Master Physics of Complex Systems (PCS)

STATISTICAL FIELD THEORY AND SOFT MATTER

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Année 2023/24

Université Paris Cité

Contents

Chapter 1

BASIC STATISTICAL FIELD THEORY TOOLS

A)   Einstein summation and tensors

1)   Einstein convention

The Einstein summation convention consists in implicitly summing over the dummy indices repeated exactly twice.

In each term of an expression, write down mentally all the possible terms by varying the dummy indices over their range $\{1 \ldots d\}$ and sum everything. An index is dummy if does not have another meaning elsewhere.

Example:

$$\boldsymbol{x}^2 = x_i x_i \quad \text{(summation)} \tag{1.1}$$
$$z_k = x_k y_k \quad \text{(no summation)}. \tag{1.2}$$

The first one means $\boldsymbol{x}^2 = x_1^2 + x_2^2 + x_3^2$ in three dimensions. In the second one, k is not dummy since it appears on the right-hand side. Further training in **tutorials**.

2)   Tensors

Here we deal only with cartesian tensors (tensors in orthonormal bases). A rank 2 tensor $\boldsymbol{T}$ is a linear mapping from a vectorial space $\mathcal{E}$ onto itself:

$$\boldsymbol{w} = \boldsymbol{T} \cdot \boldsymbol{v}. \tag{1.3}$$

Note that the 'dot' here does not represent a scalar product.

An example is the polarisation vector, $\boldsymbol{P} = \boldsymbol{\epsilon} \cdot \boldsymbol{E} + O(E^2)$: a linear function of $\boldsymbol{E}$ for small fields, not necessarily parallel to $\boldsymbol{E}$ (the tensor $\boldsymbol{\epsilon}$ can be anisotropic).

In an orthonormal basis $\{\boldsymbol{e}_i\}$, the linear mapping from $\boldsymbol{v}$ to $\boldsymbol{w}$ involves n^2 numbers T_{ij} (its components) and takes thus the form

$$w_i = T_{ij}v_j. \tag{1.4}$$

The space of the 2-tensors can be identified with $\mathcal{E}_2 = \mathcal{E} \otimes \mathcal{E}$ (cf. quantum mechanics[1]) via the definition:

$$(\boldsymbol{e}_i \otimes \boldsymbol{e}_j) \cdot \boldsymbol{v} = \boldsymbol{e}_i(\boldsymbol{e}_j \cdot \boldsymbol{v}), \quad \forall \boldsymbol{v}, \tag{1.5}$$

which justifies the use of the 'dot' notation introduced in (1.3).

Then any 2-tensor can be decomposed as

$$\boldsymbol{T} = T_{ij}\boldsymbol{e}_i \otimes \boldsymbol{e}_j. \tag{1.6}$$

Indeed $\boldsymbol{T} \cdot \boldsymbol{v} = T_{ij}\boldsymbol{e}_i \otimes \boldsymbol{e}_j \cdot v_k\boldsymbol{e}_k = T_{ij}v_k\boldsymbol{e}_i\delta_{jk} = (T_{ij}v_j)\boldsymbol{e}_i = \boldsymbol{w}$.

Higher-rank tensors

A rank n tensor is a linear mapping from $\mathcal{E}$ to $\mathcal{E}_{n-1}$. For instance, a 3-tensor $\boldsymbol{U}$ is a linear mapping from $\mathcal{E}$ to $\mathcal{E} \otimes \mathcal{E}$:

$$\boldsymbol{T} = \boldsymbol{U} \cdot \boldsymbol{v}, \quad T_{ij} = U_{ijk}v_k. \tag{1.7}$$

It appears naturally whenever a tensor depends linearly on a vector, or, equivalently, whenever a vector depends linearly on two vectors:

$$w_i = (U_{ijk}v_j)v_k' = U_{ijk}v_jv_k'. \tag{1.8}$$

Change of basis

To change basis, one considers the orthogonal passage matrix O, the columns of which are the images of the basis vectors:

$$\boldsymbol{e}_i' = O_{ji}\boldsymbol{e}_j. \qquad (O_{ji}, \text{ not } O_{ij}) \tag{1.9}$$

From $\boldsymbol{v} = v_i'\boldsymbol{e}_i'$ on easily finds the transformation

$$v_i = O_{ij}v_j'. \tag{1.10}$$

Likewise, from $\boldsymbol{T} = T_{ij}'\boldsymbol{e}_i' \otimes \boldsymbol{e}_j'$ on easily finds the transformation

$$T_{ij} = O_{ik}O_{j\ell}T_{k\ell}'. \tag{1.11}$$

Hence, each component of a n-tensor transforms exactly as a vector.

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[1]The vectorial space of dimension d^2 generated by the basis $\{\boldsymbol{e}_i \otimes \boldsymbol{e}_j\}$

An important rule follows: a set of numbers $\{T_{ij}\}$ describes a 2-tensor if and only if it changes as indicated above in a change of basis.

It follows that multiplying tensors and vectors components together builds higher-rank tensors. For instance $T_{ij}a_k$ is a 3-tensor, $F_{ijk}G_{\ell m}$ is a 5-tensor. This follows directly from the way each transforms by means of products of $O_{\alpha\beta}$.

Also, *contracting*, i.e., summing over two indices with the Einstein convention, builds lower-rank tensors. For instance $T_{ijk}b_k = u_{ij}$ is a 2-tensor, etc. This follows from the fact that, since O is orthogonal, i.e., $\mathsf{O}^{-1} = \mathsf{O}^t$, we have $O_{k\ell}O_{km} = O_{mk}^{-1}O_{k\ell} = \delta_{ml}$ ensuring that the results does transform as a 2-tensor.

B)　Functional derivatives

1)　Definition

A functional $f[h]$ is a *function of the function* $x \to h(x)$. If h is a field, $f[h]$ is a function of the field $\boldsymbol{r} \to h(\boldsymbol{r})$. A functional is thus a function of a continuous infinite number of variables.

Example: The energy of the electrical field in vacuum is a functional:

$$\mathcal{E}[\boldsymbol{E}] = \int d^3r \, \frac{\epsilon_0}{2} \boldsymbol{E}^2(\boldsymbol{r}). \tag{1.12}$$

To define the functional derivatives of $f[h]$, one considers a small variation $h(x) \to h(x) + \delta h(x)$ of the function. It implies a variation $\delta f = f[h + \delta h] - f[h]$ of the functional. It is generally possible cast it in the form

$$\delta f = \delta f_1 + \delta f_2 + \delta f_3 \ldots$$
$$= \int dx \, \alpha(x)\delta h(x) + \frac{1}{2}\int dx \, dy \, \beta(x,y)\delta h(x)\delta h(y) + \frac{1}{3!}\int dx \, dy \, dz \ldots \tag{1.13}$$

which is simply the continuous generalization of the Taylor expansion of a function $f(h_1, \ldots, h_n)$ of many variables. Then *by definition*

$$\alpha(x) \stackrel{\text{def.}}{=} \frac{\delta f}{\delta h(x)}, \tag{1.14}$$

$$\beta_s(x,y) \stackrel{\text{def.}}{=} \frac{\delta^2 f}{\delta h(x)\delta h(y)} \quad (\beta_s = \beta \text{ symmetrized}), \quad \ldots \tag{1.15}$$

are the *first derivative of f with respect to h at point x*, the *second derivative of f with respect to h at points x and y*, etc.

If $h(\boldsymbol{x})$ is a field, the integrals in (1.13) should be over space ($\int d^dx \ldots$). Training in **tutorials**.

2)   Properties

All the rules concerning the partial derivatives can be applied. The following properties hold (f, g and u are functionals, a is a function and α a real):

$$\frac{\delta(f+g)}{\delta h(x)} = \frac{\delta f}{\delta h(x)} + \frac{\delta g}{\delta h(x)}, \qquad \frac{\delta(\alpha f)}{\delta h(x)} = \alpha \frac{\delta f}{\delta h(x)}. \tag{1.16}$$

$$\frac{\delta(fg)}{\delta h(x)} = f \frac{\delta g}{\delta h(x)} + g \frac{\delta f}{\delta h(x)}. \tag{1.17}$$

$$f[h] = a(g[h]) \quad \Rightarrow \quad \frac{\delta f}{\delta h(x)} = \frac{\delta g}{\delta h(x)} a'(g[h]) \quad \text{(composition)}. \tag{1.18}$$

$$f[h] = g[u[h]] \quad \Rightarrow \quad \frac{\delta f}{\delta h(x)} = \int dy \, \frac{\delta g}{\delta u(y)} \frac{\delta u(y)}{\delta h(x)} \quad \text{(chain rule)}. \tag{1.19}$$

In the last example, u is a function $u(x)$, since we consider $g[u]$, but it is also a functional of h, as indicated. One can write it as $u(x; h)$.

C)   Functional integrals

In statistical field theory one often encounters integrals in the form (here a partition function):

$$Z = \int \mathcal{D}[\phi] \, e^{-\beta H[\phi]}, \tag{1.20}$$

where $\phi(x)$, for $x \in [0, L]$, is a field (here for a finite system in one dimension).

The meaning of $\int \mathcal{D}[\phi]$ is *integrate over all possible realizations of $\phi(x)$*. As such it is not well defined: one needs to specify the space of functions over which the integration is made and the associated measure.

In physics, usually, the prescription is the following. The space is discretized with a small cutoff a: $x_i = na$, $n \in [0, N]$, $N = L/a$, $\phi_i = \phi(x_i)$. Then

$$\int \mathcal{D}[\phi] \equiv \int \left(\prod_{i=0}^{N} d\phi_i \right). \tag{1.21}$$

The result therefore depends on our choice of regularization/measure (yet, fortunately, some parts of a functional integral are universal).

D)   Gaussian integrals

1)   One dimension

In one dimension the Gaussian integral is

$$I_1 = \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2+xy} = \left(\frac{a}{2\pi}\right)^{-1/2} e^{\frac{1}{2}y^2/a} \qquad (a>0). \tag{1.22}$$

This is easy to deduce from the area $\sqrt{\pi}$ below the Gaussian e^{-x^2}.

Rule to remember: Prefactor $[a/(2\pi)]^{-1/2}$ multiplied by a conjugate Gaussian with the sign changing, the $1/2$ remaining, the coefficient changed into its inverse, and the variable changed into its conjugate.

2) N dimensions

In N dimensions the Gaussian integral reads:

$$I_N = \int \left(\prod_{i=1}^{N} d\phi_i\right) e^{-\frac{1}{2}\phi_i A_{ij}\phi_j + \phi_i\psi_i} = \left(\det \frac{\mathsf{A}}{2\pi}\right)^{-1/2} e^{\frac{1}{2}\psi_i A_{ij}^{-1}\psi_j} \qquad (\mathsf{A}>0). \tag{1.23}$$

where $\mathsf{A}>0$ means that all the eigenvalues of the (symmetrizable) matrix A are strictly positive. Note that the rule above applies.

3)   Functional Gaussian integral

The functional Gaussian integral is

$$I = \int \mathcal{D}[\phi]\, e^{-\frac{1}{2}\int d^dx\, d^dy\, \phi(\boldsymbol{x})A(\boldsymbol{x},\boldsymbol{y})\phi(\boldsymbol{y}) + \int d^dx\, \phi(\boldsymbol{x})\psi(\boldsymbol{x})}$$

$$= \left(\det \frac{\mathsf{A}}{2\pi}\right)^{-1/2} e^{\frac{1}{2}\int d^dx\, d^dy\, \psi(\boldsymbol{x})A^{-1}(\boldsymbol{x},\boldsymbol{y})\psi(\boldsymbol{y})}, \tag{1.24}$$

where A is the matrix obtained upon regularizing the functional integral. Again the rule above applies.

The inverse kernel $A^{-1}(\boldsymbol{x},\boldsymbol{y})$ is defined by a straightforward generalization of the rule $A_{ij}^{-1}A_{jk} = \delta_{ik}$, i.e.,

$$\int d^dy\, A^{-1}(\boldsymbol{x},\boldsymbol{y})A(\boldsymbol{y},\boldsymbol{z}) = \delta(\boldsymbol{x}-\boldsymbol{z}). \tag{1.25}$$

NB. With that you can demonstrate the exponential part of the result (1.24) just by completing the square and making a change of variable.

E)   Fourier transform

1)   Infinite system

The convention in statistical field theory is the following. To a function $f(\boldsymbol{x}) \in \mathbb{R}$ we associate its Fourier transform $f(\boldsymbol{q})$ such that

$$f(\boldsymbol{x}) = \int \frac{d^d q}{(2\pi)^d}\, f(\boldsymbol{q})\, e^{i\boldsymbol{q}\cdot\boldsymbol{x}} \equiv \int_{\boldsymbol{q}} f(\boldsymbol{q})\, e^{i\boldsymbol{q}\cdot\boldsymbol{x}}, \tag{1.26}$$

Note that since $f \in \mathbb{R}$, we have $f(-\boldsymbol{q}) = f(\boldsymbol{q})^\star$. All properties and formulas derive simply from the fundamental relation:

$$\int d^d x\, e^{i\boldsymbol{q}\cdot\boldsymbol{x}} = (2\pi)^d \delta(\boldsymbol{q}), \quad \text{(or the same with } \boldsymbol{x} \leftrightarrow \boldsymbol{q}\text{).} \tag{1.27}$$

For instance, it is straightforward (by replacing $f(\boldsymbol{x})$ by its Fourier expansion) to show the inverse relation:

$$\int d^d x\, f(\boldsymbol{x})\, e^{-i\boldsymbol{q}\cdot\boldsymbol{x}} = f(\boldsymbol{q}). \tag{1.28}$$

2)   Finite continuous system (discrete Fourier transform in a box)

It is often convenient to put the system in a finite box of volume $V = L^d$, and take periodic boundary conditions (PBC).

