Statistical physics of polymerized membranes

D. Mouhanna

LPTMC - UPMC - Paris 6

J.-P. Kownacki (LPTM - Univ. Cergy-Pontoise, France)
K. Essafi (OIST, Okinawa, Japan)
O. Coquand (LPTMC- Univ. Paris 6)

Functional Renormalization - from quantum gravity and dark energy to ultracold atoms and condensed matter

IWH Heidelberg, March 7-10 2017

Outline

Introduction

- membranes: D-dimensional extended objects embedded in a d-dimensional space subject to quantum and/or thermal fluctuations

- fluctuating membranes / random surfaces occur in several domains:

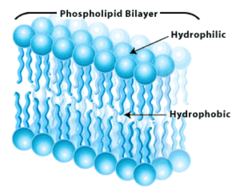
- chemical physics / biology :

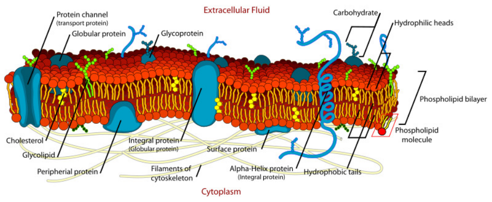
(Aronovitz - Lubensky, Helfrich, David - Guitter, Le Doussal - Radzihovsky, Nelson - Peliti,'70's- 90's)

$\Longrightarrow$ structures made of amphiphile molecules (ex: phospholipid)

- one hydrophilic head
- hydrophobic tails

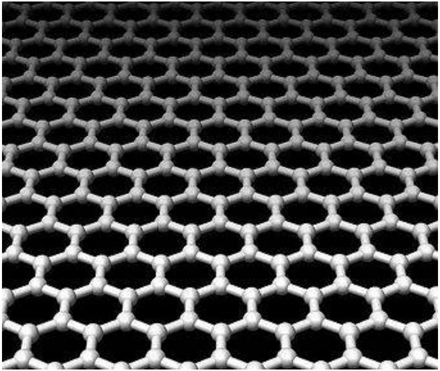
$\Longrightarrow$ bilayers:





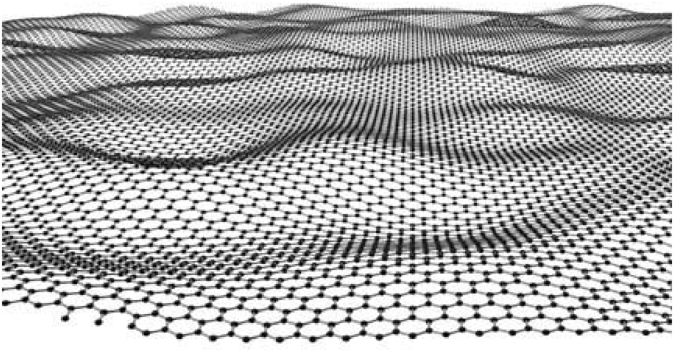
- condensed matter physics: graphene, silicene, phosphorene ...

  uni-layers of atoms located on a honeycomb lattice
- striking properties:
  - high electronic mobility, transmittance, conductivity,...



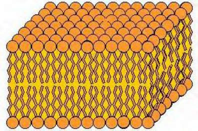
- mechanical properties: both extremely strong and soft material:

  $\Longrightarrow$ example of genuine 2D fluctuating membrane



Fluid *vs* polymerized membranes

Properties of fluid membranes



- very weak interaction between molecules
  $\Longrightarrow$ free diffusion inside the membrane plane
  $\Longrightarrow$ no shear modulus

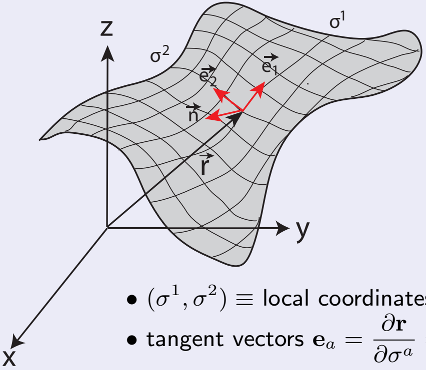
- very small compressibility and elasticity

$\Longrightarrow$ main contribution to the energy: *bending energy*

Energy:

- point of the surface described by the embedding:

