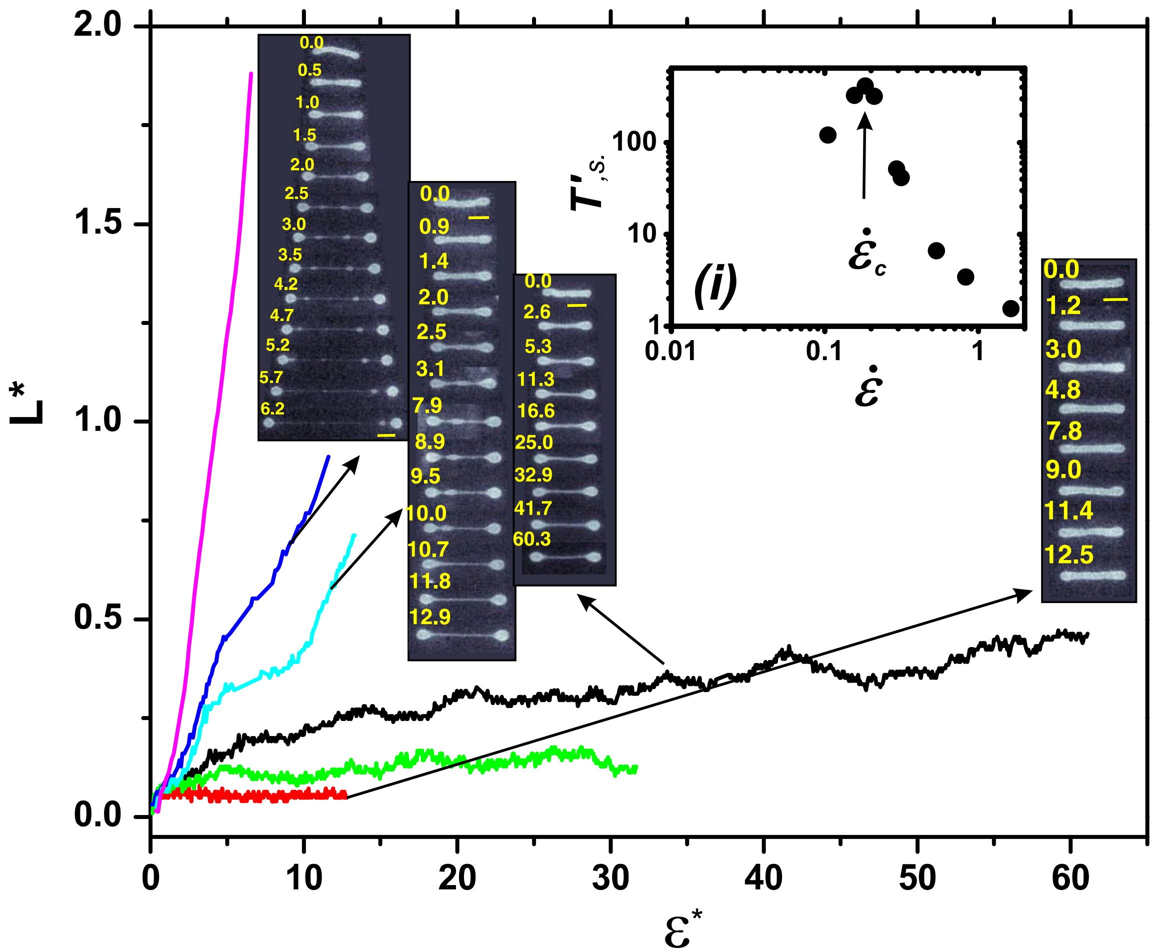
Stretching Transition

In strong elongational flows tubular vesicles are transformed into dumbbells and experience pearling instability.