Having $f(\boldsymbol{x} + L\boldsymbol{e}_j) = f(\boldsymbol{x})$, $\forall \boldsymbol{x}$ and $\forall j$, requires $q_j L$ multiple of 2π, hence

$$f(\boldsymbol{x}) = \frac{1}{L^d} \sum_{\boldsymbol{q}} f_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{x}}, \qquad \boldsymbol{q} = \frac{2\pi}{L}(n_1, \ldots, n_d)^t, \quad n_i \in \mathbb{Z}, \tag{1.29}$$

with, because f is real, $f_{-\boldsymbol{q}} = f_{\boldsymbol{q}}^\star$. The prefactor choice $1/V$ makes the correspondence with the continuous description straightforward, as in the thermodynamic limit $\sum_{\boldsymbol{q}} \simeq L^d \int d^d q/(2\pi)^d$.
   The fundamental relation is

$$\int_V d^d x\, e^{i\boldsymbol{q}\cdot\boldsymbol{x}} = L^d \delta_{\boldsymbol{q},\boldsymbol{0}}, \tag{1.30}$$

Indeed, the integral vanishes due to the quantification, except if $\boldsymbol{q} = \boldsymbol{0}$. The inverse transform follows:

$$\int_V d^d x\, f(\boldsymbol{x}) e^{-i\boldsymbol{q}\cdot\boldsymbol{x}} = f_{\boldsymbol{q}}. \tag{1.31}$$

Then, we can show that $\delta(\boldsymbol{x}) = L^{-d} \sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{x}}$ (it is actually a periodic Dirac comb). Indeed, for a generic function f, we have $\int d^d x\, f(\boldsymbol{x}) L^{-d} \sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{x}_0)} = L^{-d} \sum_{\boldsymbol{q}} e^{-i\boldsymbol{q}\cdot\boldsymbol{x}_0} f_{-\boldsymbol{q}} = f(\boldsymbol{x}_0)$.
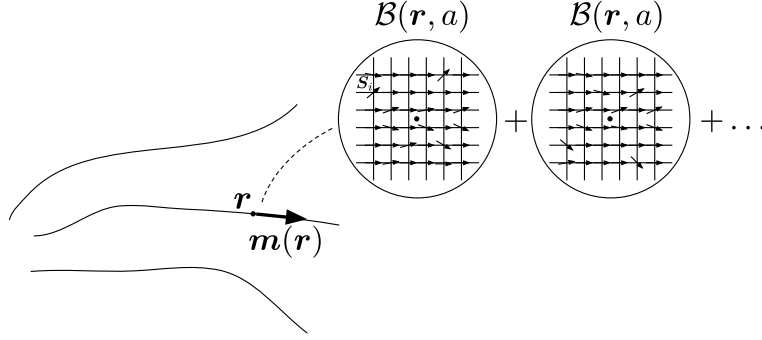
Figure 1.1: Continuous field $\boldsymbol{m}(\boldsymbol{r})$ for an *XY* model (Ising-like model with 2D spins), obtained by *spatially* averaging the spins over a ball $\mathcal{B}(\boldsymbol{r}, a)$. Several possible spin configurations in the ball $\mathcal{B}(\boldsymbol{r}, a)$ are represented. The + signs illustrate the sum over all the microstates α that are compatible with the field $\boldsymbol{m}$, which enters the effective Hamiltonian in the coarse-graining procedure defining.

F) Coarse graining and effective Hamiltonian

Consider a real, complicated, system:

$$\text{Microstates: } \{\alpha\}, H_\alpha, \tag{1.32}$$

$$P_\alpha = \frac{1}{Z} e^{-\beta H_\alpha}, \tag{1.33}$$

$$Z = \sum_\alpha e^{-\beta H_\alpha}. \tag{1.34}$$

Then, define a field by a coarse-graining procedure:

$$\phi(\boldsymbol{r}) = \text{spatial average of some quantity of interest in a ball } \mathcal{B}(\boldsymbol{r}, a), \tag{1.35}$$

of radius a centered on the point $\boldsymbol{r}$, where a is a cutoff length. Fig. 1.1 shows this procedure in a 2D XY model, where the field is $\boldsymbol{m}(\boldsymbol{r})$ (instead of $\phi(\boldsymbol{r})$). For instance for a magnetic material the quantity of interest can be the spins (Ising like).

1) Effective Hamiltonian

The probability density of a realization of the field allows us to define an effective Hamiltonian $\mathcal{H}[\phi]$ for the field $\phi(\boldsymbol{r})$:

$$P[\phi] = \frac{1}{Z} \sum_{\alpha \to [\phi]} e^{-\beta H_\alpha} \stackrel{\text{def.}}{=} \frac{1}{Z} e^{-\beta \mathcal{H}[\phi]}, \tag{1.36}$$

$$\implies \quad \mathcal{H}[\phi] \stackrel{\text{def.}}{=} -k_{\mathrm{B}} T \ln \sum_{\alpha \to [\phi]} e^{-\beta H_\alpha}, \tag{1.37}$$

The partition function is obtained by the usual procedure, but from a functional integral:

$$\implies \quad Z = \sum_\alpha e^{-\beta H_\alpha} = \int \mathcal{D}[\phi] \sum_{\alpha \to [\phi]} e^{-\beta H_\alpha} = \int \mathcal{D}[\phi]\, e^{-\beta \mathcal{H}[\phi]}. \qquad (1.38)$$

Power series expansion of the effective Hamiltonian

It is usually much too difficult to actually compute the functional $\mathcal{H}[\phi]$. However, we may often expand it in power series of some small quantity (the field, or its gradient, in general), and determine its form from symmetry arguments[2].

There are two rules to follow in the construction of the power-series expansion of the effective Hamiltonian:

1. R1: **Each term must be scalar**[3], as $\mathcal{H}$ itself.

2. R2: **Each term must be invariant under the symmetry operations that leave the disordered (or undeformed) phase invariant.**

NB. (R2) If there is no symmetry breaking, each term must simply be invariant under the symmetry operations that leave the phase invariant.

The example of the paramagnetic–ferromagnetic transition

Consider a magnetic system in d dimensions, with $\boldsymbol{m}(\boldsymbol{r}) \in \mathbb{R}^n$ the magnetization defined by a coarse-graining procedure.

The interactions are short ranged, so the effective Hamiltonian $\mathcal{H}[\phi]$ can be written as an integral over the volume of a density h that depends on the local field and its gradients:

$$\mathcal{H}[\boldsymbol{m}] = \int d^d x\, h(\{m_\mu\}, \{\partial_i m_\mu\}, \ldots). \qquad (1.39)$$

In the vicinity of the pamamagnetic–ferromagnetic transition, m is small, so we can expand h in power series of $\boldsymbol{m}$ and its gradients. Following the rules above, this gives:

$$\mathcal{H}[\boldsymbol{m}] = \int d^d x \left[\frac{1}{2} r(T) \boldsymbol{m}^2 + \frac{1}{2} c(T) \sum_{\mu=1}^n (\boldsymbol{\nabla} m_\mu)^2 + u(T) \left(\boldsymbol{m}^2\right)^2 + \ldots \right] \qquad (1.40)$$

The coefficients $r, c, u \ldots$ depend on temperature, since they originate from a coarse-graining procedure.

Let us derive this expansion using rules R1 and R2. The paramagnetic (disordered) phase is isotropic: all directions of $\boldsymbol{m}$ are equivalent and all directions of space are equivalent. The corresponding symmetry groups are the orthogonal groups $O(n)$ and $O(d)$.

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[2]Similarly, we don't know the exact deformation energy of a spring, but we may write it as $E \simeq \frac{1}{2} k x^2$ and gain physical insight from that.

[3]i.e., invariant under a change of orthonormal basis (it must not depend on how *we* orient the basis).

- Is there a term linear in m in the Hamiltonian density? Its most general form would be $a_\mu m_\mu$. From R1, the coefficients a_μ must be the components of a vector of $\mathbb{R}^n$. From R2, this vector cannot encode any direction in $\mathbb{R}^n$, otherwise a rotation of $\boldsymbol{m}$ would change the energy. So $a_\mu = 0$ and there is no linear term.

- The most general form of the term quadratic in m is $\frac{1}{2}r_{\mu\nu}m_\mu m_\nu$. From R1, $r_{\mu\nu}$ must be a tensor of $\mathbb{R}^n$. From R2, it must not encode any direction in $\mathbb{R}^n$, otherwise a rotation of $\boldsymbol{m}$ would change the energy. So it must be isotropic: $r_{\mu\nu} = r\delta_{\mu\nu}$. Hence the result $r_{\mu\nu}m_\mu m_\nu = \frac{1}{2}r\,\boldsymbol{m}^2$.

- Consider now the term quadratic in m and quadratic in the gradient. Its most general form is $\frac{1}{2}c_{ij\mu\nu}(\partial_i m_\mu)(\partial_j m_\nu)$. From R1, $c_{ij\mu\nu}$ must be a 2-tensor of $\mathbb{R}^d$, for i and j, and a 2-tensor of $\mathbb{R}^n$, for μ and ν. From R2, it must not encode any direction in $\mathbb{R}^n$ nor in $\mathbb{R}^d$. So, $c_{ij\mu\nu} = c\,\delta_{\mu\nu}\delta_{ij}$, and we have

$$\frac{1}{2}c(\partial_i m_\mu)(\partial_i m_\mu) = \frac{1}{2}c\sum_{\mu=1}^{n}(\boldsymbol{\nabla}m_\mu)^2. \tag{1.41}$$

- Consider finally the term quartic in m. Its most general form is $u_{\mu\nu\rho\sigma}m_\mu m_\nu m_\rho m_\sigma$. From R1 and R2, $u_{\mu\nu\rho\sigma}$ must be a fully isotropic 4-tensor of $\mathbb{R}^n$. It is a theorem that isotropic high-rank tensors can only be constructed with the Kronecker delta (the isotropic 2-tensor). Its most general form is thus

$$u_{\mu\nu\rho\sigma} = u_1\delta_{\mu\nu}\delta_{\rho\sigma} + u_2\delta_{\mu\rho}\delta_{\nu\sigma} + u_3\delta_{\mu\sigma}\delta_{\nu\rho}. \tag{1.42}$$

This yields $u\,m_\mu m_\mu m_\rho m_\rho = u(\boldsymbol{m}^2)^2$, with $u = u_1 + u_2 + u_3$. It is worth noticing that the result is not $\sum_{\mu=1}^{n}m_\mu^4$.

2) Average field and correlation functions

To determine those quantity one introduces formally an external field:

$$\mathcal{H}_h = \mathcal{H}[\phi] - \int d^d x\, h(\boldsymbol{x})\phi(\boldsymbol{x}). \tag{1.43}$$

The partition function and the free energy become functionals of h:

$$Z[h] = \int \mathcal{D}[\phi]\, e^{-\beta\mathcal{H}_h[\phi]}, \qquad F[h] = -k_\mathrm{B}T\ln Z[h]. \tag{1.44}$$

Then (see **tutorials**) we have

$$\langle\phi(\boldsymbol{x})\rangle = -\frac{\delta F}{\delta h(\boldsymbol{x})}, \tag{1.45}$$

$$C(\boldsymbol{x},\boldsymbol{y}) = -k_\mathrm{B}T\frac{\delta^2 F}{\delta h(\boldsymbol{x})\delta h(\boldsymbol{y})}, \tag{1.46}$$

where $C(\boldsymbol{x},\boldsymbol{y}) = \langle\phi(\boldsymbol{x})\phi(\boldsymbol{y})\rangle - \langle\phi(\boldsymbol{x})\rangle\langle\phi(\boldsymbol{y})\rangle$ is the correlation function. Note that is also equal to $\langle\delta\phi(\boldsymbol{x})\delta\phi(\boldsymbol{y})\rangle$ with $\delta\phi(\boldsymbol{x}) = \phi(\boldsymbol{x}) - \langle\phi(\boldsymbol{x})\rangle$.

G)   Mean-field approximation

In statistical field theory, the mean-field approximation is performed by evaluating the partition function using the saddle-point method (see SFT course).

This amounts to calculating the most probable field, $\phi_{\mathrm{mf}}(\boldsymbol{x})$. It is the one that maximizes the probability density $P[\phi] = Z^{-1}\exp(-\beta\mathcal{H}[\phi])$, hence the one that minimizes the effective Hamiltonien:

$$\min(\mathcal{H}[\phi]) \longrightarrow \phi_{\mathrm{mf}}(\boldsymbol{x}). \tag{1.47}$$

In the mean-field approximation, we neglect the fluctuations around ϕ_{mf}, so

$$\langle\phi(\boldsymbol{x})\rangle \overset{\mathrm{m.f.}}{=} \phi_{\mathrm{mf}}(\boldsymbol{x}). \tag{1.48}$$

H)   Gaussian model

The Gaussian model is a field theory where the effective Hamiltonian is Gaussian (quadratic). Let us consider generically a scalar field $\phi(\boldsymbol{x})$ with Hamiltonian

$$\mathcal{H}[\phi] = \int d^d x \left[\frac{a}{2}\phi^2 + \frac{b}{2}(\boldsymbol{\nabla}\phi)^2 + \frac{c}{2}(\boldsymbol{\nabla}^2\phi)^2\right]. \tag{1.49}$$

The following calculations are detailed in the **tutorials**.