$\mathbf{r}$: $\boldsymbol{\sigma} = (\sigma^1, \sigma^2) \to \mathbf{r}(\sigma^1, \sigma^2) \in \mathbb{R}^d$



- $(\sigma^1, \sigma^2) \equiv$ local coordinates on the membrane
- tangent vectors $\mathbf{e}_a = \dfrac{\partial \mathbf{r}}{\partial \sigma^a} = \partial_a \mathbf{r} \qquad a = 1, 2$
- a unit norm vector normal to $(\mathbf{e}_1, \mathbf{e}_2)$: $\hat{\mathbf{n}} = \dfrac{\mathbf{e}_1 \times \mathbf{e}_2}{|\mathbf{e}_1 \times \mathbf{e}_2|}$

- curvature tensor $\mathbf{K}$: $K_{ab} = -\hat{\mathbf{n}}.\,\partial_b \mathbf{e}_a = \mathbf{e}_a.\,\partial_b \hat{\mathbf{n}}$
- K_{ab} can be locally diagonalized with eigenvalues K_1 and K_2
    - mean or *extrinsic* curvature:

$$H = \frac{1}{2}(K_1 + K_2) = \frac{1}{2}\mathrm{Tr}\,\mathbf{K}$$

    - Gaussian or *intrinsic* curvature: $K = K_1\, K_2 = \det K_a{}^b$
      $\Rightarrow$ no role in fixed topology (Gauss-Bonnet theorem)

$\Longrightarrow$ bending energy:

$$F = \frac{\kappa}{2}\int d^2\boldsymbol{\sigma}\,\sqrt{g}\; H^2$$

- $g_{\mu\nu} = \partial_\mu \mathbf{r}.\partial_\nu \mathbf{r} \equiv$ metric induced by the embedding $\mathbf{r}(\boldsymbol{\sigma})$
- $\sqrt{g}$ ensures reparametrization invariance of F

Low-temperature fluctuations in fluid membranes

- a remark: with $\partial_a \hat{\mathbf{n}} = K_{ab}\ \mathbf{e}^b$ one has:

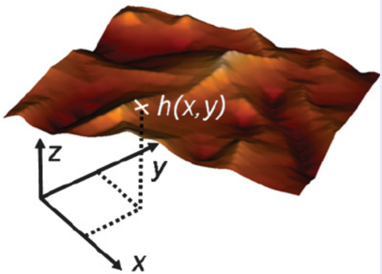
$$F = \frac{\kappa}{2} \int d^2\boldsymbol{\sigma}\ (\partial_a \hat{\mathbf{n}})^2 \quad \text{or} \quad F = -\frac{\kappa'}{2} \sum_{\langle i,j \rangle} \hat{\mathbf{n}}_i . \hat{\mathbf{n}}_j$$

where $\hat{\mathbf{n}}_i$ is a unit normal vector on the plaquette i

- very close to a $O(N)$ nonlinear σ-model / Heisenberg spin system:

- with (rigidity) coupling constant κ
- with "spins" living on a fluctuating surface
- with d playing the role of the number of components N

- Low temperature: Monge parametrization
  $x = \sigma_1$, $y = \sigma_2$ and $z = h(x, y)$ with *h* height, capillary mode



- $\mathbf{r}(x, y) = (x, y, h(x, y))$
- $\hat{\mathbf{n}}(x, y) = \dfrac{(-\partial_x h, -\partial_y h, 1)}{\sqrt{1 + |\boldsymbol{\nabla} h|^2}}$
- $\hat{\mathbf{n}}(x, y).\,\mathbf{e_z} = \cos\theta(x, y) = \dfrac{1}{\sqrt{1 + |\boldsymbol{\nabla} h|^2}}$

- Free energy:

$$F \simeq \frac{\kappa}{2} \int d^2\mathbf{x} \; (\Delta h)^2 + \mathcal{O}(h^4)$$

- flat phase ? $\Longrightarrow$ fluctuations of $\theta(x,y)$?

$$\langle \theta(x,y)^2 \rangle = k_B T \int d^2 q \; \frac{1}{\kappa \, q^2} \simeq \frac{k_B T}{\kappa} \ln\left(\frac{L}{a}\right) \to \infty$$