Stretching: Critical slowdown

Vesicle relaxation is slowed down in the vicinity of the critical strain rate



Vesicle membrane

- Two-dimensional incompressible liquid
- Rigid with respect to bending deformations
- Surface tension is not constant, but rather an adjusting quantity similar to pressure
- Impermeability and incompressibility implies the conservation of excess area Δ

$$A = (4\pi + \Delta)R^2 \qquad V = (4\pi/3)\,R^3$$

Theoretical description

- 3d Stokes equation inside and outside with membrane stresses as boundary conditions
- 2d Stokes equation on the membrane
- Nonlinear and Nonlocal (integral) boundary equations describe the dynamics

Parameters

- Viscosity ratio $\tilde{\eta}/\eta \approx 0.5 \div 5$
- Membrane viscosity $\zeta/\eta R \ll 1$
- Excess area $\Delta \approx 0.1 \div 5$
- Strain rate $s\eta R^3/\kappa \approx 0.1 \div 100$
- Relative vorticity $\omega/s \approx 0.1 \div 10$
- Temperature $T/\kappa \approx 0.05 \ll 1$

Quasi-spherical vesicles

Equations are strongly simplified for $\Delta \ll 1$

Vesicle shape is parameterized as $r = R(1+u)$

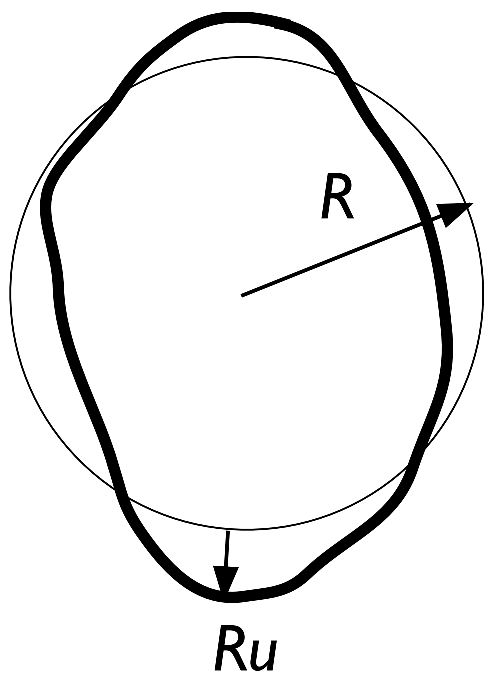
$$u(t,\theta,\phi) = \sum u_{lm}(t) Y_{lm}(\theta,\phi)$$

Excess area conservation law:

$$\sum |u_{lm}|^2 = \Delta$$

Spectral distribution:

$$\Delta_l = \sum_m |u_{lm}|^2$$



Dynamical equations

Vesicle dynamic is described by

$$\hat{a}(\partial_t - \omega\partial_\varphi)u = 10 s_{ij}\frac{r_i r_j}{r^2} - \frac{1}{\eta r_0^3}\frac{\delta\mathcal{F}}{\delta u}$$

where $\mathcal{F} = \int dA\left(\sigma + \frac{\kappa}{2}H^2\right)$

In the leading order over $\sqrt{\Delta}$ only the second order harmonics is excited:

$$u = \frac{\sqrt{5\Delta}}{4\sqrt{2\pi}}\left[\frac{\sin\Theta}{\sqrt{3}}(1 - 3\cos^2\theta) + \cos\Theta\sin^2\theta\cos(2\varphi - 2\Phi)\right]$$

$$a = \frac{16}{3}\left(1 + \frac{23}{32}\frac{\tilde{\eta}}{\eta} + \frac{\zeta}{2\eta r_0}\right)$$

Dynamical equations 2

The resulting system of equations:

$$\tau\dot{\Phi} = \tfrac{S}{2}\left[\frac{\cos(2\Phi)}{\cos\Theta} - \Lambda\right],$$

$$\tau\dot{\Theta} = -S\sin\Theta\sin(2\Phi) + \cos(3\Theta)$$

where $\tau = \frac{7\sqrt{\pi}}{12\sqrt{10}}\frac{a\eta r_0^3}{\kappa\sqrt{\Delta}}$ and

$$S = \frac{14\pi}{3\sqrt{3}}\frac{s\eta r_0^3}{\kappa\Delta},$$

$$\Lambda = \frac{\sqrt{3}}{4\sqrt{10\pi}}\frac{\sqrt{\Delta}\,a\omega}{s}.$$

Only two parameters left!