The Hamiltonian can be rewritten as

$$\mathcal{H}[\phi] = \frac{1}{2}\int d^d x\, d^d y\, \phi(\boldsymbol{x})H(\boldsymbol{x},\boldsymbol{y})\phi(\boldsymbol{y}), \tag{1.50}$$

with

$$H(\boldsymbol{x},\boldsymbol{y}) = \mathcal{L}\delta(\boldsymbol{x}-\boldsymbol{y}) = (a - b\boldsymbol{\nabla}^2 + c\boldsymbol{\nabla}^2\boldsymbol{\nabla}^2)\delta(\boldsymbol{x}-\boldsymbol{y}). \tag{1.51}$$

Adding an external field as previously, the partition function (1.44) takes the form of a standard functional Gaussian integral. Calculating it yields

$$F[h] = F_0 - \frac{1}{2}\int d^d x\, d^d y\, h(\boldsymbol{x})G(\boldsymbol{x},\boldsymbol{y})h(\boldsymbol{y}), \qquad G(\boldsymbol{x},\boldsymbol{y}) = H^{-1}(\boldsymbol{x},\boldsymbol{y}). \tag{1.52}$$

We deduce

$$\langle\phi(\boldsymbol{x})\rangle = -\left.\frac{\delta F}{\delta h(\boldsymbol{x})}\right|_{h=0} = 0, \tag{1.53}$$

and

$$C(\boldsymbol{x},\boldsymbol{y}) = -k_{\mathrm{B}}T\frac{\delta^2 F}{\delta h(\boldsymbol{x})\delta h(\boldsymbol{y})} = k_{\mathrm{B}}T\, G(\boldsymbol{x},\boldsymbol{y}), \tag{1.54}$$

In addition, it can be shown that $G(\boldsymbol{x}, \boldsymbol{y}) = G(\boldsymbol{x} - \boldsymbol{y})$ with $G(\boldsymbol{x})$ the Green function of $\mathcal{L}$. Thus, solving for the Green function in Fourier space, we obtain finally

$$C(\boldsymbol{x}, \boldsymbol{y}) = k_{\mathrm{B}}T \int_{\boldsymbol{q}} \frac{e^{i\boldsymbol{q}\cdot(\boldsymbol{x}-\boldsymbol{y})}}{a + bq^2 + cq^4}. \tag{1.55}$$

This is a result to remember: **the correlation function of a Gaussian theory is equal to $k_{\mathrm{B}}T$ multiplied by the Green function of the operator associated with the Hamiltonian.**
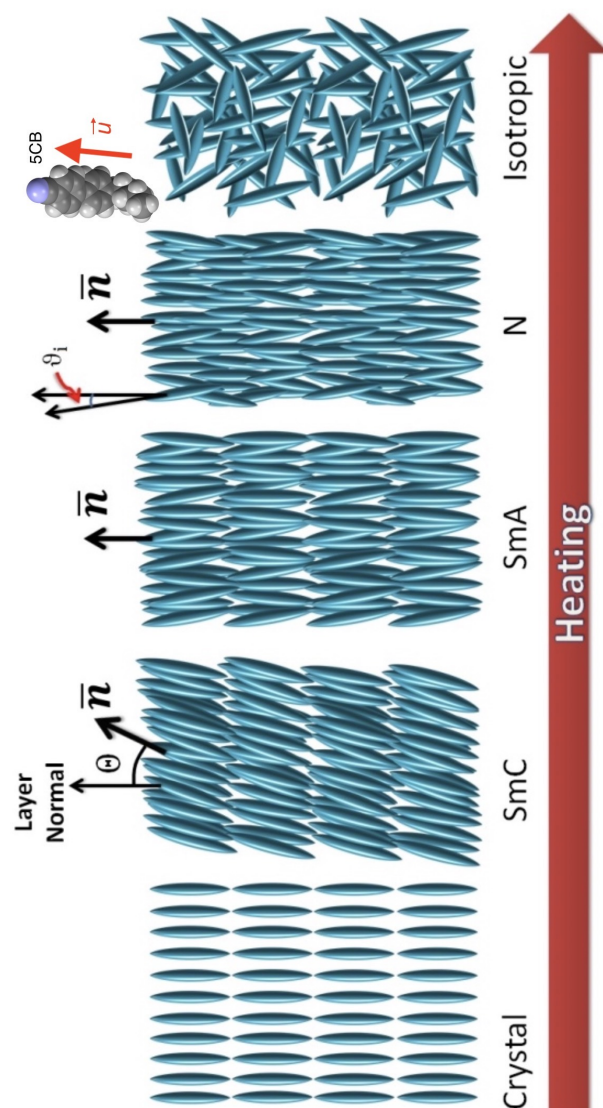
Chapter 2

NEMATIC LIQUID CRYSTALS

Figure 2.1: Schematic liquid crystal phases (Dierking et al.) and a 5CB molecule.

In a ferromagnet, the spins align (imperfectly) along a common direction,

In a nematic[1], the molecules align (imperfectly) along a common **axis**.

Choosing a unit vector $\boldsymbol{n}$ (or $-\boldsymbol{n}$) parallel to this axis defines the **director $\boldsymbol{n}$** of the nematic phase (see Fig. 2.1).

$$\boldsymbol{n} \Longleftrightarrow -\boldsymbol{n}. \tag{2.1}$$

Both the isotropic phase and the nematic phase are liquids: the positions of the molecules are completely random (not true for the smectic phases).

A) Molecular orientations in the nematic phase

The molecules that form nematic phases are called *nematogens*. They are not ideal ellipsoids as in Fig. 2.1. They are usually elongated polar molecules like the 5CB molecule in Fig. 2.1.

Let $\boldsymbol{u}$ be a vector attached to a molecule, oriented from tail to head

The exact orientation of a molecule can be specified by three angles (θ, ϕ, ψ), where $(\theta, \phi) = \boldsymbol{u}$, with $\cos\theta = \boldsymbol{u} \cdot \boldsymbol{n}$, and ψ is the intrinsic rotation angle of the molecule around $\boldsymbol{u}$.

The probability density $f(\boldsymbol{u}, \psi)$ that a molecule has the orientation $(\boldsymbol{u}, \psi)$ is uniform in the isotropic phase:

$$f(\boldsymbol{u}, \psi) = f_0 \quad \text{(isotropic phase)}. \tag{2.2}$$

In the **nematic phase**, f depends only on θ and it has a inversion symmetry:

$$f(\theta, \phi, \psi) = f_1(\boldsymbol{u}) = f_2(\theta) \tag{2.3}$$
$$f_1(-\boldsymbol{u}) = f_1(\boldsymbol{u}). \qquad (\theta \to \pi - \theta, \phi \to \phi + \pi) \tag{2.4}$$

In other words the direction in which the molecule points ($\boldsymbol{u}$ or $-\boldsymbol{u}$) and its intrinsic rotation (ψ) are statistically irrelevant. This is why in Fig. 2.1 the molecules are depicted as simple ellipsoids (average molecule).

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[1]an ordinary nematic

B)   Definition of a nematic phase

Phases are characterized by their symmetries (not by the shape and organization of their constituants).

The isotropic phase is an ordinary liquid: it is invariant under all translation and under the point group $O(3)$ of the transformations that leave the sphere invariant.

The **nematic phase** is an anisotropic liquid. It has a reduced symmetry. **By definition** it is invariant under

- all translations.

- the point group $D_{\infty h}$ of the transformation that leave the cylinder invariant (Schoenflies notation).

Problem: Consider a dense system of elongated molecules, with no positional order, that are randomly (imperfectly) oriented perpendicular to an axis Δ. This is obviously a very different situation from Fig. 2.1. Is this a nematic phase ?

C)   Nematic field and order-parameter

Ferromagnet

In a magnet the order-parameter is the average of the spin $\boldsymbol{S}_i$. The field is constructed from the local spatial average of the spins:

$$\boldsymbol{m}(\boldsymbol{r}) = [\boldsymbol{S}_i]_{\mathcal{B}(\boldsymbol{r},a)}, \tag{2.5}$$

and the order parameter (in a uniform magnet):

$$\begin{aligned} \boldsymbol{M} &= \langle \boldsymbol{m}(\boldsymbol{r}) \rangle \\ &= \langle\, [\boldsymbol{S}_i]_{\mathcal{B}(\boldsymbol{r},a)}\, \rangle = [\, \langle \boldsymbol{S}_i \rangle\,]_{\mathcal{B}(\boldsymbol{r},a)} = \langle \boldsymbol{S}_i \rangle, \end{aligned} \tag{2.6}$$

is nonzero in the ferromagnetic phase and zero in the paramagnetic phase.

Nematic

In a nematic, the order-parameter cannot be the average of the orientation of one molecular $\boldsymbol{u}_i$, as this vanishes by symmetry (no vector possesses $D_{\infty h}$ symmetry):

$$\langle \boldsymbol{u}_i \rangle = \int d\Omega\, \boldsymbol{u} f_1(\boldsymbol{u}) = \int d\Omega'\, (-\boldsymbol{u}') f_1(\boldsymbol{u}') = 0. \tag{2.7}$$

A natural candidate is therefore the tensor even in $\boldsymbol{u}_i$:

$$\langle \boldsymbol{u}_i \otimes \boldsymbol{u}_i \rangle \neq 0 \qquad \text{(nematic phase)}, \tag{2.8}$$

$$\langle \boldsymbol{u}_i \otimes \boldsymbol{u}_i \rangle = \frac{1}{3}\boldsymbol{I} \qquad \text{(isotropic phase)}, \tag{2.9}$$
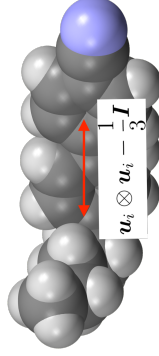
Figure 2.2: Microscopic tensor attached to a nematogen

To obtain an object with an average that vanishes in the isotropic phase, we therefore substract $\frac{1}{3}\boldsymbol{I}$ to construct the nematic field and the order parameter:

$$\boldsymbol{q}(\boldsymbol{r}) = \left[\boldsymbol{u}_i \otimes \boldsymbol{u}_i - \frac{1}{3}\boldsymbol{I}\right]_{\mathcal{B}(\boldsymbol{r},a)} \tag{2.10}$$

The order-parameter of a uniform nematic phase is therefore

$$\boldsymbol{Q} = \langle \boldsymbol{q}(\boldsymbol{r}) \rangle = \langle \boldsymbol{u}_i \otimes \boldsymbol{u}_i - \frac{1}{3}\boldsymbol{I}\rangle \tag{2.11}$$

Scalar nematic order-parameter

By construction $\boldsymbol{q}$ is a symmetric, traceless tensor. In a given basis, it has thus 5 independent components. In general, its three eigenvalues are all different, so it is called *biaxial* (two special axes can be identified).

However, due to the $D_{\infty h}$ symmetry of the nematic phase, $\boldsymbol{Q}$ is symmetric, traceless and *uniaxial* along $\boldsymbol{n}$ (or $-\boldsymbol{n}$). Choosing $\boldsymbol{z} \parallel \boldsymbol{n}$ makes $\boldsymbol{Q}$ diagonal with $Q_{xx} = Q_{yy} \neq Q_{zz}$.

It is convenient to define the *scalar order-parameter*:

$$S = \frac{3}{2}Q_{zz}. \tag{2.12}$$

We have then $\boldsymbol{Q} = \text{diag}(-\frac{1}{3}S, -\frac{1}{3}S, \frac{2}{3}S)$ in the (x, y, z) basis, i.e.,

$$\boldsymbol{Q} = S\left(\boldsymbol{n} \otimes \boldsymbol{n} - \frac{1}{3}\boldsymbol{I}\right). \tag{2.13}$$

We have then $S = 1$ if all the molecules are perfectly parallel or anti-parallel to $\boldsymbol{n}$, as is obvious from (2.11), and $S = 0$ in the isotropic phase. So S is the scalar order-parameter and $\boldsymbol{Q}$ is the tensorial order-parameter, while $\boldsymbol{n}$ is the director.

The statistical field theory will however be constructed from the field $\boldsymbol{q}(\boldsymbol{r})$, a biaxial symmetric traceless tensorial field.

D) Nematic effective Hamiltonian (close to the isotropic phase)

The interactions in a nematic phase are short ranged (van der Waals forces), so the effective Hamiltonian can be expanded, close to the isotropic phase, in the form of a local functional of q_{ij} and its gradients $q_{ij,k} = \partial q_{ij}(\boldsymbol{x})/\partial x_k$, etc.

The most general expansion up to order 4 complying with the symmetries is

$$\mathcal{H}[\boldsymbol{q}] = \int d^3x \, f(q_{ij}, q_{ij,k}, \dots), \tag{2.14}$$

$$f = \frac{1}{2}a(T)q_{ij}q_{ij} - \frac{1}{3}c(T)q_{ij}q_{jk}q_{ki} + \frac{1}{4}d_1(T)(q_{ij}q_{ij})^2 + \frac{1}{4}d_2(T)q_{ij}q_{jk}q_{k\ell}q_{\ell i} + \dots$$

$$+ \frac{1}{2}L_1(T)q_{ij,k}q_{ij,k} + \frac{1}{2}L_2(T)q_{ij,k}q_{kj,i} + \dots \tag{2.15}$$

In the following we shall call $\Phi(\boldsymbol{q})$ the non-gradient terms.

Let us comment on this expansion (we shall see more in the **tutorials**):

Linear term

The most general linear term is $\alpha_{ij}q_{ij}$, with α_{ij} a tensor (R1). It must be isotropic (R2) like the disordered phase, so $\alpha_{ij} = \alpha\delta_{ij}$, yielding $\alpha q_{ii} = 0$ as $\boldsymbol{q}$ is traceless. So the linear term vanishes.

Quadratic term

The most general quadratic term is $a_{ijk\ell}q_{ij}q_{k\ell}$, with $a_{ijk\ell}$ a 4-tensor (R1). It must be isotropic (R2), so it has to be constructed with Kroneckers deltas only. So $a_{ijk\ell} = a_1\delta_{ij}\delta_{k\ell} + a_2\delta_{ik}\delta_{j\ell} + a_3\delta_{i\ell}\delta_{jk}$. This yields $a_1q_{ii}q_{kk} + a_2q_{ij}q_{ij} + a_3a_2q_{ij}q_{ji} = (a_2+a_3)q_{ij}q_{ij}$, since $\boldsymbol{q}$ is traceless and symmetric. Calling $a = \frac{1}{2}(a_2 + a_3)$ we get $\frac{1}{2}aq_{ij}q_{ij}$.

Temperature dependance of the coefficients

If there is an isotropic–nematic transition at a temperature T_{NI}, it is a reasonable assumption that $a(T)$ *changes sign at some temperature* $T^\star$, going from $a > 0$ for $T > T^\star$ to $a < 0$ for $T < T^\star$. The most probable configuration, for small $\boldsymbol{q}$'s will then be $\boldsymbol{q} = 0$ at high temperature and $\boldsymbol{q} \neq 0$ at low temperature.

Since "most probable" and "average" are two different things, we do not expect $T_{\mathrm{NI}} = T^\star$, but the two should be rather close.

We thus assume

$$a(T) = a_0(T - T^\star) + O[(T - T^\star)^2] \tag{2.16}$$

$$c(T), d_1(T), d_2(T), L_1(T), L_2(T) > 0 \quad \text{(all positive).} \tag{2.17}$$

The other coefficients must be *all positive*, at least in the vicinity of the transition (where we make use of $\mathcal{H}$). For d_1 and d_2 this is required for stability reasons: if one was negative the probability of a uniform nematic phase would diverge with $\boldsymbol{q}$ (and we would need sixth-order terms to stabilize the Hamiltonian[2]). For c it is a convenient assumption (no loss of generality): if that is not the case, we can define $\boldsymbol{q}' = -\boldsymbol{q}$ and we are back to the situation $c > 0$ for $\boldsymbol{q}'$.

Consider now L_1 and L_2. Real nematics are spatially uniform at equilibrium. It can be shown that L_1 and L_2 must be positive for the associated terms to be always positive, so that spatially modulated conformations are penalized with respect to uniform situations.

E)   First-order nematic–isotropic transition (in mean field)

Within mean-field theory the order parameter $\boldsymbol{Q}(\boldsymbol{r})$ is given by the field $\boldsymbol{q}(\boldsymbol{r})$ that minimizes the effective Hamiltonian $\mathcal{H}[\boldsymbol{q}]$.