$\Longrightarrow$ no long-range order between the normals

At next order in h, κ is renormalized and decreased at long distances.:

$$\kappa_R(q) = \kappa - \frac{3k_BT}{2\pi}\left(\frac{d}{2}\right)\ \ln\left(\frac{1}{qa}\right)$$

$\Longrightarrow$ divergence of $\langle\theta(x,y)^2\rangle$: worse

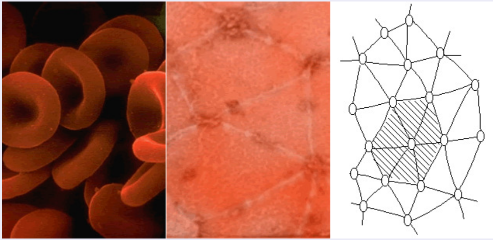
$\Longrightarrow$ strong analogy with 2D-NLσ model:

- correlations: $\langle \hat{\mathbf{n}}(\mathbf{r}).\hat{\mathbf{n}}(\mathbf{0})\rangle \sim e^{-r/\xi}$
- correlation length – mass gap: $\xi \simeq a\, e^{4\pi\kappa/3k_BTd}$
- $d/2 \Longrightarrow N-2$
- nothing really new . . .

Polymerized membranes

ex:

- organic: red blood cell, . . .
- inorganic: graphene, phosphorene, . . .

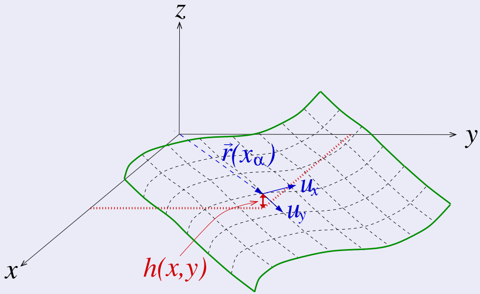


- made of molecules linked by $V(|\mathbf{r_i} - \mathbf{r_j}|)$

$\Longrightarrow$ free energy built from both bending and elastic energy

Free energy and low-temperature fluctuations in polymerized membranes

- reference configuration: $\mathbf{r}_0(x,y) = (x, y, z=0)$
- fluctuations: $\mathbf{r}(x,y) = \mathbf{r}_0 + u_x\,\mathbf{e}_1 + u_y\,\mathbf{e}_2 + h\,\hat{\mathbf{n}}$



stress tensor: $u_{ab} = \frac{1}{2}\left(\partial_a \mathbf{r}.\partial_b \mathbf{r} - \partial_a \mathbf{r}_0.\partial_b \mathbf{r}_0\right) = \frac{1}{2}\left(\partial_a \mathbf{r}.\partial_b \mathbf{r} - \delta_{ab}\right)$

$$\Longrightarrow \; u_{ab} = \frac{1}{2}\left[\partial_a u_b + \partial_b u_a + \partial_a \mathbf{u}.\partial_b \mathbf{u} + \partial_a h\, \partial_b h\right]$$

- u_ν describes the longitudinal – phonon-like – degrees of freedom
- h describes height, capillary – degrees of freedom

- free energy:

$$F \simeq \int d^2\mathbf{x} \; \left[\frac{\kappa}{2}(\Delta h)^2 + \mu (u_{ab})^2 + \frac{\lambda}{2}(u_{ab})^2\right]$$

$\kappa \equiv$ bending rigidity $\quad \lambda,\, \mu \equiv$ elastic coupling constants

- non-trivial coupling between longitudinal - in plane - and height fluctuations $\Longrightarrow$ *frustration* of height fluctuations

Gaussian approximation on phonon fields:

$$u_{ab} \simeq \frac{1}{2}\left[\partial_a u_b + \partial_b u_a + \partial_a h\, \partial_b h\right]$$

integrate over u:

$$F_{eff} = \frac{\kappa}{2}\int d^2\mathbf{x}\ (\Delta h)^2 + \frac{\mathcal{K}}{8}\int d^2\mathbf{x}\left(P^T_{ab}\,\partial_a h\,\partial_b h\right)^2$$

- $P^T_{ab} = \delta_{ab} - \partial_a\partial_b/\nabla^2$
- κ bending, rigidity coupling constant
- $\mathcal{K} = 4\mu(\lambda+\mu)/(2\mu+\lambda)$: Young elasticity modulus

- Self-consistent screening approximation (SCSA)
  $\sim$ Schwinger-Dyson equation closed at large d

$$\kappa_{eff}(\mathbf{q}) = \kappa + k_B T \mathcal{K} \int d^2k \frac{\left[\hat{q}_a\, P^T_{ab}\, \hat{q}_b\right]^2}{\kappa_{eff}(\mathbf{q}+\mathbf{k})|\mathbf{q}+\mathbf{k}|^4}$$

$$\Longrightarrow \kappa_{eff}(\mathbf{q}) \sim \frac{\sqrt{k_B T \mathcal{K}}}{q}$$ rigidity increased by fluctuations !