“Linear” equations

Without high-order free energy corrections, equations have the following form:

$$\tau\dot{\Theta} = -S\sin\Theta\sin 2\Phi$$
$$\tau\dot{\Phi} = S\left(\frac{\cos 2\Phi}{\cos\Theta} - \Lambda\right)$$

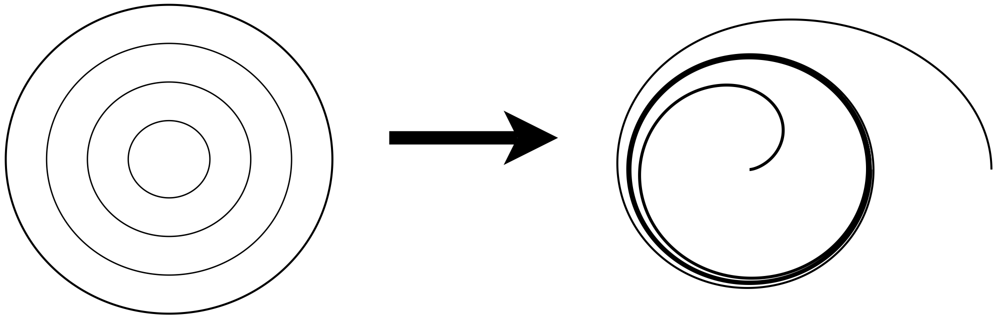
They possess an integral of motion

$$\partial_t \sin\Theta/(\Lambda - \cos\Theta\cos 2\Phi) = 0$$

Long-time behavior depends on initial conditions!