Because the space is invariant by translation and we expect the nematic phase to be uniaxial, we look for a uniform uniaxial nematic field[3]:

$$\boldsymbol{Q}(\boldsymbol{r}) = \boldsymbol{Q}_0 \qquad \text{(uniaxial).} \tag{2.18}$$

So we minimize $\Phi(\boldsymbol{Q})$ with $Q_{ij} = S(n_i n_j - \frac{1}{3}\delta_{ij})$ uniform. Substituting, we find

$$\Phi(S) = A(T - T^\star)S^2 - CS^3 + DS^4 + \dots \tag{2.19}$$

with

$$A = \frac{1}{3}a_0 > 0, \quad c = \frac{2}{27}c > 0, \quad D = \frac{1}{18}\left(2d_1 + d_2\right) > 0. \tag{2.20}$$

To do these calculations one can use matrix products and traces, or use Einstein's summation convention:

$$
\begin{aligned}
q_{ij}q_{ij} &= S^2 \left(n_i n_j - \frac{1}{3}\delta_{ij} \right)\left(n_i n_j - \frac{1}{3}\delta_{ij} \right) \\
&= S^2 \left(n_i n_i n_j n_j - \frac{2}{3}n_i n_j \delta_{ij} + \frac{1}{9}\delta_{ij}\delta_{ij} \right) \\
&= S^2 \left(1 - \frac{2}{3} + \frac{1}{3} \right) = \frac{2}{3}S^2,
\end{aligned}
\tag{2.21}
$$

since $n_i n_i = 1$ as the director is unitary and $\delta_{ii} = 3$ (in three dimensions).

---

[2]and fifth-order terms. That is actually a possibility, but it requires a separate study.

[3]In principle, we should check that there does not exist a lower biaxial minimum (depending on the values of the Hamiltonian's coefficients).
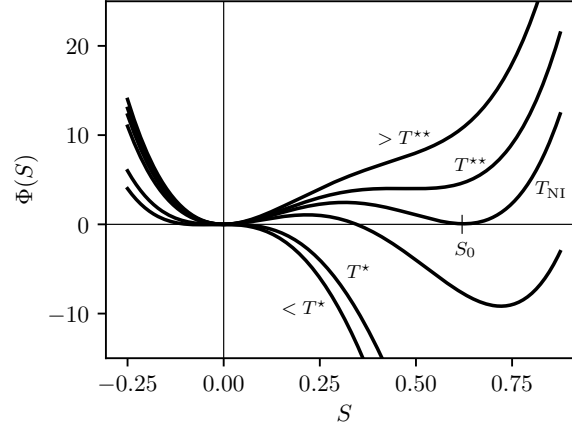
Figure 2.3: Mean-field (Landau) potential versus order-parameter in a typical first-order phase transition. The phase transition is at $T = T_{\mathrm{NI}}$. The temperature $T^\star$ and $T^{\star\star}$ are the lowest temperature below which the isotropic phase can exist (in a metastable state) and the highest temperature above which the nematic phase can exist (in a metastable state), respectively. The order at the transition is S_0. When $S_0 \ll 1$ the transition is said to be weakly first-order (i.e., almost second-order).

F)   Elasticity

For $T \ll T_{NI}$, the scalar-order parameter S can be considered constant (with a value very close to the minimum of $\Phi(S)$). However, although the ground state corresponds to a uniform $\boldsymbol{n}$, the local director $\boldsymbol{n}(\boldsymbol{r})$ can easily be distorted on large scales by the action of external boundary forces (fig. 2.4). This is a form of *elasticity*, since the nematic will relax to a uniform state if the external constraints are relaxed.

This director field $\boldsymbol{n}(\boldsymbol{r})$, in the SFT sense, can easily be obtained from the coarse-graining procedure: since $\boldsymbol{q}$ is symmetric and traceless (and not far from being uniaxial if the coarse-graining length is large), $\boldsymbol{n}(\boldsymbol{r})$ is simply defined as the eigenvenvector of $\boldsymbol{q}$ with largest eigenvalue (in absolute value)[4].

As derived in the **tutorials**, the elastic free energy deformation associated with the field $\boldsymbol{n}(\boldsymbol{r})$ has the form (first derived by F. C. Frank):

$$F[\boldsymbol{n}] = \int d^3r \left[\frac{1}{2}K_1 \left(\operatorname{div}\boldsymbol{n}\right)^2 + \frac{1}{2}K_2 \left(\boldsymbol{n}\cdot\operatorname{rot}\boldsymbol{n}\right)^2 + \frac{1}{2}K_3 \left(\boldsymbol{n}\times\operatorname{rot}\boldsymbol{n}\right)^2 \right], \qquad (2.22)$$

where the K_i's are three independent elastic constants. These three terms correspond to deformations of the type "splay", "twist" and "bend", respectively.

---

[4]One can write without loss of generality $\boldsymbol{q}(\boldsymbol{r}) = \operatorname{diag}(-\frac{1}{3}S + b, -\frac{1}{3}S - b, \frac{2}{3}S)$, which defines S, b and $\boldsymbol{n}$.
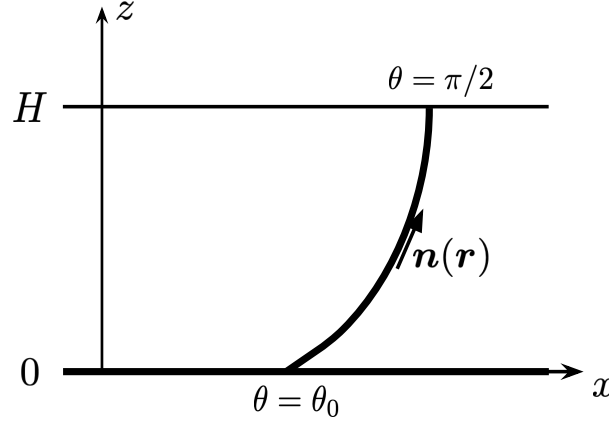
Figure 2.4: Smooth director distorsion caused by antagonistic "anchorings", i.e., antagonistic orientations of the director at the boundaries, in a hybrid cell. The nematic occupies the volume between $z = 0$ and $z = H$. The upper boundary fixes $\theta = \pi/2$ (strong anchoring). The lower boundary sets a preferred energy for $\theta = 0$ (weak anchoring), but the elastic torque coming from the bulk violates this preference.

G)   Topological defects

Definition: a *singularity* is a region where the director is not defined (it would be multivalued).

Definition: a transformation preserves the *topology* if it preserves the neighborhood relation between the points. For example, deforming a piece of clay preserves its topology, but breaking or punching a hole in it does not.

Definition: **Topological defects are singular regions of low dimension (e.g., points or lines) that are surrounded by order-parameter configurations that cannot be transformed to a homogeneous ground state via (spatially) continuous deformations.**

In nematics topological defects are called *disclinations*, i.e., defects relative to the inclination of the director ($\neq$ dislocations in crystals).

In the example of Fig. 2.4, there is no defect, since the director field can be continuously distorted to $\boldsymbol{n}(\boldsymbol{r}) = \boldsymbol{e}_z$, $\forall \boldsymbol{r}$.

Consider now the radial director field, $\boldsymbol{n}(r, \theta, \phi) = \boldsymbol{e}_r$. There is no way to continuously deform it in order to obtain a uniform state $\implies$ There is a point disclination at the origin.

Definitions:

- We now call $\boldsymbol{n}$ the order-parameter.

- We call "texture" the field $\boldsymbol{n}(\boldsymbol{r})$ (one can choose $\boldsymbol{n}$ or $-\boldsymbol{n}$ but in a continuous, consistent way).

- The order-parameter space, P_1, is the unit circle, where $\boldsymbol{n}$ is defined, but with *opposite points identified* (so that it is actually $\boldsymbol{n} \otimes \boldsymbol{n}$ that counts). In 3D it is the unit sphere with opposite points identified, called P_2.

1) Two dimensional nematic

The textures shown in Fig. 2.5 (right), with their central defects, are *disclinations*.
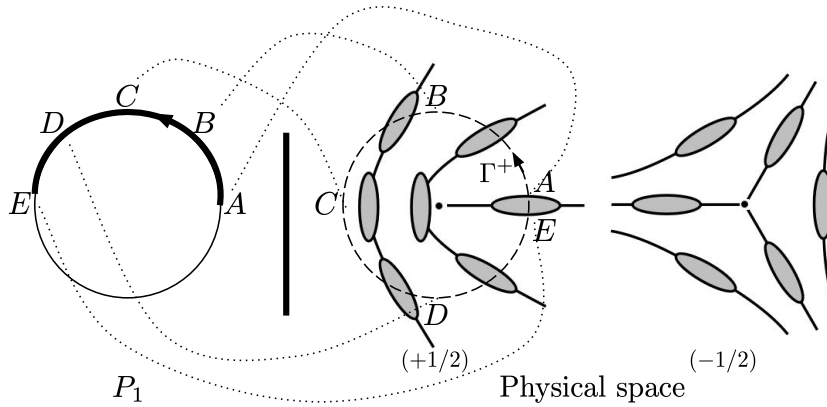
Figure 2.5: (Right) $+1/2$ and $-1/2$ disclination in the physical space. The ellipsoids represent the (headless) director $\boldsymbol{n} \otimes \boldsymbol{n}$. The dotted circle is an oriented path Γ^+ surrounding the $+1/2$ defect. (Left) Mapping to a path in the order parameter space P_1.

Identifying defects

Defects are identified by mapping a contour in physical space to a path in order-parameter space (Fig. 2.5)[5]. If the path in order-parameter space cannot be continuously shrunk to a point, the physical path surrounds a defect (or more than one).

In Fig. 2.5, there is no way to shrink the path in P_1 to a point, since A and E are the *same point*[6]

---

[5]The contour must not cross a singularity
[6]Any continuous distorsion will move $A \to A'$ and $E \to E'$ but will leave $A' \equiv E'$.

Topological charge

Along a path Γ^+ in physical space, oriented positively (counterclockwise), the topological charge is defined as

$$C(\Gamma^+) = \frac{1}{2\pi} \oint_{\Gamma^+} d\theta = \frac{\theta_f - \theta_i}{2\pi} = m, \qquad m \in \{\ldots, -\tfrac{3}{2}, -\tfrac{1}{2}, 0, \tfrac{1}{2}, \tfrac{3}{2} \ldots\}, \qquad (2.23)$$

with $\theta = \widehat{(\boldsymbol{n}, \boldsymbol{e}_x)}$. Indeed, since there is no singularity on the path, $\theta_f = \theta_i \; [\pi]$.

Thus only defects of half-integer charge are possible (see the $+\tfrac{1}{2}$ and the $-\tfrac{1}{2}$ charges in Fig. 2.5). They are not topologically equivalent since the path in P_1 goes clockwise for the $+1/2$ defect and counterclockwise for the $-1/2$ defect.

The charge is conserved, since splitting a contour Γ^+ into two sub-coutours gives

$$\int_{\Gamma^+} d\theta = \int_{\Gamma_1^+} d\theta + \int_{\Gamma_2^+} d\theta \qquad \Longrightarrow \qquad m = m_1 + m_2. \qquad (2.24)$$
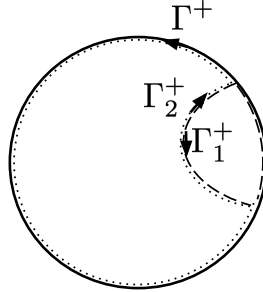
Figure 2.6: Path decomposition illustrating the conservation of the topological charge. Γ^+: solid line, Γ_1^+: dashed line, Γ_2^+: dotted line.

Defects localization.—If we find $m_1 + m_2 \neq 0$, but $m_1 = 0$, then we know that $m_2 \neq 0$, so the defect(s) is inside Γ_2. We can further split Γ_2 and go down localizing the defects.

2)   Three dimensional nematics

In 2D there are only point defects. Indeed, any angular discontinuity through a line can be spread into a continuous splay or bend deformation. Likewise in 3D there are only *line and point defects* (no walls).

Line defects

Consider in real space a closed contour Γ^+ and a line singularity that goes through it (Fig. 2.7).

The only stable line topological defects are those of 1/2 (with no sign), corresponding to a line in P_2 joining two opposite (i.e., identical) points. Indeed, because the line can roll on the P_2 sphere, any other path in P_2 can either be shrunk to such a line (1/2 disclination) or to a point (no defect).
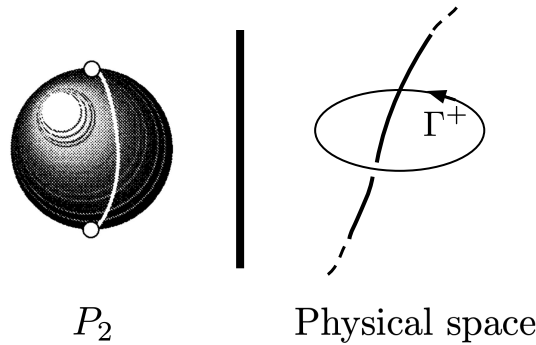

$$P_2 \qquad \text{Physical space}$$

Figure 2.7: Line defect in 3D real space (right) and the corresponding path in P_2 (left) showing a 1/2 defect. In physical space, this line must either close into a loop or end on some boundary surface.

Example 1: Consider the 3D line defects obtained by translating the $\pm 1/2$ defects of Fig. 2.5 perpendicularly to the plane of the page. Since P_1 has now become P_2 it is possible to rotate the path in order-parameter space around the horizontal axis of Fig. 2.5 in order to go from one situation to another: they are thus topologically equivalent.

Example 2: Consider a $+1$ defect in 2D. Consider then the 3D line defect obtained by translation. The image on P_2 of a coutour surrounding it is an equatorial circle. It can be shrunk to the north pole (rotating all directors towards the north pole), so it is not a defect.

Point defects (hedgehogs)

Consider in real space a spherical contour Ω surrounding a point singularity and the mapping of the director on P_2 (Fig. 2.8).

The topological charge q is defined in this way:

- If each point of P_2 is visited *1 time or less*: the charge is $q = 0$. For instance the texture is defect-free as the mapping can be shrunk continuously to a point.

- If each point of P_2 is visited *at least 1 time, but not at least 2 times*: the charge is $q = 1$. For instance there is a radial defect.
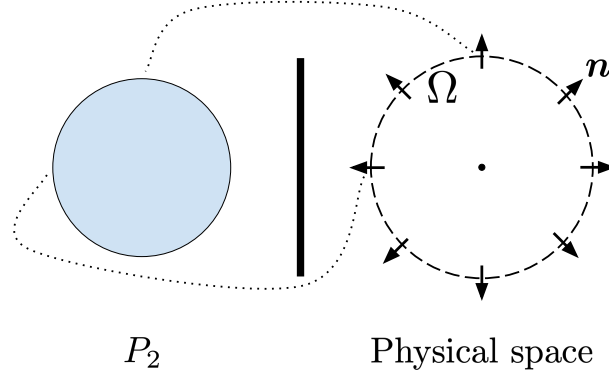
P_2 Physical space

Figure 2.8: (Right) Point disclination of charge 1 in 3D real space. The director field is radial: $\boldsymbol{n}(r, \theta, \phi) = \boldsymbol{e}_r$ in spherical coordinates. The dotted circle is the path Ω surrounding the central defect. (Left) Mapping onto P_2, covering all of it once exactly.