- normal fluctuations:

$$\langle \theta(x,y)^2 \rangle = k_B T \int d^2q \, \frac{1}{\kappa_{eff}(\mathbf{q}) q^2} < \infty!$$

$\Longrightarrow$ Long-range order between normals even in $D = 2$!

- polymerized membranes $\Longrightarrow$ possibility of spontaneous symmetry breaking in $D = 2$ and even in $D < 2$

$\Longrightarrow$ low-temperature - flat - phase with non-trivial correlations in the I.R.

$$\begin{cases} G_{hh}(\mathbf{q}) \sim q^{-(4-\eta)} \\ \\ G_{uu}(\mathbf{q}) \sim q^{-(6-D-2\eta)} \end{cases}$$

with $\eta \neq 0 \Longrightarrow$ associated *e.g.* to stable sheet of graphene

Perturbative approach of the flat phase

(Aronovitz and Lubensky'88)

- Field theory of the flat phase:

$$F \simeq \int d^2\mathbf{x} \left[\frac{\kappa}{2}(\Delta h)^2 + \mu(u_{ab})^2 + \frac{\lambda}{2}(u_{aa})^2\right]$$

$\Longrightarrow$ perturbative expansion in $\bar{\lambda} \equiv \lambda/\kappa^2$ and $\bar{\mu} \equiv \mu/\kappa^2$ in $D_{uc} = 4 - \epsilon$

- non-trivial fixed point governs the flat phase
- increasing rigidity $\kappa_{eff}(\mathbf{q}) \sim q^{-\eta} \Longrightarrow$ orientational order $\nearrow$
- decreasing elasticity $\mathcal{K}_{eff}(\mathbf{q}) \sim q^{\eta} \Longrightarrow$ positional disorder $\searrow$

$\simeq$ ripples formation

However:

- flat phase properties: very poorly determined in $D = 2$ because $D_{uc} = 4$
- SCSA or weak-coupling tedious beyond leading order due to
  - derivative interaction
  - multiplicity of fields: h, u
  - propagator structure:

Capillary modes: $G_{\alpha\beta}(q^2) = \dfrac{\delta_{\alpha\beta}}{\kappa\, q^4}$

Phonon modes: $G_{ij}(q^2) = G_1(q^2)\left[\delta_{ij} - \frac{q_i\, q_j}{q^2}\right] + G_2(q^2)\,\frac{q_i\, q_j}{q^2}$

with:

$$
\begin{aligned}
G_1(q^2) &= \frac{1}{\kappa\, q^4 + \zeta^2\, \mu\, q^2} \\
G_2(q^2) &= \frac{1}{\kappa\, q^4 + \zeta^2\, (2\mu + \lambda)\, q^2}
\end{aligned}
$$

FRG approach to polymerized membranes

(Kownacki and D.M.'08, Essafi, Kownacki and D.M.'14, Coquand and D.M.'16)

- Effective action: $\Gamma_k[\partial_\mu \mathbf{r}]$ expanded around the flat phase configuration:

$$\mathbf{r}(\mathbf{x}) = \zeta \sum_{\alpha=1}^{D} x_\alpha \, \mathbf{e}_\alpha$$

