Université Paris Cité

Academic year 2023-2024

M2 PCS — Statistical field theory and soft matter
TD n°3 : Interfaces

1 Christoffel symbols (algebra homework)

The Christoffel symbols of a surface parametrized by $\boldsymbol{R}(u^1, u^2)$ are defined by the fundamental relation $\partial_i \boldsymbol{t}_j = \Gamma^k_{ij} \boldsymbol{t}_k + L_{ij} \boldsymbol{n}$, where $\boldsymbol{t}_j = \partial_j \boldsymbol{R}$, $\partial_j = \partial / \partial u^j$ and $\boldsymbol{n} \propto \boldsymbol{t}_1 \times \boldsymbol{t}_2$ is the normal to the surface. The purpose of this exercice is (i) to obtain the explicit formula:

$$\Gamma^m_{jk} = \frac{1}{2} g^{im} \left(\partial_k g_{ij} + \partial_j g_{ki} - \partial_i g_{jk} \right), \tag{1}$$

(ii) to demonstrate the relation

$$\Gamma^j_{ji} = \partial_i \ln \sqrt{g}, \tag{2}$$

and (iii) to deduce that the covariant derivative of the metric vanishes.

1. Show that $\partial_i \boldsymbol{t}_j = \partial_j \boldsymbol{t}_i$ and deduce that $\Gamma^k_{ij} = \Gamma^k_{ji}$ (lower indices symmetry).
2. Show that $\partial_k g_{ij} = \Gamma^\ell_{ik} g_{j\ell} + \Gamma^\ell_{jk} g_{i\ell}$
3. Calculate $\partial_k g_{ij} + \partial_j g_{ki} - \partial_i g_{jk}$ (circular permutations), and deduce (1).
4. By summing over all the values of the dummy indices i and j, show that $\Gamma^j_{j1} = \frac{1}{2} \left(g^{11} \partial_1 g_{11} + g^{22} \partial_1 g_{22} + 2 g^{12} \partial_1 g_{12} \right)$.
5. Using $g^{11} = g^{-1} g_{22}$, etc. (as g^{ij} is the inverse matrix of g_{ij}), deduce (2).
6. Using question 2 and the definition of the covariant derivative, show that

$$D_k g_{ij} = 0, \quad D_k g = 0. \tag{3}$$

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2 Laplace's law

The effective Hamiltonian of a system of two fluids in contact through an interface $\boldsymbol{R}(u^1, u^2)$ is given by the sum of a surface term and a volume pressure term:

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_V = \gamma \int d^2u \sqrt{g} - \int d^3r \, P(\boldsymbol{r}). \tag{4}$$

Here, γ is the surface free energy (surface tension) and $d^2u \sqrt{g} = dA$ is the area element along the interface and the integral. Note that the corrections due to the curvature of the interface have been neglected.

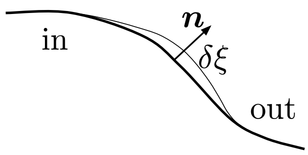

Figure 1: Normal variation of the shape of the interface.

The term $\mathcal{H}_V$ features the integral of the pressure field $P(\boldsymbol{r})$ over the entire volume of the system. It accounts for the work of the pressure forces when the interface is moved. Indeed, if the interface is shifted by $\delta\boldsymbol{R} = \boldsymbol{n}\delta\xi$, the variation of $\mathcal{H}_V$ is

$$\delta\mathcal{H}_V = -\int d^2u\sqrt{g}\,(P_{\text{in}} - P_{\text{out}})\,\delta\xi, \tag{5}$$

where P_{out} is the pressure field on the side to which the interface normal $\boldsymbol{n}$ points, and P_{in} is the pressure field on the other side. The pressure is indeed generally discontinuous at the interface. For instance, for a drop in contact with its vapor, we have $P_{\text{out}} = P_0$ in the vapor, with P_0 the constant atmospheric pressure, and $P_{\text{in}} = P_1 - \rho g z$, with P_1 a constant, ρ the mass density of the liquid and z the upward vertical coordinate

The aim of this problem is to find the equation that determines the shape of the interface that minimizes $\mathcal{H}$, i.e., Laplace's equation. It determines the "equilibrium shape" of the interface, or, more precisely, the most probable configuration of the interface.