- If each point of P_2 is visited *at least 2 times, but not at least 3 times*: the charge is $q = 2$.

- etc.

It can be shown that the charge q is given by the following topological invariant:

$$q = \frac{1}{8\pi} \oint dS_i \, \epsilon_{ijk} \, \boldsymbol{n} \cdot (\partial_j \boldsymbol{n} \times \partial_k \boldsymbol{n}) . \tag{2.25}$$

Exemples of topologically equivalent point defects of topological charge 1 are given below:

(a)   (b)   (c)
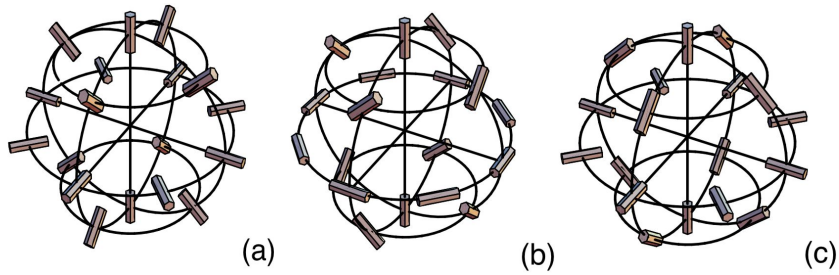
Figure 2.9: Three topologically equivalent hedgehogs of strength 1 (from Lubensky et al.). (a) A radial hedgehog in which the director points radially outward from a central point. (b) A circular hedgehog obtained from a radial hedgehog by rotating the director at every point through $\pi/2$ about the vertical axis. (c) A hyperbolic hedgehog obtained from the radial hedgehog by rotating the director at every point by π about the vertical axis.

Chapter 3

INTERFACES
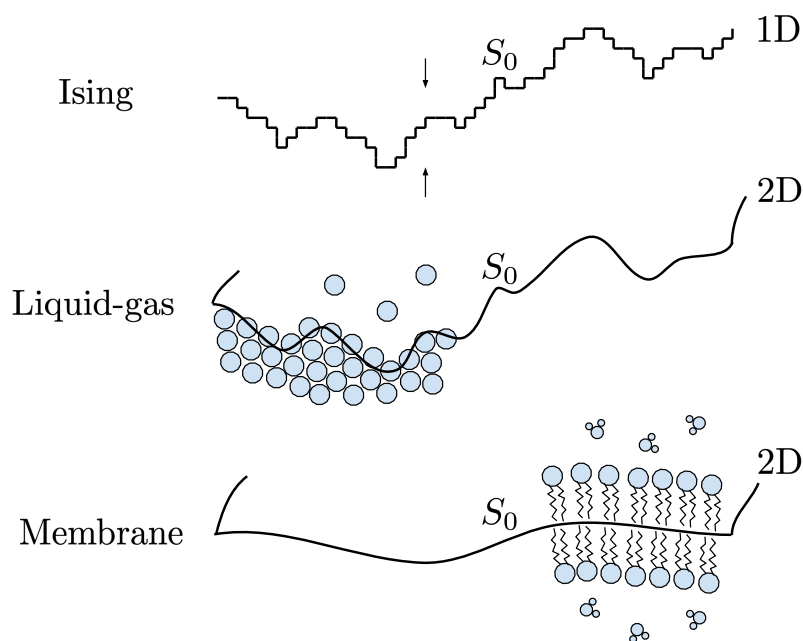
Figure 3.1: Microscopic interfaces S_0 for various coexisting phases.

A)   Coarse-graining and description by a field

Consider a system made of two phases that are in contact through an interface S_0, e.g., the 1D interface between a spin-up and a spin-down domain in the Ising model, the 2D interface between a liquid phase and its coexisting gas, a biological membrane made by a bilayer of phospholipids in an aqueous solvent (see Fig. 3.1).

In field theory, a microscopic resolution of the interface is not desired. To coarse-grain the interface (Fig. 3.2, left), we associate to each point $\boldsymbol{r}_0$ of S_0 a point $\boldsymbol{R}$ of a lower resolution interface S by averaging $\boldsymbol{r}$ over a ball $\mathcal{B}(\boldsymbol{r}_0, a)$.

29
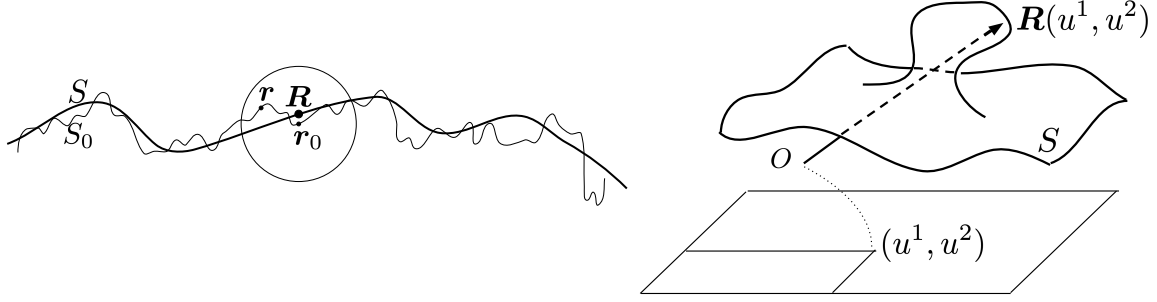
Figure 3.2: Coarse-graining of a microscopic interface (left) and definition of a field $\boldsymbol{R}(\{u^i\})$ describing the resulting low-resolution interface (right).

Whatever the complexity of S, it can mathematically be represented by a field

$$\boldsymbol{R}(u^1, u^2), \tag{3.1}$$

describing the mapping from $\boldsymbol{u} = (u^1, u^2)$ spanning a domain of $\mathbb{R}^2$, to the surface S, as illustrated in Fig. 3.2 (right).

For instance, if the interface has the topology of a rectangle (but a complicated shape), we can take $u^1 \in [0, L_1]$ and $u_2 \in [0, L_2]$, thinking of them as x and y, with $L_1 = L_2 = 1$ or any fixed value we wish (Fig. 3.2). If the interface is very strongly distorted but has the topology of a sphere, we can take $u^1 \in [0, \pi]$ and $u^2 \in [0, 2\pi]$, thinking of them as θ and ϕ, with periodic boundary conditions on u_2.

Then one can define an effective Hamiltonian associated with $\boldsymbol{R}(u^1, u^2)$ from the sum over all the physical microstates $\alpha \in \mathcal{E}[\boldsymbol{R}]$ that yield the same shape $\boldsymbol{R}$:

$$\mathcal{H}[\boldsymbol{R}] = -k_\mathrm{B} T \ln \sum_{\alpha \in \mathcal{E}[\boldsymbol{R}]} e^{-\beta H_\alpha}. \tag{3.2}$$

We end up (conceptually) with a field theory describing the interface.

B) Differential geometry of surfaces (metric tensor, curvature tensor)

At each point of the surface, parametrized by $\boldsymbol{R}(u^1, u^2)$, we can introduce a basis $(\boldsymbol{t}_1, \boldsymbol{t}_2)$ of tangent vectors, defined through

$$\boldsymbol{t}_i = \frac{\partial \boldsymbol{R}}{\partial u^i} \equiv \partial_i \boldsymbol{R}. \tag{3.3}$$

Note that the basis $(\boldsymbol{t}_1, \boldsymbol{t}_2)$ changes from point to point and is *not* orthonormal. It is therefore useful to introduce a dual basis $(\boldsymbol{t}^1, \boldsymbol{t}^2)$ such that

$$\boldsymbol{t}^i \cdot \boldsymbol{t}_j = \mathrm{Kronecker}(i, j) \equiv g^i_j \qquad \text{(new notation)}. \tag{3.4}$$
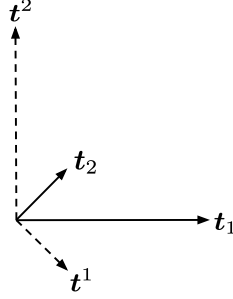
Figure 3.3: Dual bases $(\boldsymbol{t}_1, \boldsymbol{t}_2)$ and $(\boldsymbol{t}^1, \boldsymbol{t}^2)$ in the local tangent plane.

The two bases are "mutually orthonormal" (Fig. 3.3).

Then any tangent vector $\boldsymbol{V}$ can be written in two forms:

$$\boldsymbol{V} = V^i \boldsymbol{t}_i, \qquad \boldsymbol{V} = V_i \boldsymbol{t}^i. \tag{3.5}$$

which defines the "covariant" composants $V^i = \boldsymbol{V} \cdot \boldsymbol{t}^i$ and the "contravariant" composants $V_i = \boldsymbol{V} \cdot \boldsymbol{t}_i$ of the tangent vector.

Metric tensor

The metric tensor is defined by

$$g_{ij} = \boldsymbol{t}_i \cdot \boldsymbol{t}_j \qquad \text{(symmetric)}. \tag{3.6}$$

The actual tensor is actually the object

$$\boldsymbol{g} = g_{ij} \boldsymbol{t}^i \otimes \boldsymbol{t}^j. \tag{3.7}$$

Like vectors, tensors have covariant and contravariant components (or mixed). It is easy to show that $g^{ij} = \boldsymbol{t}^i \cdot \boldsymbol{t}^j$ and that $g^i_j = \boldsymbol{t}^i \cdot \boldsymbol{t}_j$ is the Kronecker delta, in agreement with the new notation above.

Proof: Let us write $\boldsymbol{g} = g_{ij} \boldsymbol{t}^i \otimes \boldsymbol{t}^j$ as some factor times $\boldsymbol{t}_k \otimes \boldsymbol{t}_\ell$:

$$\boldsymbol{g} = g_{ij} \left(\boldsymbol{t}^i \cdot \boldsymbol{t}^k \right) \boldsymbol{t}_k \otimes \left(\boldsymbol{t}^j \cdot \boldsymbol{t}^\ell \right) \boldsymbol{t}_\ell \tag{3.8}$$

$$g^{k\ell} = (\boldsymbol{t}_i \cdot \boldsymbol{t}_j) \left(\boldsymbol{t}^i \cdot \boldsymbol{t}^k \right) \left(\boldsymbol{t}^j \cdot \boldsymbol{t}^\ell \right) = \boldsymbol{t}^k \cdot \boldsymbol{t}^\ell \tag{3.9}$$

Then, we have

$$g_{ij} g^{jk} = (\boldsymbol{t}_i \cdot \boldsymbol{t}_j)(\boldsymbol{t}^j \cdot \boldsymbol{t}^k) = \boldsymbol{t}_i \cdot \boldsymbol{t}^k = g_i^k \tag{3.10}$$

therefore g^{ij} is the inverse matrix of g_{ij}.

Exercice: show that the tensor $\boldsymbol{g}$, i.e., $\boldsymbol{g} = g_{ij} \boldsymbol{t}^i \otimes \boldsymbol{t}^j$, is actually the identity tensor (a constant tensor).

Solution: $\boldsymbol{g} \cdot \boldsymbol{V} = (\boldsymbol{t}_i \cdot \boldsymbol{t}_j) \boldsymbol{t}^i \otimes \boldsymbol{t}^j \cdot \boldsymbol{V} = (\boldsymbol{t}_i \cdot \boldsymbol{t}_j) \boldsymbol{t}^i V^j = (\boldsymbol{t}_i \cdot \boldsymbol{V}) \boldsymbol{t}^i = \boldsymbol{V}, \forall \boldsymbol{V}.$

Raising and lowering of indices

The metric tensor allows to transform covariant indices into contravariant indices and vice-versa:

$$g_{ij}V^j = V_i, \quad g^{ij}V_j = V^i, \quad g^{jk}T_{ik} = T_i{}^j, \quad \ldots \tag{3.11}$$

The proof is straightforward:

$$g_{ij}V^j = \boldsymbol{t}_i \cdot \boldsymbol{t}_j V^j = \boldsymbol{t}_i \cdot \boldsymbol{V} = V_i, \quad \text{etc.} \tag{3.12}$$

Scalars, vectors and tensors

Using changes of parametrization (hence of bases, see below), it can be shown that multiplying vector or tensor components makes higher-order tensors:

$$V_i T^{jk} = U_i{}^{jk} \quad \text{3-tensor (mixed components).} \tag{3.13}$$

Contracting pairs of dummy *covariant/contravariant* indices via Einstein summation preserves the scalar, vector or tensor character:

$$V_i W^i (= V^i W_i) \quad \text{scalar,} \tag{3.14}$$

$$T_{ij}V^j \quad \text{vector (covariant component),} \tag{3.15}$$

$$T_i{}^i (= T^i{}_i = T_i{}^i) \quad \text{trace of a tensor (scalar).} \tag{3.16}$$

When changing parametrization, the coordinates $\{u^i\}$ of a point M become $\{u'^i\}$, with a mapping $u'^1 = f(u^1, u^2)$ and $u'^2 = g(u^1, u^2)$. Then

$$V'^i = \frac{\partial u'^i}{\partial u^k} V^k, \quad V_i' = \frac{\partial u^k}{\partial u'^i} V_k, \tag{3.17}$$

with obvious generalization to tensors, each component behaving as a vector. The proof is straightforward:

$$\boldsymbol{V} = V^k \boldsymbol{t}_k = V^k \frac{\partial \boldsymbol{R}}{\partial u^k} = V^k \frac{\partial \boldsymbol{R}}{\partial u'^i} \frac{\partial u'^i}{\partial u^k} = V^k \boldsymbol{t}_i' \frac{\partial u'^i}{\partial u^k}. \tag{3.18}$$

For the covariant composants, start with $V_i = \boldsymbol{V} \cdot \boldsymbol{t}_i$ and proceed in a similar way.

Proof of (3.14): $V_i W^i = g_{ik}V^k g^{i\ell}W_\ell = g_k^\ell V^k W_\ell = V^k W_k$. To show that this quantity is a scalar, let us show that it does not change if we change parametrization:

$$V'^i W_i' = \frac{\partial u'^i}{\partial u^k} V^k \frac{\partial u^\ell}{\partial u'^i} W_\ell = \frac{\partial u^\ell}{\partial u'^i} \frac{\partial u'^i}{\partial u^k} V^k W_\ell = V^\ell W_\ell. \tag{3.19}$$

The last equality follows from the chain rule which gives a Kronecker delta in front of $V^k W_\ell$. The same method can be used to prove that products and contractions preserve the tensor character.