$$\begin{aligned}
\Gamma_k\left[\partial_\mu \mathbf{r}\right] \; &= \int d^D\mathbf{x} \, \frac{Z}{2} \left(\partial_\alpha \partial_\alpha \mathbf{r}\right)^2 + \\
&+ u_1 \left(\partial_\alpha \mathbf{r}.\partial_\beta \mathbf{r} - \zeta^2 \, \delta_{\alpha\beta}\right)^2 + \; u_2 \left(\partial_\alpha \mathbf{r}.\partial_\alpha \mathbf{r} - D \, \zeta^2\right)^2 \\
&+ \ldots \\
&+ \ldots \\
&+ u_{10} \left(\partial_\alpha \mathbf{r}.\partial_\beta \mathbf{r} - \zeta^2 \, \delta_{\alpha\beta}\right) \left(\partial_\beta \mathbf{r}.\partial_\gamma \mathbf{r} - \zeta^2 \, \delta_{\beta\gamma}\right) \times \\
&\qquad \left(\partial_\gamma \mathbf{r}.\partial_\delta \mathbf{r} - \zeta^2 \, \delta_{\gamma\delta}\right) \; \left(\partial_\delta \mathbf{r}.\partial_\alpha \mathbf{r} - \zeta^2 \, \delta_{\delta\alpha}\right)
\end{aligned}$$

- Flat phase: $\eta = 0.849$ (SCSA: 0.821 (Le Doussal and Radzihovsky'92)

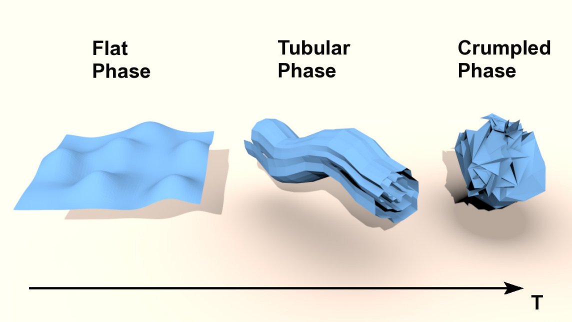
  MC computation with a interatomic potential for graphene: $\eta = 0.850$! (Los, Katsnelson, Yazyev, Zakharchenko and Fasolino'09)

- amazingly:
  - no correction beyond the leading order in field: $(\partial r)^4$! (Essafi, Kownacki and D.M.'14)
  - almost no correction beyond the leading order in field-derivatives ∂^4 ! (Braghin and Hasselmann'10)

- key point: graphene very well described by the ordered phase of a derivative-"ϕ^4-like" theory at leading order !

Extension to membranes in various physical situations :

- anisotropic membranes $\Longrightarrow$ tubular phase
  (Essafi, Kownacki and D.M.'11)
  - production of organic nanotubes
  - applications in bio- and nano-technology (drug delivery devices, electrochemical sensors, etc)



- anisotropy between the x and y directions

$$\Gamma_k[\mathbf{r}] = \int dx\ dy \left\{ \frac{Z_y}{2}(\partial_y^2 \mathbf{r})^2 + t_x(\partial_x \mathbf{r})^2 + \frac{u_y}{2}(\partial_y \mathbf{r}.\partial_y \mathbf{r} - \zeta_y^2)^2 \right\}$$

- transition between a crumpled phase with $\zeta_y = 0$ at high T and a tubular phase with $\zeta_y \neq 0$ at low T

- general phenomenon of *anisotropic scaling*: $q_\perp \propto q_y^2$
  - Lifshitz critical behaviour: disordered+homogenous ordered+ spatially modulated, phases meet together
  - Horava-Lifshitz theory/gravity: breaks Lorentz invariance

    $$S = \int dt\ d^D x \left\{ \frac{1}{2}(\partial_t \phi)^2 - \frac{1}{2}(\partial_i^{\mathbf{z}} \phi)^2 + V(\phi) \right\}$$

    $\Longrightarrow$ improves UV behaviour

Upper critical dimension: $D = 5/2$ "very close" to $D = 2$

$\Longrightarrow \epsilon = 5/2 - D$ in good position ?

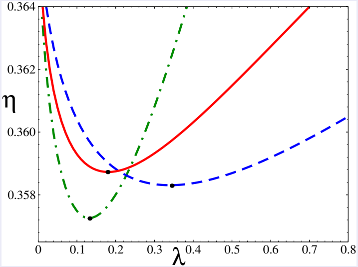
- perturbatively: $\eta = -0.0015 < 0$! (rigidity: $\kappa \sim 1/q^{\eta}$)

  ϵ-expansion: *"unreliable" and "qualitatively wrong"*

  (Radzihovsky and Toner'95)

- FRG approach:

(Essafi, Kownacki and D.M.'11)



$\eta = 0.358(4) > 0$ to be compared to MC data ...