1. For a variation $\delta\boldsymbol{R}$ of the interface, show that $\delta g = g\left(g^{22}\delta g_{22} + g^{11}\delta g_{11} + 2g^{12}\delta g_{12}\right)$.

2. Deduce that

$$\delta\sqrt{g} = \sqrt{g}\,\boldsymbol{t}^i\cdot\delta\boldsymbol{t}_i. \tag{6}$$

3. Show that $\delta\boldsymbol{t}_i = D_i\delta\boldsymbol{R}$.

4. By using the eq. (2) above, show that the covariant divergence can be expressed as

$$D_iV^i = \frac{1}{\sqrt{g}}\,\partial_i\left(\sqrt{g}\,V^i\right). \tag{7}$$

and deduce that the surface integral $\int d^2u\sqrt{g}\,D_iV^i$ of a covariant divergence reduces to a boundary term.

5. Show then that

$$\delta\mathcal{H}_S = -\gamma\int d^2u\sqrt{g}\,K_i^i\boldsymbol{n}\cdot\delta\boldsymbol{R} + \text{boundary terms} \tag{8}$$

6. Deduce Laplace's law:

$$\gamma\,(c_1 + c_2) = P_{\text{out}} - P_{\text{in}}. \tag{9}$$

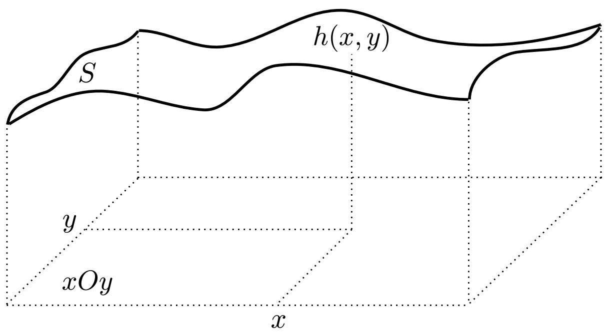

Figure 2: Monge parametrization.

3 Interface curvature in the Monge jauge

In the Monge parametrization, a surface is described by its height $z = h(x,y)$ above a reference plane (x,y) in orthonormal coordinates, as shown in Fig. 2. The corresponding shape field is therefore

$$\boldsymbol{R}(x,y) = x\boldsymbol{e}_x + y\boldsymbol{e}_y + h(x,y)\boldsymbol{e}_z. \tag{10}$$

This corresponds to a standard surface parametrization with $u^1 \equiv x$ and $u^2 \equiv y$.

1. With $h_x = \partial h/\partial x$, etc., show that the metric tensor is given by

$$g_{ij} = \begin{pmatrix} 1+h_x^2 & h_x h_y \\ h_x h_y & 1+h_y^2 \end{pmatrix} \tag{11}$$

2. Calculate $g = \det g_{ij}$ and the contravariant components g^{ij} of the metric tensor.

3. Deduce that the area element is given by

$$dA = \sqrt{1+(\boldsymbol{\nabla} h)^2}\, dx\, dy. \tag{12}$$

4. Calculate the normal $\boldsymbol{n} = \boldsymbol{t}_1 \times \boldsymbol{t}_2 / |\boldsymbol{t}_1 \times \boldsymbol{t}_2|$.

5. Show that the curvature tensor is given by

$$K_{ij} = \frac{1}{\sqrt{g}} \begin{pmatrix} h_{xx} & h_{xy} \\ h_{xy} & h_{yy} \end{pmatrix}. \tag{13}$$

6. Show then that

$$K_i^j = \frac{1}{g^{3/2}} \begin{pmatrix} \left(1+h_y^2\right) h_{xx} - h_x h_y h_{xy} & \left(1+h_y^2\right) h_{xy} - h_x h_y h_{yy} \\ \left(1+h_x^2\right) h_{xy} - h_x h_y h_{xx} & \left(1+h_x^2\right) h_{yy} - h_x h_y h_{xy} \end{pmatrix}. \tag{14}$$

7. Deduce that the sum of the principal curvatures is given by the exact formula

$$c_1 + c_2 = \frac{h_{xx}\left(1+h_y^2\right) + h_{yy}\left(1+h_x^2\right) - 2h_{xy}h_x h_y}{\left(1+h_x^2+h_y^2\right)^{3/2}}. \tag{15}$$

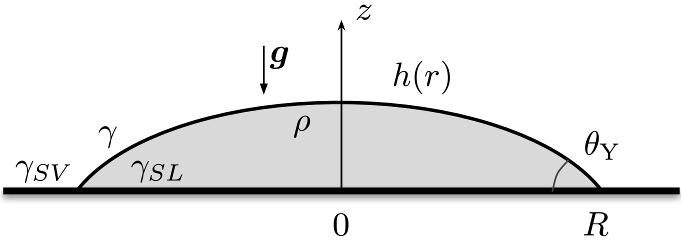

Figure 3: Drop wetting a substrate in the gravity field.