Length and area

The elementary length ds associated with $d\boldsymbol{R} = (du^1, du^2)$ is given by

$$ds^2 = g_{ij} \, du^i \, du^j. \tag{3.20}$$

This follows simply from $ds^2 = d\boldsymbol{R} \cdot d\boldsymbol{R}$ and $d\boldsymbol{R} = \boldsymbol{t}_i du^i$.

The elementary area covered on the surface when we move the coordinates by du^1 and du^2, with $d^2u = du^1 \, du^2$, is given by

$$dA = \sqrt{g} \, d^2u, \tag{3.21}$$

where

$$g = \det(g_{ij}). \tag{3.22}$$

is the determinant of the metric tensor. Note that g is not a scalar (it depends on the parametrization).

Proof: $dA = ||\boldsymbol{t}_1 du^1 \times \boldsymbol{t}_2 du^2|| = \sqrt{(\boldsymbol{t}_1 \times \boldsymbol{t}_2)^2} \, d^2u$, with $(\boldsymbol{t}_1 \times \boldsymbol{t}_2)^2 = (t_1)^2(t_2)^2 \sin^2\theta = (t_1)^2(t_2)^2 - (\boldsymbol{t}_1 \cdot \boldsymbol{t}_2)^2 = g_{11} \, g_{22} - (g_{12})^2 = g$, where θ is the angle between $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$.

Covariant derivative

The covariant gradient $\boldsymbol{\nabla V}$ of a tangential vector field $\boldsymbol{V}$ is, by definition, its *tangential* gradient, such that[1]

$$(d\boldsymbol{V})_\parallel = d\boldsymbol{R} \cdot \boldsymbol{\nabla V}, \tag{3.23}$$

where $(d\boldsymbol{V})_\parallel$ is the projection of $d\boldsymbol{V}$ onto the tangent plane[2]. It can be shown that the components $D_i V^j$ of $\boldsymbol{\nabla V}$ are given by

$$D_i V^j = \partial_i V^j + \Gamma_{ik}^j V^k, \tag{3.24}$$

where the Christoffel symbols (not tensors) are defined through the variation of the tangential vectors

$$\partial_i \boldsymbol{t}_j = \Gamma_{ij}^k \boldsymbol{t}_k + L_{ij} \boldsymbol{n} \qquad \text{(definition of } \Gamma_{ij}^k\text{)}. \tag{3.25}$$

A direct formula for Γ_{ij}^k and the demonstration that is is symmetric for $i \leftrightarrow j$ will be given in the **tutorials**.

---

[1]Note that a tensor $\boldsymbol{a} \otimes \boldsymbol{b}$ acts *on the right* in the manner $\boldsymbol{V} \cdot \boldsymbol{a} \otimes \boldsymbol{b} = (\boldsymbol{V} \cdot \boldsymbol{a})\boldsymbol{b}$, actually behaving like its transpose $\boldsymbol{b} \otimes \boldsymbol{a}$.

[2]Why that? From the point of view of a 2D being that would live inside the surface of a sphere, the unit vector $\boldsymbol{e}_\phi$ of the spherical coordinates is constant as one moves along the equator. But it's 3D variation is actually normal to the sphere. We want it to vanish, so we must substract the normal component.

By definition, for scalars the covariant derivative coincides with the partial derivative:

$$D_i f \overset{\text{def.}}{=} \partial_i f \qquad (f \text{ scalar}). \tag{3.26}$$

Note that $\boldsymbol{R}$ is a scalar, i.e., a scalar with respect to surface parametrization (but not with respect to a change of the 3D basis).

For contravariant coordinates

$$D_i V_j = \partial_i V_j - \Gamma_{ij}^k V_k, \tag{3.27}$$

and the generalization to tensors is straightforward: $D_i T^{jk} = \partial_i T^{jk} + \Gamma_{i\ell}^j T^{\ell k} + \Gamma_{i\ell}^k T^{j\ell}$ (each component behaves as a vector component).

The product rule applies:

$$D_i(xy) = (D_i x)y + x D_i y \qquad (x, y \text{ scalars, or vectors/tensors components}) \tag{3.28}$$

but the covariant derivatives *do not* commute, i.e., $D_i D_j \neq D_j D_i$.

An important property (see **tutorials**) is that the covariant derivative of the metric tensor vanishes:

$$D_i g_{jk} = 0, \tag{3.29}$$

and, as a consequence $D_i g = 0$, since $g = g_{11} g_{22} - (g_{12})^2$.

Some demonstration follows. The gradient $\boldsymbol{\nabla} f$ of a scalar f is quite simple. It is defined through the relations

$$df = du^i \partial_i f = du^i \, \boldsymbol{t}_i \cdot (\partial_j f) \boldsymbol{t}^j = d\boldsymbol{R} \cdot \boldsymbol{\nabla} f, \qquad \Longrightarrow \qquad (\boldsymbol{\nabla} f)_j = \partial_j f. \tag{3.30}$$

For a vector, the difficulty comes from the fact that the variation of $\boldsymbol{V} = V^i \boldsymbol{t}_i$ involves also that of $\boldsymbol{t}_i$. We therefore need a *connection*, a relation between nearby tangent vectors. It is defined through the Christoffel symbols (and the second fundamental form L_{ij}):

$$\partial_i \boldsymbol{t}_j = \Gamma_{ij}^k \boldsymbol{t}_k + L_{ij} \boldsymbol{n}. \tag{3.31}$$

We have then

$$d\boldsymbol{V} = du^i \partial_i (V^j \boldsymbol{t}_j) = du^i \left[(\partial_i V^j) \boldsymbol{t}_j + V^j (\Gamma_{ij}^k \boldsymbol{t}_k + L_{ij} \boldsymbol{n}) \right], \tag{3.32}$$

$$(d\boldsymbol{V})_\parallel = du^i (\partial_i V^j + \Gamma_{ik}^j V^k) \boldsymbol{t}_j. \tag{3.33}$$

Since we can rewrite (3.23) as

$$(d\boldsymbol{V})_\parallel = du^i \boldsymbol{t}_i \cdot (D_k V^j) \boldsymbol{t}^k \otimes \boldsymbol{t}_j = du^i (D_i V^j) \boldsymbol{t}_j, \tag{3.34}$$

we obtain the formula (3.24).

Curvature tensor

The curvature tensor is defined by

$$\boldsymbol{K}_{ij} = D_i \boldsymbol{t}_j \quad \text{(symmetric tensor)}. \tag{3.35}$$

Note that these are the *components* of the curvature tensor, and that they are each actually 3D vectors. So the above object is quite complicated.

As a 3D vector, however, it is simply normal to the surface:

$$\boldsymbol{K}_{ij} = K_{ij}\, \boldsymbol{n}. \tag{3.36}$$

It follows that

$$K_{ij} = \boldsymbol{n} \cdot \partial_i \boldsymbol{t}_j\,, \tag{3.37}$$

which gives an easy way to compute the curvature tensor.

The demonstrations of these assertions follow. First the symmetry property: $\boldsymbol{K}_{ij} = D_i \partial_j \boldsymbol{R} = \partial_i \partial_j \boldsymbol{R} + \Gamma_{ij}^k \partial_k \boldsymbol{R} = \boldsymbol{K}_{ji}$, since $\Gamma_{ij}^k = \Gamma_{ji}^k$. Then, since the covariant derivative $D_i(\boldsymbol{t}_j \cdot \boldsymbol{t}_k)$ of the metric tensor vanishes, we have

$$\boldsymbol{t}_k \cdot \boldsymbol{K}_{ij} = \boldsymbol{t}_k \cdot D_i \boldsymbol{t}_j = -\boldsymbol{t}_j \cdot D_i \boldsymbol{t}_k = -\boldsymbol{t}_j \cdot \boldsymbol{K}_{ik} \tag{3.38}$$

$$= \boldsymbol{t}_i \cdot \boldsymbol{K}_{kj} = -\boldsymbol{t}_k \cdot \boldsymbol{K}_{ij} = 0. \tag{3.39}$$

Therefore the curvature tensor is normal: $\boldsymbol{K}_{ij} = K_{ij}\, \boldsymbol{n}$. It follows that $K_{ij} = \boldsymbol{n} \cdot D_i \boldsymbol{t}_j = \boldsymbol{n} \cdot (\partial_i \boldsymbol{t}_j - \Gamma_{ij}^k \boldsymbol{t}_k) = \boldsymbol{n} \cdot \partial_i \boldsymbol{t}_j$.

Principal curvatures

Since K_{ij} is symmetric, two scalar quantities can be defined from the real eigenvalues of K_i^j (at each point of the surface). Because $\boldsymbol{K}$ is a tensor, these scalars are independent of the parametrization and they are called the principal curvature $\{c_1, c_2\}$.

Indeed, we can always locally choose a flat metric, i.e., a parametrization $\boldsymbol{R}(s^1, s^2)$ such that s^1 and s^2 are the curvilinear coordinate along two perpendicular directions (Fig. 3.4). Then $(\boldsymbol{t}_1, \boldsymbol{t}_2)$ is orthornormal, and from 1D geometry, we know that $\partial \boldsymbol{t}_1 / \partial s_1 \propto \boldsymbol{n}$ with the coefficient been the curvature along the associated line drawn on the surface. If we rotate $(\boldsymbol{t}_1, \boldsymbol{t}_2)$ so as to diagonalize $\boldsymbol{K}$ we get the principal curvatures.

The principal curvatures are thus given by the relations:

$$c_1 + c_2 = K_i^i \quad \text{(total curvature, or twice the mean curvature)}, \tag{3.40}$$

$$c_1 c_2 = \det(K_i^j) = \frac{1}{2}(K_i^i K_j^j - K_i^j K_j^i) \quad \text{(Gaussian curvature)}. \tag{3.41}$$
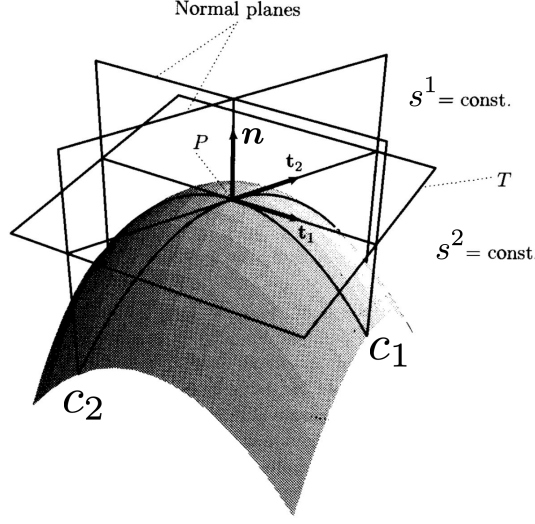
Figure 3.4: Principal curvatures c_1 and c_2 at a point of the surface. They are actually the maximum and minimum curvatures of the lines obtained by cutting the surface by a normal plane. Here the Gaussian curvature is $c_1 c_2 > 0$. When it is negative, the surface locally looks as a saddle. (Adapted from the book of Lubensky et al.)

where we have used the usual relation for 2×2 matrices $\det(A) = \frac{1}{2}[(\mathrm{tr}A)^2 - \mathrm{tr}A^2]$.

An interesting property is that the 3-tensor "gradient of curvature" is fully symmetric:

$$D_i K_{jk} = D_j K_{ik} \tag{3.42}$$

Proof: $D_i K_{jk} = D_i(\boldsymbol{n} \cdot D_j \boldsymbol{t}_k) = \boldsymbol{n} \cdot D_i D_j \boldsymbol{t}_k$. Indeed, $D_i \boldsymbol{n}$ is tangential, while $D_j \boldsymbol{t}_k$ is normal, thus the other term vanishes. Then we proceed as follows (using $\boldsymbol{n} \perp \boldsymbol{t}_k$):

$$\boldsymbol{n} \cdot D_i D_j \boldsymbol{t}_k = \boldsymbol{n} \cdot \left(\partial_i D_j \boldsymbol{t}_k - \Gamma_{ij}^\ell D_\ell \boldsymbol{t}_k - \Gamma_{ik}^\ell D_j \boldsymbol{t}_\ell \right) = \boldsymbol{n} \cdot \left(\partial_i \partial_j \boldsymbol{t}_k - \partial_i \left(\Gamma_{jk}^\ell \boldsymbol{t}_\ell \right) - \Gamma_{ij}^\ell \partial_\ell \boldsymbol{t}_k - \Gamma_{ik}^\ell \partial_j \boldsymbol{t}_\ell \right)$$
$$= \boldsymbol{n} \cdot \left(\partial_i \partial_j \boldsymbol{t}_k - \Gamma_{jk}^\ell \partial_i \boldsymbol{t}_\ell - \Gamma_{ij}^\ell \partial_\ell \boldsymbol{t}_k - \Gamma_{ik}^\ell \partial_j \boldsymbol{t}_\ell \right) = \boldsymbol{n} \cdot D_j D_i \boldsymbol{t}_k \,, \tag{3.43}$$

since the last expression is symmetric with respect to the exchange of i and j.

C)   Effective Hamiltonian

Assuming no long-range forces among the constituents of the interface and its surrounding phases, the effective Hamiltonian can be written as a surface integral:

$$\mathcal{H}[\boldsymbol{R}] = \int d^2 u \, \sqrt{g} \, h(u^1, u^2), \tag{3.44}$$

where h is the density of Hamiltonian.

1) Helfrich Hamiltonian

To construct the effective Hamiltonian, we need to determine which variables it depends on and identify a small parameter for the series expansion.

The energy density h should not change if we translate or rotate the patch of interface located at (u^1, u^2), so it cannot depend on $\boldsymbol{R}$ nor on $\boldsymbol{t}_i = \partial_i \boldsymbol{R}$. It will depend however on the the second derivative of $\boldsymbol{R}$, i.e., the curvature tensor K_{ij}. For small local deformations, this is a good parameter for the power series expansion.

Each term of the expansion should be scalar (R1). In the undistorted state, the interface is flat, isotropic (and translation invariant). So each term must comply with this symmetry (R2). The power series expansion of h is thus

$$h = \gamma + \lambda^{ij} K_{ij} + \kappa^{ijk\ell} K_{ij} K_{k\ell} + \ldots \qquad (3.45)$$

with λ^{ij} and $\kappa^{ijk\ell}$ isotropic (R2) tensors (R1). These tensors must be constructed from the identity tensor g^{ij} (recall that g_i^j is Kronecker).