- effects of quantum fluctuations on the flat phase of polymerized membrane / graphene
(quantum fluctuation important up to T $\sim$ 1000 K)

- perturbative approach: (Kats and Lebedev.'14, Amorim et al'14)
quantum membranes at $T = 0$ asymptotically free in the UV !
$\Longrightarrow$ unstable wrt quantum fluctuations !

preliminary work: FRG flow from the effective action for quantum membranes (Coquand and D.M.'16)

$$\Gamma[\mathbf{r}] = \int_0^\beta d\tau \int d^D x \left\{ \frac{\rho}{2}(\partial_\tau \mathbf{r})^2 + \frac{\kappa}{2}(\partial_\gamma \partial_\gamma \mathbf{r})^2 + \frac{\mu_k}{4}\left(\partial_\gamma \mathbf{r}.\partial_\nu \mathbf{r} - {\zeta_k}^2 \delta_{\gamma\nu}\right)^2 + \frac{\lambda_k}{8}\left(\partial_\gamma \mathbf{r}.\partial_\gamma \mathbf{r} - D{\zeta_k}^2\right)^2 \right\}$$

RG equations $\overline{\lambda}_k$, $\overline{\mu}_k$ and ζ_k

- quantum membranes governed by a IR trivial fixed point
  $\Longrightarrow$ stability of quantum membranes at T=0
- cross-overs:
  - quantum to classical regime
  - classical weak-coupling to classical strong-coupling regime

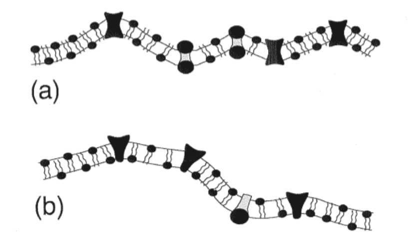
  $\Longrightarrow$ improved with respect to SCSA approach

(see O. Coquand, ERG 2016 and Phys. Rev. E 94, 032125 (2016))

- effect of disorder

origin: imperfect polymerization, protein, etc

  - isotropic defects $\Longrightarrow$ elastic disorder
  - anisotropic defect $\Longrightarrow$ curvature disorder



Hamiltonian:

$$H[\mathbf{r}] = \int \mathrm{d}^D x \left\{ \frac{\kappa}{2} \left(\partial_\mu \partial_\mu \mathbf{r}(\mathbf{x}) - \frac{\mathbf{c}(\mathbf{x})}{\kappa} \right)^2 + \lambda \left(\partial_\mu \mathbf{r}(\mathbf{x}).\partial_\nu \mathbf{r}(\mathbf{x}) - \zeta^2 \delta_{\mu\nu} (1 + 2\, m(x)) \right)^2 + \mu \left(\partial_\mu \mathbf{r}(\mathbf{x}).\partial_\mu .\mathbf{r}(\mathbf{x}) - \zeta^2 D (1 + 2\, m(x)) \right)^2 \right\}$$

with $\mathbf{c}(\mathbf{x})$ and $m(x)$ Gaussian random fields

- average over (quenched) disorder using replica trick:

$$F = \overline{\log Z} = \lim_{n \to 0} \frac{Z^n - 1}{n}$$

$\Longrightarrow$ effective action with interacting replica :

$$\Gamma[\mathbf{r}] = \int \mathrm{d}^d x \sum_{\alpha} \left\{ \frac{\overline{\kappa}}{2}\Big(\partial_i\partial_i \mathbf{r}^\alpha(\mathbf{x})\Big)^2 + \frac{\overline{\lambda}}{8}\Big(\partial_i \mathbf{r}^\alpha(\mathbf{x}).\partial_i \mathbf{r}^\alpha(\mathbf{x}) - D\zeta^2\Big)^2 + \frac{\overline{\mu}}{4}\Big(\partial_i \mathbf{r}^\alpha(\mathbf{x}).\partial_j \mathbf{r}^\alpha(\mathbf{x}) - \zeta^2\delta_{ij}\Big)^2 \right\}$$
$$- \frac{\overline{\Delta}_\kappa}{2} \sum_{\alpha,\beta} \partial_i\partial_i \mathbf{r}^\alpha(\mathbf{x}).\partial_j\partial_j \mathbf{r}^\beta(\mathbf{x})$$
$$- \frac{\overline{\Delta}_\lambda}{8} \sum_{\alpha,\beta} \Big(\partial_i \mathbf{r}^\alpha(\mathbf{x}).\partial_i \mathbf{r}^\alpha(\mathbf{x}) - D\zeta^2\Big)\Big(\partial_j \mathbf{r}^\beta(\mathbf{x}).\partial_j \mathbf{r}^\beta(\mathbf{x}) - D\zeta^2\Big)$$
$$- \frac{\overline{\Delta}_\mu}{8} \sum_{\alpha,\beta} \Big(\partial_i \mathbf{r}^\alpha(\mathbf{x}).\partial_j \mathbf{r}^\alpha(\mathbf{x}) - \zeta^2\delta_{ij}\Big)\Big(\partial_i \mathbf{r}^\beta(\mathbf{x}).\partial_j \mathbf{r}^\beta(\mathbf{x}) - \zeta^2\delta_{ij}\Big)$$