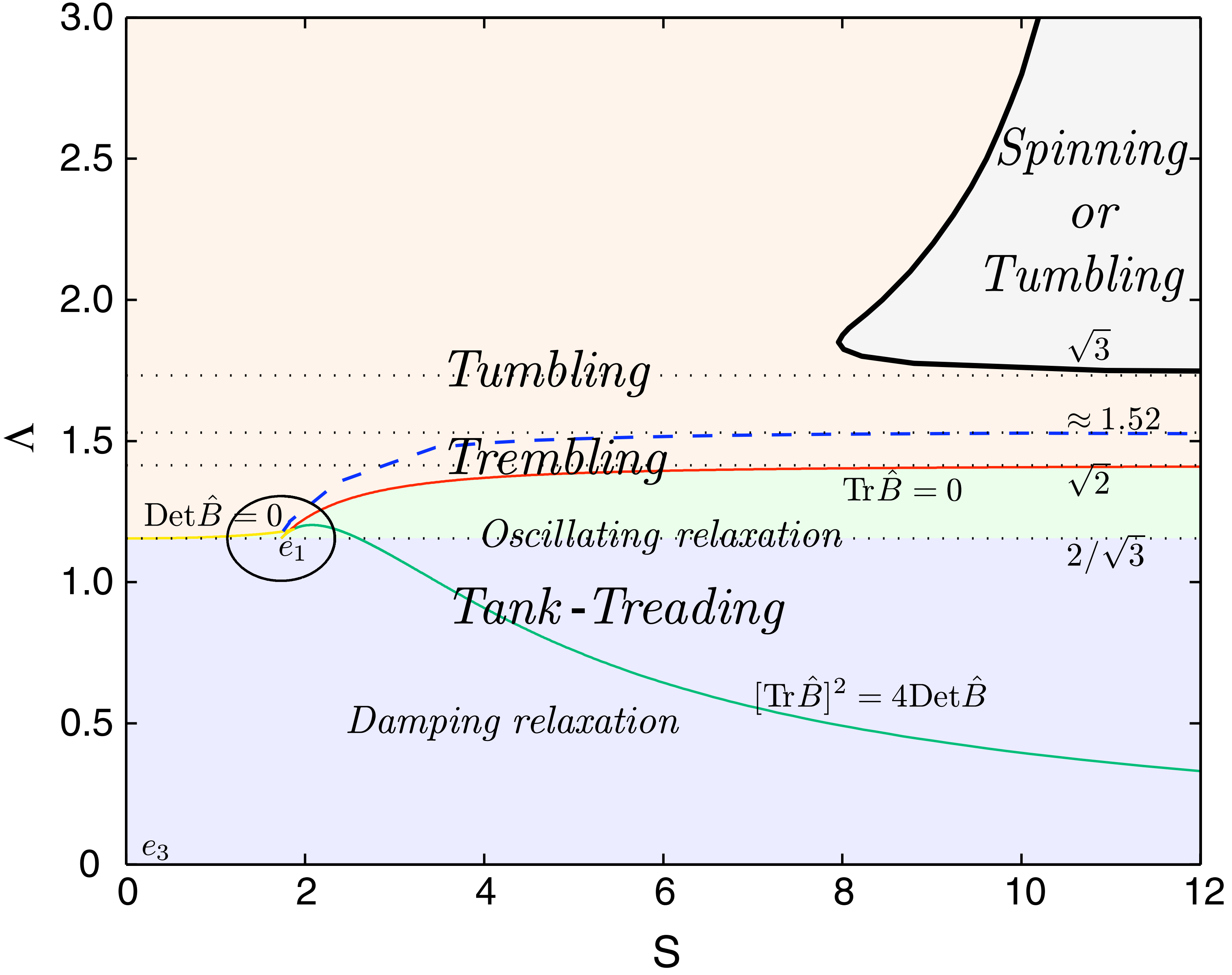
“Nonlinear” corrections

Small non-linear corrections coming from the membrane free energy break integrability and produce limit cycles.