The linear term h_1 is obtained from $\lambda^{ij} = \lambda g^{ij}$, yielding

$$h_1 = \lambda g^{ij} K_{ij} = \lambda K_i^i = \lambda(c_1 + c_2). \qquad (3.46)$$

The quadratic term h_2 is obtained from the most general isotropic 4-tensor: $\kappa^{ijk\ell} = \kappa_1 g^{ij} g^{k\ell} + \kappa_2 g^{ik} g^{j\ell} + \kappa_3 g^{i\ell} g^{jk}$. Inserting it in h_2 amounts to doing the sum of all possible contractions, yielding

$$h_2 = \kappa_1 K_i^i K_k^k + (\kappa_2 + \kappa_3) K_i^\ell K_\ell^i \qquad (3.47)$$

$$= \frac{1}{2} \kappa (c_1 + c_2)^2 + \bar{\kappa} c_1 c_2, \qquad (3.48)$$

where we have used (3.40) and (3.41), i.e., $K_i^i K_k^k = (c_1 + c_2)^2$ and $K_i^\ell K_\ell^i = (c_1 + c_2)^2 - 2c_1 c_2$.

We arrive at the general interface Hamiltonian, or Helfrich Hamiltonian:

$$\mathcal{H} = \int dA \left[\gamma + \lambda(c_1 + c_2) + \frac{1}{2} \kappa (c_1 + c_2)^2 + \bar{\kappa} c_1 c_2 + \ldots \right], \qquad (3.49)$$

featuring 4 parameters:

- γ: surface tension

- λ: coefficient of spontaneous curvature

- κ: bending rigidity

- $\bar{\kappa}$: Gaussian bending rigidity

$\longrightarrow$ **Tutorials, sheet 3, exercices (1), 2 and 3.**

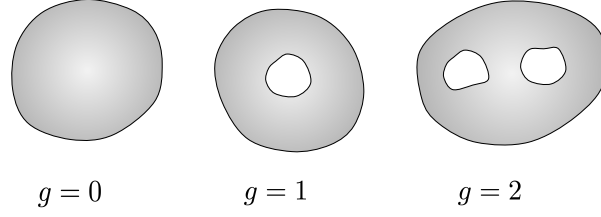$$g = 0 \qquad\qquad g = 1 \qquad\qquad g = 2$$

Figure 3.5: Closed surfaces with increasing genus.

2)   Gauss-Bonnet theorem

Theorem: The integral of the Gaussian curvature $c_1 c_2$ on a smooth close surface *does not* depend on the shape of the surface; it depends only on its *topology*. Or, if the surface has a planar topology, it depends only on how the membrane is shaped at its boundary.

More precisely, for a closed surface,

$$\oint dA\, c_1 c_2 = 4\pi(1 - g) \qquad \text{(Gauss Bonnet)}, \tag{3.50}$$

where g is the genus of the surface, i.e., the number of holes in it (Fig. 3.5).

3)   Monge jauge and small deformations

The Monge jauge is a convenient and intuitive way to parametrize an interface. The shape of the surface is described by a function

$$z = h(x, y) \tag{3.51}$$

giving the height of the membrane above each point of the (x, y) plane (Fig. 3.6).

We now have a 2D field $h(x, y)$ describing the shape of the interface. Note that strong deformations, like shapes with overhangs, cannot be described in this way.

Using covariant differential geometry (see **tutorials**) it can be shown that

$$dA = \sqrt{1 + (\boldsymbol{\nabla} h)^2}\, dx\, dy. \tag{3.52}$$

and

$$c_1 + c_2 = \frac{h_{xx}\left(1 + h_y^2\right) + h_{yy}\left(1 + h_x^2\right) - 2h_{xy}h_x h_y}{\left(1 + h_x^2 + h_y^2\right)^{3/2}}. \tag{3.53}$$
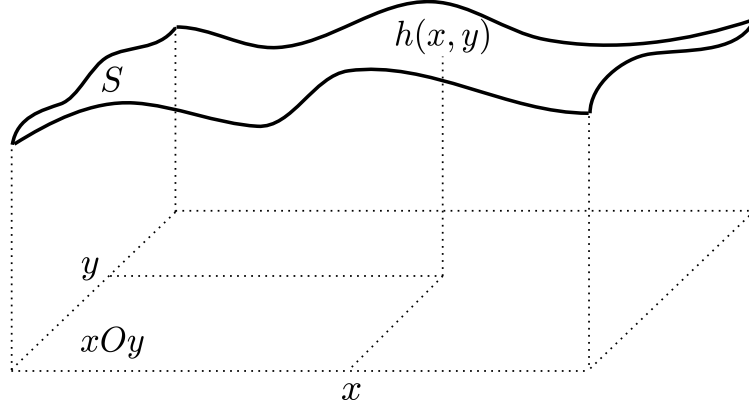
Figure 3.6: Monge parametrization.

Small deformations limit

The Monge jauge is particularly convenient in the limit of small deformations with respect to a flat shape. NB. It is not h that is small, but its derivatives.

We set $h_x = O(\epsilon)$ and $h_y = O(\epsilon)$, i.e., more precisely $h_x = \epsilon f(x,y)$ and $h_y = \epsilon g(x,y)$, with f and g of order 1. Then, to order ϵ^2, we have

$$dA = dx\,dy\left[1 + \frac{1}{2}(\boldsymbol{\nabla}h)^2\right] + O(\epsilon^4) \tag{3.54}$$

and

$$c_1 + c_2 = h_{xx} + h_{yy} + O(\epsilon^3). \tag{3.55}$$

Therefore, keeping only second derivatives and $O(\epsilon^2)$ terms, we have

$$\mathcal{H} = \int dA\left[\gamma + \lambda(c_1 + c_2) + \frac{1}{2}\kappa(c_1 + c_2)^2 + \text{B.T.}\right] \tag{3.56}$$

$$= \int dx\,dy\left[1 + \frac{1}{2}(\boldsymbol{\nabla}h)^2 + O(\epsilon^4)\right]\left[\gamma + \lambda\boldsymbol{\nabla}^2 h + \frac{1}{2}\kappa\left(\boldsymbol{\nabla}^2 h\right)^2 + O(\epsilon^3)\right]. \tag{3.57}$$

We have discarded the $c_1 c_2$ term, because its integral over the surface does not depend on the shape of the membrane thanks to the Gauss-Bonnet theorem (for fixed borders or an infinite membrane).

– The constant term $\gamma \int dx\,dy$ can be discarded as it is independent of the shape of the membrane).

– The term $\lambda\nabla^2 h$ can be discarded as it is a divergence. At this order it contributes then only a boundary term.

Therefore, up to terms $O(\epsilon^4)$, the effective Hamiltonian reduces to

$$\mathcal{H}[h] \simeq \int dx\, dy \left[\frac{1}{2}\gamma \left(\boldsymbol{\nabla} h\right)^2 + \frac{1}{2}\kappa \left(\boldsymbol{\nabla}^2 h\right)^2 \right] + O(\epsilon^3). \qquad (3.58)$$

Truncating the theory at this order, we therefore have a Gaussian field theory for the field $h(\boldsymbol{r})$, where $\boldsymbol{r} = (x, y)$, in which the first term describes the cost of increasing the area of the interface and the second one the cost of bending it.

4)   Effective Hamiltonian for phase boundaries and membranes

Phase boundaries

For an interface between two phases (liquid-gas, Ising, etc.), the constants κ and γ depend on the molecules constituting the phases (or on the coupling between the spins), and to a lesser extent on the temperature T.

It turns out that the quantity $\sqrt{\kappa/\gamma}$ (dimension of a length) is microscopic. It is then legitimate to neglect the bending term in our field theory. The effective Hamiltonian for a phase boundary (pb) reduces therefore to

$$\mathcal{H}_{pb} = \int d^2 r\, \frac{\gamma}{2} \left(\boldsymbol{\nabla} h\right)^2. \qquad (3.59)$$

Justification: let us perform a Fourier transform: $h(\boldsymbol{r}) = \int_{\boldsymbol{q}} h(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}}$. In terms of $h(\boldsymbol{q})$, the Hamiltonian becomes $\mathcal{H} = \int_{\boldsymbol{q}} (\gamma q^2 + \kappa q^4) |h(\boldsymbol{q})|^2$. To neglect the bending term, we need $\kappa q^2 \ll \gamma$, i.e., $q \ll \sqrt{\gamma/\kappa}$, $\forall q$. For phases boundaries, the quantity $\sqrt{\kappa/\gamma}$ arises from short-ranged molecular interactions and it is actually a molecular length[3]. So if the coarse-graining length a is much larger than this length, then all q's are much smaller that $2\pi/a$ and the conditions is verified for all q.

Membranes (free)

Biological membranes consist of lipids that have self-assembled into a bilayer in water. Their bending modulus (dimension of an energy in 2D) is of order $\kappa \approx 10 - 50\, k_{\mathrm{B}} T$ for ordinary lipids, at room temperature.

A huge difference with phase boundaries is that they are naturally tensionless $\gamma \approx 0$ (contrary to phase boundaries where γ is a material parameter). So the effective hamiltonian for a membrane (m) reduces to

$$\mathcal{H}_m = \int d^2 r\, \frac{\kappa}{2} \left(\boldsymbol{\nabla}^2 h\right)^2. \qquad (3.60)$$

---

[3]For water in equilibrium with its vapor it is of the order of the size of the water molecules. For the Ising model, it is of the order of the lattice spacing, etc. NB. For the water-vapor interface, $\gamma \simeq 50\,\mathrm{mJ/m}^2$.

Justification: lipids are insoluble in water, so their number N in the membrane is fixed. The area per lipid a_0 is essentially constant, so the total area $A \simeq N a_0$ of the membrane is essentially fixed.

To order ϵ^2, we have thus

$$N a_0 = \int d^2r \left[1 + \frac{1}{2} \left(\boldsymbol{\nabla} h \right)^2 \right], \tag{3.61}$$

$$\int d^2r \, \frac{1}{2} \left(\boldsymbol{\nabla} h \right)^2 = N a_0 - A_0 = \text{Cst}, \tag{3.62}$$

where $A_0 = \int d^2r$ is the area of the reference plane under the membrane, assumed fixed, or fixed on average in the thermodynamic limit. The surface energy term in (3.64) is therefore a constant energy, which can be omitted.

Membranes under external tension

Now, let us imagine that the reference plane is a frame and that an external tension $\gamma > 0$ is applied onto it, with potential energy

$$U = -\gamma A_0 \qquad \text{(when } A_0 \text{ increases } U \text{ is lowered)} \tag{3.63}$$

The surface tension γ can have any value, as it is chosen by the operator (contrary to phase boundaries where it is a material parameter).

From above, $A_0 = N a_0 - \int d^2r \frac{1}{2} (\boldsymbol{\nabla} h)^2$, so for a membrane under an external tension γ, we recover

$$\mathcal{H}_{mt}[h] = \int dx \, dy \left[\frac{1}{2} \gamma \left(\boldsymbol{\nabla} h \right)^2 + \frac{1}{2} \kappa \left(\boldsymbol{\nabla}^2 h \right)^2 \right], \tag{3.64}$$

but contrary to phase boundaries, γ can be given any value.

D) Fluctuations of phases boundaries and membranes

We are interested in the general behavior of interfaces in d dimensions (although ordinary interfaces are for $d = 2$, or $d = 1$).

1) Correlation function and fluctuation spectrum

Let us apply the general results of Gaussian field theory. The effective Hamiltonian of a generic interface is

$$\mathcal{H} = \int d^2r \left[\frac{\gamma}{2} (\partial_i h) \partial_i h + \frac{\kappa}{2} (\partial_i \partial_i h) \partial_j \partial_j h \right] \tag{3.65}$$

$$= \frac{1}{2} \int d^2r \, h \left(-\gamma \partial_i \partial_i + \kappa \partial_j \partial_j \partial_i \partial_i \right) h + \text{B.T.} \tag{3.66}$$

The operator is therefore $\mathcal{L} = -\gamma\boldsymbol{\nabla}^2 + \kappa(\boldsymbol{\nabla}^2)^2$, of Green function $G(\boldsymbol{r})$ obeying $\mathcal{L}G(\boldsymbol{r}) = \delta(\boldsymbol{r})$. The correlation function is $k_{\mathrm{B}}T$ multiplied by the Green function.

Let us perform the Fourier transform $G(\boldsymbol{r}) = (1/L^d)\sum_{\boldsymbol{q}} G_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{r}}$. We therefore assume a finite size system, with $\boldsymbol{r} \in [0, L]^d$ and periodic boundary conditions[4]. We obtain[5]

$$(\gamma q^2 + \kappa q^4)G(\boldsymbol{q}) = 1. \tag{3.67}$$

The correlation function is therefore

$$\langle h(\boldsymbol{r})h(\boldsymbol{r}')\rangle = C(\boldsymbol{r} - \boldsymbol{r}') = k_{\mathrm{B}}T G(\boldsymbol{r} - \boldsymbol{r}') = \frac{k_{\mathrm{B}}T}{L^d}\sum_{\boldsymbol{q}} \frac{e^{i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{\gamma q^2 + \kappa q^4}. \tag{3.68}$$

Or, taking the thermodynamic limit ($L \to \infty$),

$$C(\boldsymbol{r}) = k_{\mathrm{B}}T \int_{\boldsymbol{q}} \frac{e^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{\gamma q^2 + \kappa q^4}. \tag{3.69}$$

Let us now determine the height fluctuation spectrum $\langle|h_{\boldsymbol{q}}|^2\rangle$, i.e., the amplitude of the modes $h_{\boldsymbol{q}}$ at thermal equilibrium. We first look for the correlation function in Fourier space $\langle h_{\boldsymbol{q}} h_{\boldsymbol{q}'}\rangle$:

$$\langle h(\boldsymbol{r})h(\boldsymbol{r}')\rangle = \frac{k_{\mathrm{B}}T}{L^d}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{q}'} \frac{e^{i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{\gamma q^2 + \kappa q^4}\delta_{\boldsymbol{q}+\boldsymbol{q}'} \tag{3.70}$$

$$= \frac{k_{\mathrm{B}}T}{L^d}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{q}'} \frac{e^{i\boldsymbol{q}\cdot\boldsymbol{r}} e^{i\boldsymbol{q}'\cdot\boldsymbol{r}'}}{\gamma q^2 + \kappa q^4}\delta_{\boldsymbol{q}+\boldsymbol{q}'}, \tag{3.71}$$

which implies

$$\langle h_{\boldsymbol{q}} h_{\boldsymbol{q}'}\rangle = k_{\mathrm{B}}T \frac{L^d \delta_{\boldsymbol{q}+\boldsymbol{q}'}}{\gamma q^2 + \kappa q^4}, \tag{3.72}$$

and therefore, taking $\boldsymbol{q}' = -\boldsymbol{q}$,

$$\langle|h_{\boldsymbol{q}}|^2\rangle = \frac{k_{\mathrm{B}}T L^d}{\gamma q^2 + \kappa q^4}. \tag{3.73}$$

For phase boundaries we will take $\kappa = 0$ and for membranes $\gamma = 0$ (in the absence of an externally applied tension).