4 Wetting drop

A drop of liquid of mass density ρ is deposited on a substrate in a room on earth where gravity is g. It has the surface tension γ. The energy of the substrate–vapor interface is γ_{SV} and the energy of the substrate–liquid interface is γ_{SL}. Since we expect the drop to have rotational symmetry, we model its shape in the Monge jauge in polar coordinates by the height function

$$z = h(r), \quad r \in [0, R], \tag{16}$$

independent of the polar angle θ. Seen from above the drop takes a circular shape of radius R. We assume that we can use the Monge jauge in the limit of small deformations.

1. Work out the effective Hamiltonian $\mathcal{H}[h]$ of the drop. Show that it take the form

$$\mathcal{H}[h] = \int_0^R 2\pi r\, dr \left(\frac{1}{2}\gamma h'^2 + \frac{1}{2}\rho g h^2\right) + (\gamma + \gamma_{SL} - \gamma_{SV})\, \pi R^2. \tag{17}$$

2. To look for the situation of minimum energy, we make the variation $h(r) \to h(r) + \delta h(r)$ and $R \to R + \delta R$, where both δh and δR are assumed to be $O(\epsilon)$. In the following, all the variations will be performed at $O(\epsilon)$. Show that

$$\delta h(R) = -h'(R)\, \delta R. \tag{18}$$

3. Let $\mathcal{H}^\star = \mathcal{H} + PV$, where V is the volume. Minimizing $\mathcal{H}$ at fixed volume is equivalent to minimizing $\mathcal{H}^\star$ without constraints. Show that

$$\delta\mathcal{H}^\star = \int_0^R 2\pi r\, dr \left[\gamma h' \delta h' + P\delta h + \rho g h \delta h\right] + 2\pi R \left[\frac{\gamma}{2} h'^2(R) + \Gamma\right] \delta R, \tag{19}$$

where $\Gamma = \gamma + \gamma_{SL} - \gamma_{SV}$.

4. Deduce the two equations that characterize the equilibrium of the drop:

$$\gamma\, \frac{1}{r} \left(r h'\right)' = P + \rho g h \qquad \text{(Laplace's law)}, \tag{20}$$

$$\gamma \left(1 - \frac{1}{2} h'^2\right) = \gamma_{SV} - \gamma_{SL} \qquad \text{(Young's law)}. \tag{21}$$

5. Interpret these two equations in terms of Laplace's law, hydrostatic pressure, contact angle θ_{Y} and the balance of surface forces acting on the contact line (i.e., Young's law).

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5 The renormalization group on Gaussian interfaces

We consider an interface in d dimensions, described as $h(\boldsymbol{r})$ in the Monge jauge, with cutoff Λ in reciprocal space (i.e., $\Lambda = 2\pi/a$, where a is the small distance cutoff). It Fourier decomposition can the be written as

$$h(\boldsymbol{r}) = L^{-d} \sum_{\boldsymbol{q}\in\mathcal{E}} h_{\boldsymbol{q}}\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}}, \qquad \mathcal{E} = \{\boldsymbol{q}, q < \Lambda\}, \tag{22}$$

where L^d is the area of the projection of the interface onto the reference plane. The Hamiltonian describing the fluctuation of the interface is assumed to be Gaussian:

$$\mathcal{H}[h] = \int_{L^d} d^d r \left[\frac{\gamma}{2}\left(\boldsymbol{\nabla} h\right)^2 + \frac{\kappa}{2}\left(\boldsymbol{\nabla}^2 h\right)^2\right]. \tag{23}$$

The parameters of the system are therefore $\{\gamma, \kappa, L, \Lambda\}$. We observe the fluctuations of the interface and ask whether there is an asymptotic scale invariance (as in critical systems). In other words, do large scales behave in some way identically?