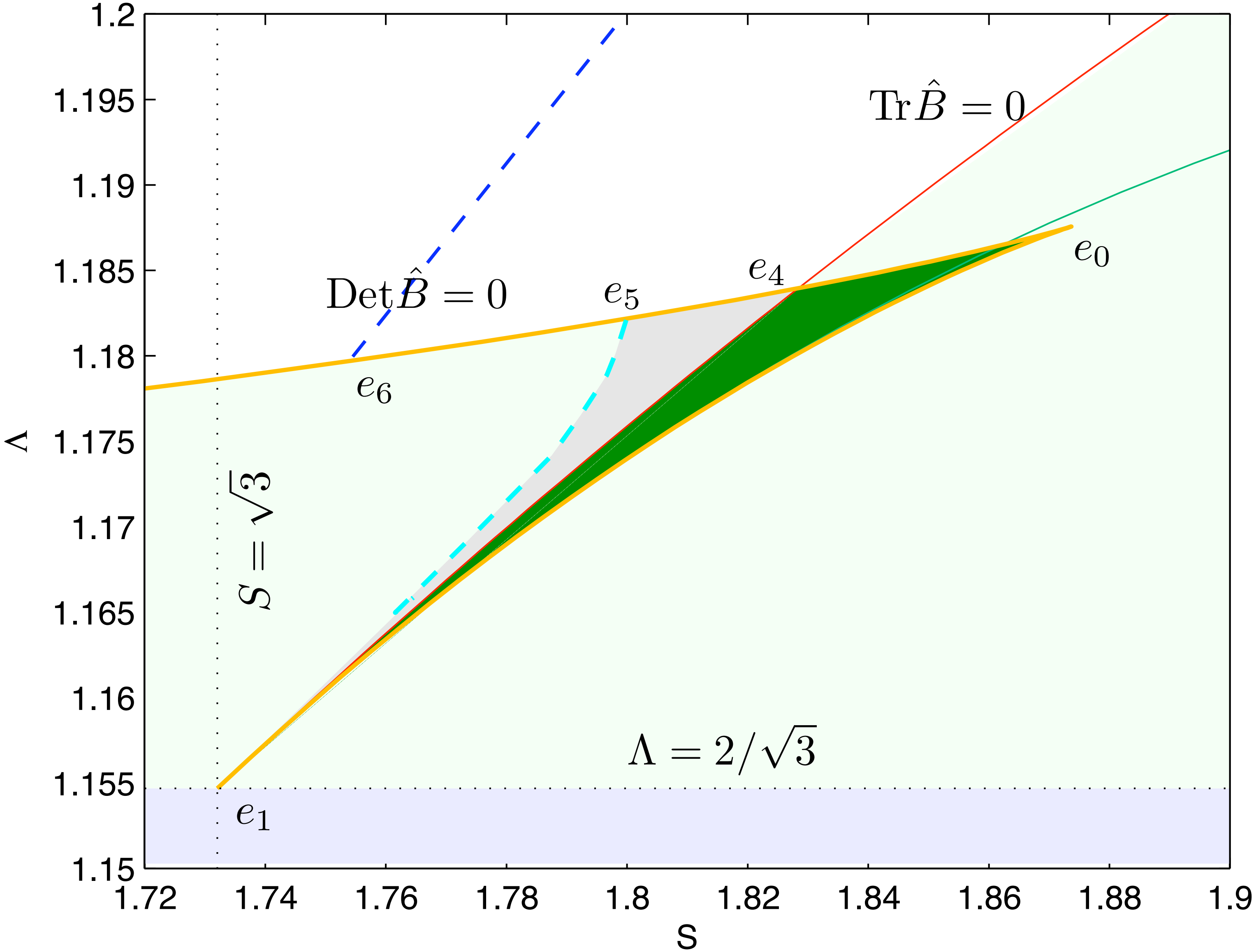


For $S \gg 1$ there are two time-scales in the problem.

Phase diagram 1



Phase Diagram 2



Critical slowdown

Vesicle dynamics is significantly slowed down in the vicinity of critical points:

- Trembling cycles: $T \sim \dfrac{\tau}{(S-\sqrt{3})^{1/2}}$
- Tumbling cycles: $T \sim \dfrac{\tau}{(S-S_c)^{1/4}\delta\Lambda^{1/2}}$
- For strong thermal fluctuations: $T \sim \dfrac{\tau}{(S-S_c)^{1/3}D^{1/3}}$