with $\overline{\Delta}_\kappa, \overline{\Delta}_\lambda, \overline{\Delta}_\mu$ disorder variances

- SCSA: (Radzihovsky and Nelson'91)

$$\kappa^D_{eff}(\mathbf{q}) = \kappa_{eff}(\mathbf{q}) + \Delta_\kappa \; \mathcal{K} \int d^2k \frac{\left[\hat{q}_a \, P^T_{ab} \, \hat{q}_b\right]^2}{{\kappa_{eff}}^2(\mathbf{q}+\mathbf{k})|\mathbf{q}+\mathbf{k}|^4}$$

$$-(\Delta_\lambda + \Delta_\mu) \; \mathcal{K}^2 \int d^2k \frac{\left[\hat{q}_a \, P^T_{ab} \, \hat{q}_b\right]^2}{\kappa_{eff}(\mathbf{q}+\mathbf{k})|\mathbf{q}+\mathbf{k}|^4}$$

  with κ_{eff} renormalized only by thermal fluctuations

- weak coupling (Morse and Lubensky'92)

  $\Longrightarrow$ stability of the ordered fixed point

- SCSA: (Radzihovsky and Nelson'91)

$$\kappa^D_{eff}(\mathbf{q}) = \kappa_{eff}(\mathbf{q}) + \Delta_\kappa\ \mathcal{K} \int d^2k \frac{\left[\hat{q}_a\, P^T_{ab}\, \hat{q}_b\right]^2}{{\kappa_{eff}}^2(\mathbf{q}+\mathbf{k})|\mathbf{q}+\mathbf{k}|^4}$$

$$-(\Delta_\lambda + \Delta_\mu)\ \mathcal{K}^2 \int d^2k \frac{\left[\hat{q}_a\, P^T_{ab}\, \hat{q}_b\right]^2}{\kappa_{eff}(\mathbf{q}+\mathbf{k})|\mathbf{q}+\mathbf{k}|^4}$$

  with κ_{eff} renormalized only by thermal fluctuations

- weak coupling (Morse and Lubensky'92)

  $\Longrightarrow$ stability of the ordered fixed point

- FRG approach (Coquand, Essafi, Kownacki, D.M.'17): *new fixed point* not seen within perturbation theory
- new failure of perturbative approach ?

Conclusion

Perturbative approaches of membranes fail in several situations

- $D = 2$ far from the upper critical dimension D_{uc}
- D_{uc} is fractional
- missing of fixed point ?
- $\ldots$

The FRG seems efficient in all these cases . . . but

Prospects

- self-avoidance (David, Duplantier, Guitter, Le Doussal, Wiese)

$$H = H_0 + \frac{b}{2} \int d^D x \, d^D y \; \delta(\mathbf{r}(\mathbf{x}) - \mathbf{r}(\mathbf{y}))$$

  $\Longrightarrow$ disappearance of the – high T – crumpled phase ?

  problem: non-locality in D-space

- graphene-like systems: interaction between electronic and membranes degrees of freedom

  $\Longrightarrow$ fermionic matter coupled to fluctuating metric

$$H = -i \int d^2 x \sqrt{g} \, \bar{\Psi} \, \gamma^a e_a^i (\partial_i + \Omega_i) \Psi$$

  with: $g_{ij} = \delta_{ij} + 2u_{ij}$

  (Coquand, Le Doussal, D.M., Radzihovsky)