To investigate this question, we observe the interface through a renormalization group (RG) "megascope" (the opposite of a microscope). It has two parameters: ℓ (anti-zoom factor) and D (amplification factor). The image we see, $h'(\boldsymbol{r}')$, is the following transformation of the direct image:

$$h'(\boldsymbol{r}') = \ell^D\, h^<(\ell \boldsymbol{r}'), \tag{24}$$

where

$$h^<(\boldsymbol{r}) = L^{-d} \sum_{\boldsymbol{q}\in\mathcal{E}^<} h_{\boldsymbol{q}}\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}}, \qquad \mathcal{E}^< = \{\boldsymbol{q}, q < \Lambda/\ell\}. \tag{25}$$

In other words, the megascope smoothes out the image of the interface by eliminating the small deformations of wavevector larger than Λ/ℓ, then it amplifies the signal by a factor ℓ^D (a scale invariant factor), then it contracts the in-plane distances by dividing $\boldsymbol{r}$ by ℓ. The result is a smaller interface, of size $L = L/\ell$, with a smoothed, amplified shape, that fluctuates with the same cutoff Λ as the real one (thanks to the in-plane contraction). Does it look like the real one? Can one find D such that the answer is yes for $\ell \to \infty$? This is how the RG seeks scale invariance.

1. Write the Fourier expansion of $h^> = h - h^<$ in the form of Eq. (46).

2. Show that $\mathcal{H}[h] = \mathcal{H}[h^<] + \mathcal{H}[h^>]$. Would that be true for a non-Gaussian model?

3. Writing the probability density for $h^<$ as $P^<[h^<] = Z^{-1}\exp(-\beta\mathcal{H}^<[h^<])$ defines $\mathcal{H}^<[h^<]$. Show that $\mathcal{H}^<[h^<] = \mathcal{H}[h^<]$ (up to an irrelevant constant). Would this very simple result be true for a non-Gaussian model?

4. Deduce that the probability density for h' is $P'[h'] = Z^{-1}\exp(-\beta\mathcal{H}'[h'])$, with

$$\mathcal{H}'[h'] = \int_{L^d} d^d r' \left[\frac{\gamma(\ell)}{2}\left(\boldsymbol{\nabla}' h'\right)^2 + \frac{\kappa(\ell)}{2}\left(\boldsymbol{\nabla}'^2 h'\right)^2\right] \tag{26}$$

(up to an irrelevant constant), with

$$\gamma(\ell) = \gamma\,\ell^{d-2D-2}, \tag{27}$$
$$\kappa(\ell) = \kappa\,\ell^{d-2D-4}, \tag{28}$$
$$L(\ell) = L\,\ell^{-1}. \tag{29}$$

5. Assuming d is large enough, represent the renormalization flow, and deduce that the correct (interesting) setting of the megascope corresponds to $D = (d-2)/2$.

6. Deduce that κ is irrelevant at large scales when $\gamma \neq 0$.

7. Let $W(\gamma,\kappa,L)$ be the typical width of the interface (omitting Λ, which remains constant during renormalization). By comparing the real interface and the megascope image for $D = (d-2)/2$, show that

$$W(\gamma,\kappa,L) = \ell^{-D}\,W(\gamma,\kappa\ell^{-2},L\ell^{-1}). \tag{30}$$

What clever choice of ℓ will give us physical insight when $L\to\infty$? It is convenient to have $\kappa\to 0$, so we want a diverging ℓ. But we don't want $L\to 0$, otherwise the interface image would diasppear. So we choose ℓ such that $L\ell^{-1} = \bar{L}$, where $\bar{L}$ is a constant.

8. Using this choice of ℓ, show that

$$W \sim L^{1-\frac{d}{2}}. \tag{31}$$

9. Deduce that the interface is flat for $d > 2$ and rough for $d < 2$, when $\gamma \neq 0$, in agreement with the results of the course.