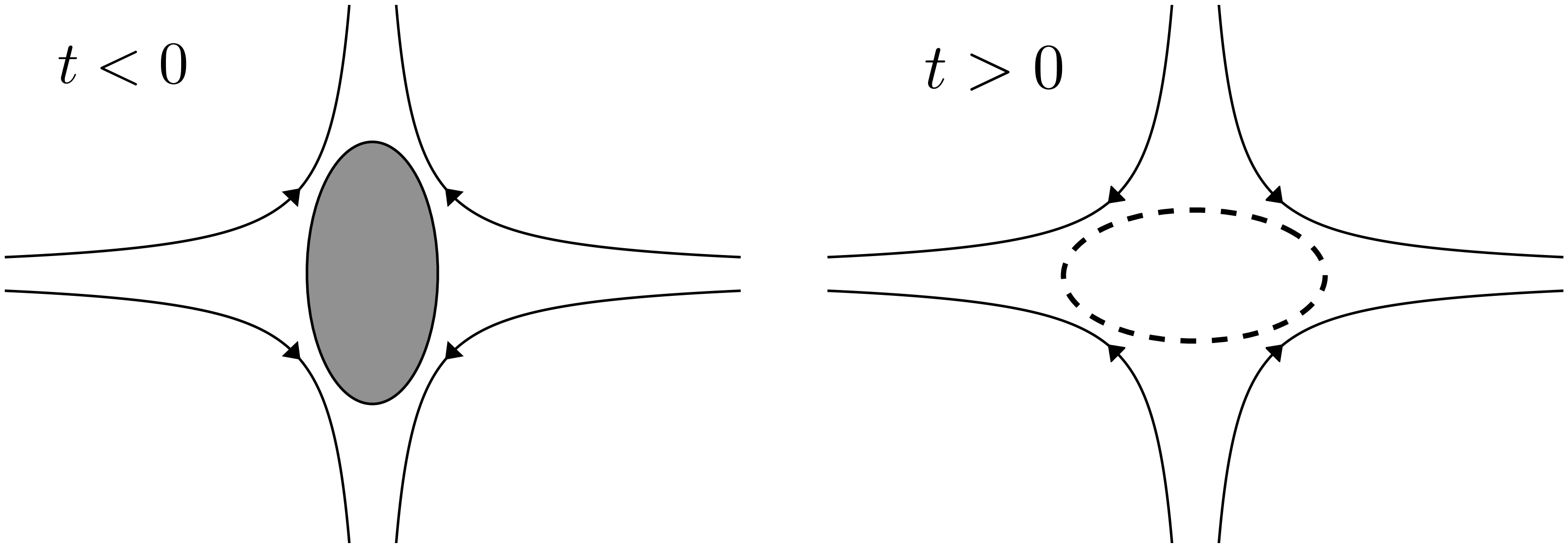
Key results

- Self-similarity of effective equations
- Complicated phase-diagram
- Multiple time-scales of the problem
- Critical slowdown

Wrinkling Experiment 1

Vesicle is immersed in non-stationary extensional flow with

$$\partial_x V_x = -\partial_y V_y = -S\,\mathrm{sign}(t)$$



After the switch of the flow direction the vesicle starts its relaxation to a new stationary state

Dynamical equations

Quasi-spherical vesicle dynamics is described by

$$\tau \dot{u}_{lm} = S(t)\delta_{l2}\delta_{m2} - (\Gamma_l + A_l\sigma)u_{lm}$$

Where $\tau = \kappa/(\eta R^3)$ is the characteristic relaxation time. $\sigma(t)$ is the average surface tension. It is a Lagrange multiplier which ensures the excess area conservation. It makes the equations strongly nonlinear!

$$\Gamma_l = \frac{(l-1)l^2(l+1)^2(l+2)}{(2l+1)(2l^2+2l-1)} \sim l^3/4, \quad l \gg 1$$

$$A_l = \frac{l(l+1)(l^2+l-2)}{(2l+1)(2l^2+2l-1)} \sim l/4$$

Surface tension and Buckling Instability

Surface tension is completely determined by the membrane shape:

$$\sigma = \frac{S(t)\mathrm{Re}[u_{22}] - \bar{\Gamma}}{\bar{A}}$$

$$\bar{\Gamma} = \sum \Gamma_l |u_{lm}|^2 \qquad \bar{A} = \sum A_l |u_{lm}|^2$$

After switching the external velocity, the surface tension becomes instantly negative:

$$\sigma(+0) = -S/A_2$$

Most unstable mode corresponds to $l_0 = \sqrt{|S|/3A_2}, \quad l \gg 1$

First stage

During the first stage of the dynamics high order harmonics grow exponentially while surface tension remains constant. The distribution is centered near $l_0 \sim \sqrt{S} \gg 1$. This stage ends when the contribution of high order harmonics to the surface tension becomes dominant:

$$(1 - |u_{22}|^2) \sim A_2/\bar{\Gamma} \sim S^{-1/2} \ll 1$$

Duration of this stage can be estimated as $\tau/S^{3/2}$

It is much smaller compared to the characteristic timescale τ/S associated with the dynamics of u_{22}.