10. Characterize the width of an interface in the two dimensional Ising model.

11. Let $\theta(\gamma,\kappa,L)$ be the typical orientational fluctuations of the interface. Using a relation similar to (59), in the limit of small angles, show that

$$\theta \sim L^{-\frac{d}{2}}, \tag{32}$$

12. Conclude that an interface under tension is oriented in all dimensions.

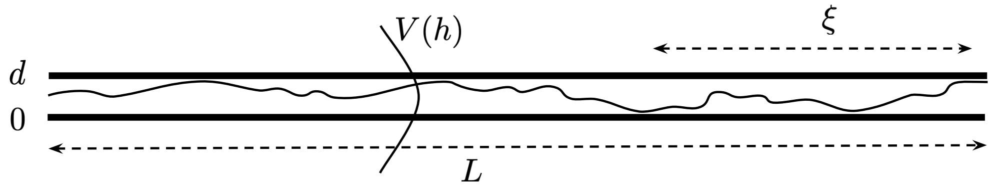

Figure 4: Fluctuating membrane exerting Helfrich forces

6 Helfrich forces

When a tensionless membrane of lateral size L is confined between two parallel plates, separated by a distance d, it exerts a pressure $P(d)$ on these plates. Indeed, a tensionless membrane is marginally rough in two dimensions, so it will always collide with the plates if it is large enough (Fig. 4). In the Monge jauge, the effective Hamiltonian of the corresponding system is given by

$$\mathcal{H} = \int d^2r \left[\frac{1}{2}\kappa(\boldsymbol{\nabla}^2 h)^2 + V(h)\right], \tag{33}$$

with

$$V(h(\boldsymbol{r})) = \begin{cases} 0 & 0 < h(\boldsymbol{r}) < d, \\ +\infty & \text{otherwise.} \end{cases} \tag{34}$$

To calculate the pressure exerted by the fluctuating membrane (Helfrich forces), we must compute the free-energy $f(d)$ per unit area of the membrane and differentiate:

$$P(d) = -\frac{\partial f}{\partial d}. \tag{35}$$

Self-consistent Gaussian approximation.—The above non-Gaussian model is very difficult to solve. A convenient strategy, which we adopt, is to approximate $V(h)$ by a quadratic potential $V(h) = \frac{1}{2}mh^2$, with $m(d)$ chosen so as to verify $\langle h^2(\boldsymbol{r})\rangle \approx d$ (as in the presence of the plates), where the symbol $\approx$ means "up to a factor of order unity". This approximation yields the correct scaling for the pressure of the Helfrich forces.

1. Using standard results on the correlation function of Gaussian models, show that

$$\langle h^2(\boldsymbol{r})\rangle \simeq \frac{k_\mathrm{B}T\xi^2}{8\kappa}, \tag{36}$$

where $\xi = (\kappa/m)^{1/4}$. To obtain this simple result, assume that $L \to \infty$ and $\xi \gg a$, where a is the microscopic cutoff of the theory.

2. Deduce that in order to match the plate problem, we need to take

$$m \approx \frac{(k_\mathrm{B}T)^2}{\kappa d^4}. \tag{37}$$

3. Without further calculations, show that ξ is the typical membrane size below which the membrane does not collide with the plates and above which it does.

4. The pressure exerted by the membrane can be estimated using a scaling argument: $f \approx k_\mathrm{B}T/\xi^2$. Justify this statement and deduce that

$$P \approx \frac{(k_\mathrm{B}T)^2}{\kappa d^3}. \tag{38}$$

5. The partition function of the system can be expressed in the reciprocal space, with $h(\boldsymbol{r}) = L^{-2}\sum_{\boldsymbol{q}} h_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{r}}$, as

$$Z = C\int\left(\prod_{\boldsymbol{q}} dh'_{\boldsymbol{q}}\, dh''_{\boldsymbol{q}}\right) e^{-\beta L^{-2}\sum_{\boldsymbol{q}}\frac{1}{2}(\kappa q^4+m)|h_{\boldsymbol{q}}|^2}, \tag{39}$$

where $h_{\boldsymbol{q}} = h'_{\boldsymbol{q}} + ih''_{\boldsymbol{q}}$. Behind the apparences, what are the correct and precise meanings of $\sum_{\boldsymbol{q}}$ and $\prod_{\boldsymbol{q}}$? Why is there a constant C?

6. Deduce that in the thermodynamic limit and up to an irrelevant additive constant, the free energy density is given by

$$f = \frac{1}{2}k_\mathrm{B}T\int\frac{d^2q}{(2\pi)^2}\,\ln\left(\kappa q^4 + m\right). \tag{40}$$

7. Conclude again that

$$P \approx \frac{(k_\mathrm{B}T)^2}{\kappa d^3} \tag{41}$$

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