Second stage

During the second stage the value of surface tension is completely determined by high order harmonics: $\sigma = -\bar{\Gamma}/\bar{A}$

Formal solution of the dynamical equation has the form

$$u_{lm}(t) = C(t)\exp(-\Gamma_l t/\tau + A_l \rho) \qquad \rho = -\int_0^t dt' \sigma(t')/\tau$$

Spectral distribution Δ_l is narrow, peaked at $l_* = \sqrt{\rho/3t}$

This yields a closed equation $\dot{\rho} = -\sigma/\tau = l_*^2 = \rho/3t$

With formal solution $\rho = c(t/\tau)^{1/3}$

Surface tension decays as $\sigma \sim (t/\tau)^{-2/3}$ and the wavelength grows as $\lambda = R/l_* \sim R(t/\tau)^{1/3}$

Third Stage

During the last stage vesicle orientation changes significantly. Due to significant decrease of surface tension the dynamics of u_{22} is trivial: $u_{22} = 1 - St/\tau$

Using the ansatz $\rho(t) = S^{1/3} f(St/\tau)$ one obtains

$$\frac{df(x)}{dx} = \frac{f(x)}{3x} + 4\frac{1-x}{2-x}\sqrt{\frac{3}{xf(x)}}$$

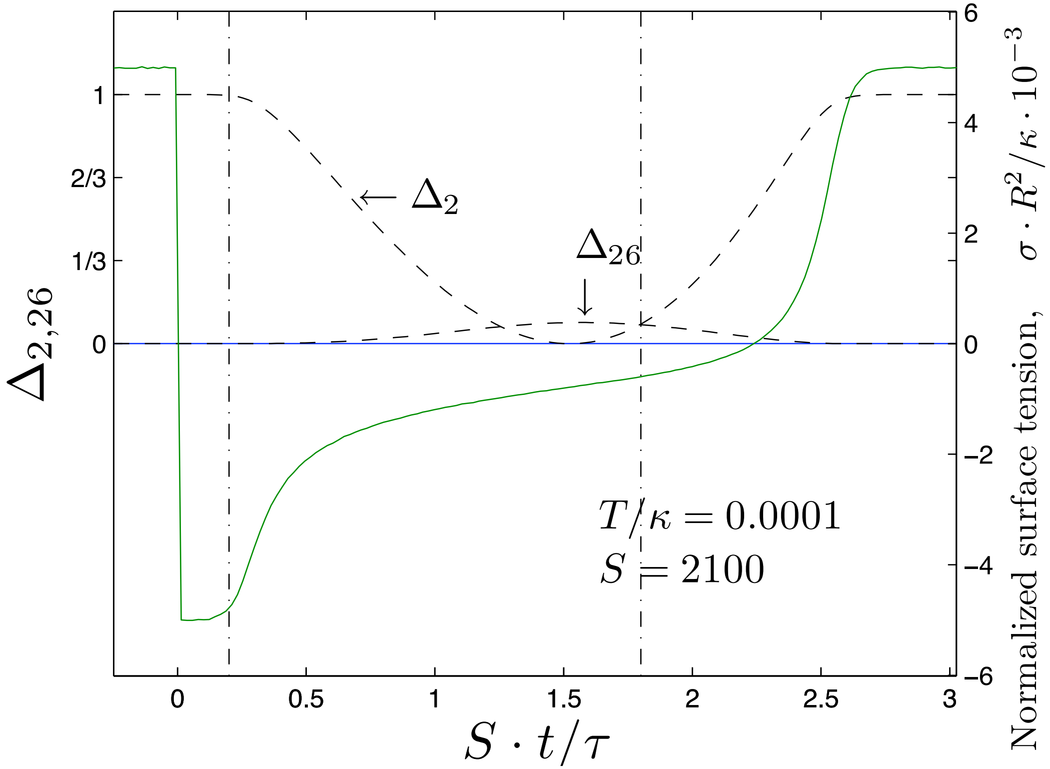
Thus, $f(x) = x^{1/3} \left[\log C\sqrt{S}x(2-x)\right]^{2/3}$

Maximal amplitude of wrinkles is achieved at $t = \tau/S$

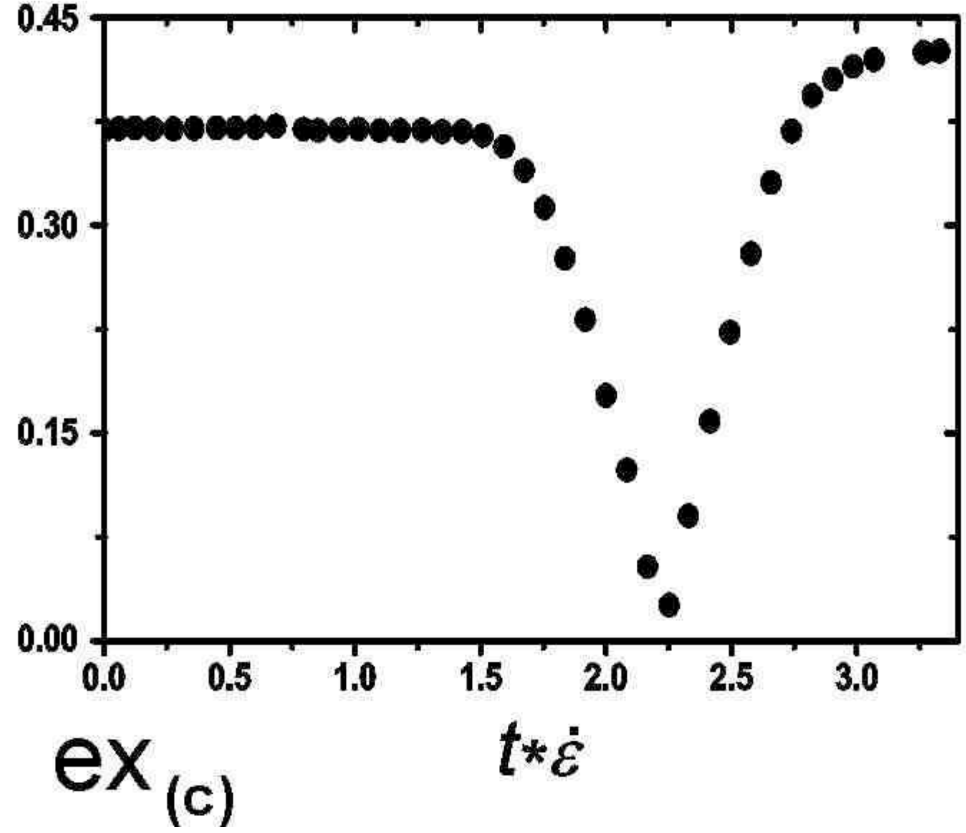
At this moment their wavelength is estimated as

$$\lambda = R/l_* \sim R\,(S\log S)^{-1/3}$$

Numerics vs experiment



Temporal dynamics



Dynamics of second harmonic excess area

Conclusions

- Vesicle membrane can experience buckling instability during the transient dynamics.
- Wrinkles wavelength smoothly grows to
$$\lambda_* \sim R(S \log S)^{-1/3}$$
- During the second stage evolution is characterized by the universal laws:
$$\lambda \propto (t/\tau)^{1/3}, \quad \sigma \propto (t/\tau)^{-2/3}$$

Challenges

- Rheology of vesicular solutions. Resonances in periodic flows ?
- Effect of membrane inclusions. Proteins, lipid rafts, multiphase membranes etc.
- Biologically relevant processes. Transport along membrane nanotubes (*Davis et. al., Nat. Rev. Mol. Cell. Bio. 2008*)
- Soft matter machines, swimming vesicles (*R. Lipowsky, 99*)