---

[4]This will be convenient for calculating the fluctuation spectrum.
[5]We have used $\delta(\boldsymbol{r}) = L^{-d}\sum_{\boldsymbol{q}} 1 e^{i\boldsymbol{q}\cdot\boldsymbol{r}}$, see chapter 1, section (E)(2).
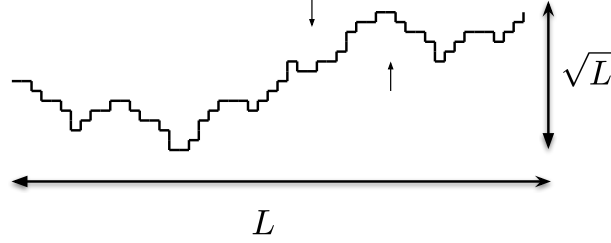
Figure 3.7: Roughness of a 1D interface in the two-dimensional Ising model.

2)   Infrared and ultraviolet divergences

We will encounter, in dimension d, integrals like

$$I(d, n) = \int_{\boldsymbol{q}} \frac{1}{q^n} \quad : \quad \text{IR divergent for } d \leq n. \tag{3.74}$$

where $\int_{\boldsymbol{q}} = \int [d^d q/(2\pi)^d]$.

Such an integral always "diverges". If it diverges for $q \to 0$ it is said to have an infrared (IR) divergence (long wavelengths), and if it diverges for $q \to \infty$ it is said to have an ultraviolet (UV) divergence (short wavelengths).

Precisely, using generalized spherical coordinates $(q, \theta_1, \ldots, \theta_{d-2}, \phi)$

$$I(d, n) = \int q^{d-1} dq \, d\Omega \, \frac{1}{q^n} = \int d\Omega \int_{\frac{2\pi}{L} \to 0}^{\frac{2\pi}{a}} \frac{dq}{q^{1+n-d}}, \tag{3.75}$$

where we have indicated the IR boundary $\approx 2\pi/L$ (with $L \to \infty$ in the thermodynamic limit) is the lateral size of the interface[6], and the UV boundary $\approx 2\pi/a$, the finite cutoff.

We *don't care* about the UV divergence, because we never have $q \to \infty$ thanks to the cutoff.

We *do care* about the IR divergence: it gives the behavior in the thermodynamic limit. The integral $I(d, n)$ diverges for $q \to 0$ when $1 + n - d \geq 1$, i.e., $d \leq n$.

3)   Width of the interface

From the correlation function (3.68) with $\boldsymbol{r}' = \boldsymbol{r}$, we obtain, for phase boundaries and tensionless membranes:

$$\langle h^2 \rangle_{pb} = \frac{k_{\mathrm{B}}T}{\gamma} \int_{\boldsymbol{q}} \frac{1}{q^2}, \quad \text{IR divergent for } d \leq D_{pb} = 2 \tag{3.76}$$

$$\langle h^2 \rangle_m = \frac{k_{\mathrm{B}}T}{\kappa} \int_{\boldsymbol{q}} \frac{1}{q^4}, \quad \text{IR divergent for } d \leq D_m = 4. \tag{3.77}$$

---

[6]The Fourier modes would be multiples of $2\pi/L$ for periodic boundary conditions, or multiples of π/L for pinned boundary conditions.

rough   2   flat

Phase boundary |———————————|———————————→ d

oriented

rough   4   flat

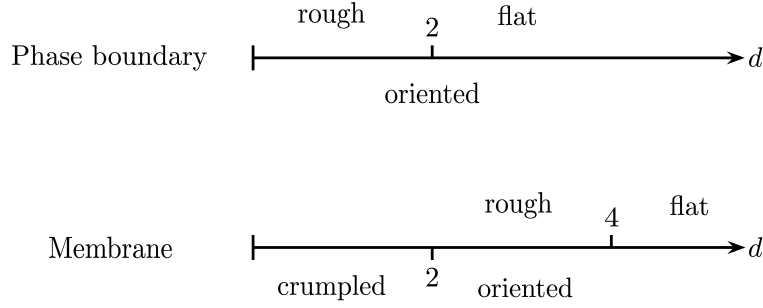Membrane |———————————|———————————→ d

crumpled   2   oriented

Figure 3.8: Rugosity and orientation behavior of phase boundaries and membranes.

- For $d > D$ (i.e., D_{pb} or D_m), the variance $\langle h^2 \rangle$ is finite (stopped UV divergence and IR convergence). The interface is "flat", since in the (thermoynamic) limit of large scales $L \to \infty$, its thickness $w = (\langle h^2 \rangle)^{1/2}$ is negligibly small.

- For $d \leq D$, the variance $\langle h^2 \rangle$ is IR-divergent, so the thickness of the interface diverges as $L \to \infty$. The interface is then qualified as "rough". Precisely,

$$w^2 \sim L^{D-d}. \tag{3.78}$$

For instance, in the 2D Ising model, the width of the interface is rough as $w_{pb} \sim L^{1/2}$, corresponding to $d = 1$ and $D = 2$ (Fig. 3.7).

4) Orientation of the interface

In the limit of small deformations, the normal to the interface (see **tutorials**) is given by $\boldsymbol{n} \simeq (-\partial_x h, -\partial_y h, 1)$, so its inclination in the x and y directions are

$$\theta_x = \partial_x h, \qquad \theta_y = \partial_y h. \tag{3.79}$$

To calculate the variance $\langle \theta_x^2 \rangle$ of the interface orientation, we proceed as follows

$$\langle h(\boldsymbol{r}) h(\boldsymbol{r}') \rangle = k \int_{\boldsymbol{q}} \frac{e^{i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{q^D}, \tag{3.80}$$

$$\langle \partial_x h(\boldsymbol{r}) \, \partial_{x'} h(\boldsymbol{r}') \rangle = k \int_{\boldsymbol{q}} (iq_x)(-iq_x) \frac{e^{i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{q^D}, \tag{3.81}$$

$$\langle \theta_x^2 \rangle = k \int_{\boldsymbol{q}} q_x^2 \frac{1}{q^\alpha} = \frac{k}{2} \int_{\boldsymbol{q}} (q_x^2 + q_y^2) \frac{1}{q^D} \tag{3.82}$$

$$= \frac{k}{2} \int_{\boldsymbol{q}} \frac{1}{q^{D-2}}, \quad \text{IR divergent for } d \leq D' = D - 2. \tag{3.83}$$

with $D = 2$ and $k = k_B T/\gamma$ for phase boundaries and $D = 4$ and $k = k_B T/\kappa$ for membranes.

The same reasoning as before applies with now $D' = D - 2$. So for $d > D'$ the variance of the orientation is finite, so the interface is "oriented", while for $d \leq D'$ the variance of the orientation diverges as $L \to \infty$, so the interface is said to be "crumpled".
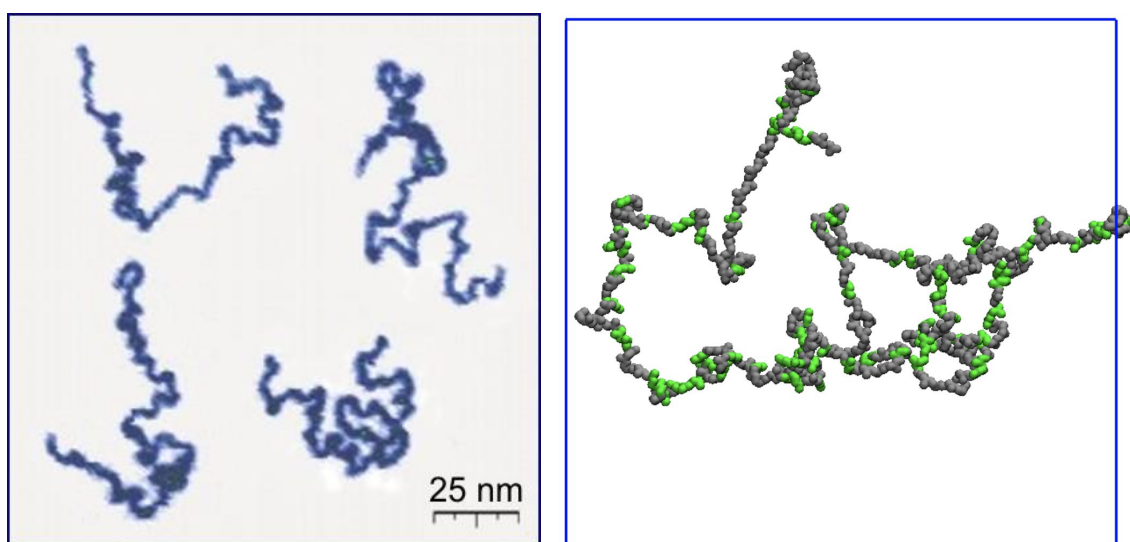
Chapter 4

Polymers

Figure 4.1: (Left) Poly(2-vinylpyridine) polymer chains on a surface, imaged with an AFM microscope in a liquid medium (Roiter et al., 2005). (Right) Molecular simulation of a polyisoprene polymer (Degiacomi et al., 2015). The cis and trans monomers are shown in gray and green, respectively.

A)   Introduction

Polymers are very long molecules (macromolecules), made by the attachement of short subunits called monomers. The monomers can be all the same (homopolymer) or different (heteropolymer). Polymers can be linear or branched. They exist naturally in the biological world (glycogen, actin, microtubules, DNA, etc.) and are synthesized in the chemical industry (polyethylene $|–CH_2–|_N$, etc.).

The polymer chain always lies in a solvent. There are two possible scenarios:

- *Good solvent conditions*: If the monomer/solvent interactions are favorable, the polymer will swell into the solvent and gain entropy (Fig. 4.1).

- *Bad solvent conditions*: If the monomers and solvent repel each other strongly, the polymer will collapse into a dense coil (despite the entropy loss).

Limited flexibility.—There is some freedom for the orientation of neighboring monomers, but also some constraints and energetical preferences:
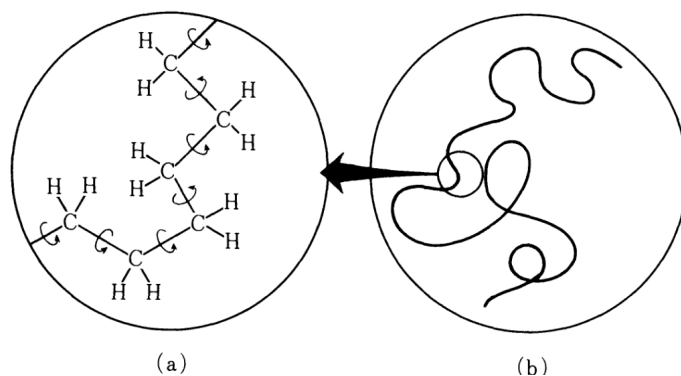

(a)   (b)

Figure 4.2: (a) Atomic structure of a polyethylene molecule. (b) Overview of the polymer. Each C–C bond is constrained to make a fixed angle θ with the next. The freedom of rotation around each C–C bond is hindered by energy preferences (from Doi's book).

Large loop interactions.—Monomers far apart along the chain can still approach each other. They undergo van der Waals interactions, and most importantly excluded volume interactions (impenetrability). This has tremendous consequences on the statistics of polymer chains.
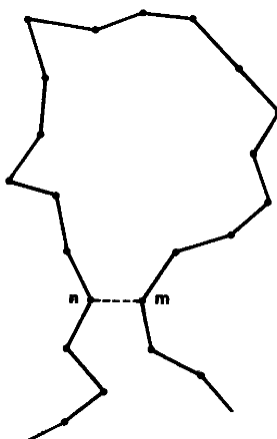

Figure 4.3: Interaction between two monomers, n and m, that are a long distance apart along the chain (from de Gennes' book).

In this chapter, we are going to focus on the *universal physical properties* of very long linear homopolymers in good solvent conditions.
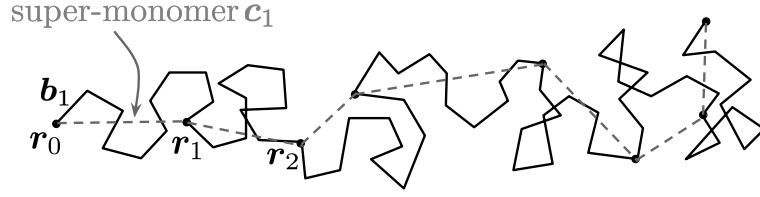
Figure 4.4: Coarse-graining of an ideal polymer chain. Sets of m consecutive monomers ($\boldsymbol{b}_i$) are grouped into super-monomers ($\boldsymbol{c}_j$). The coarse-grained polymer is the chain $\{\boldsymbol{r}_0, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_n\}$. For m very large, the distribution of the end-to-end vectors of the super-monomers is Gaussian.

B) Field theory of ideal polymer chains

An *ideal* polymer is, by definition, a polymer in which the large-loop interactions are neglected. It is thus a phantom chain that can cross itself with no penalty (limited flexibility and local interactions are taken into account, however).

As we shall see, an ideal chain is described, in the thermodynamic limit, by a *Gaussian field theory*.

1) Coarse-graining

Let us consider an ideal polymer chain made of an extremely large number $N \gg 1$ of monomers $\boldsymbol{b}_i$ of length b. Because of the limited flexibility between neighboring monomers, the correlation between monomers is *not zero*, but it does vanish exponentially at large chemical intervals $|i - j|$ (see **Tutorials**):

$$\langle \boldsymbol{b}_i \cdot \boldsymbol{b}_j \rangle \sim e^{-|i-j|/\Delta}. \tag{4.1}$$

The quantity $\ell_p = b\Delta$ is called the persistence length (persistence of orientation).

Les us form $n = N/m \gg 1$ *super-monomers* $\boldsymbol{c}_j$ by grouping together m successive monomers into one subunit (see Fig. 4.4). We assume

$$m = m_1 m_2, \qquad \text{with} \quad m_1 \gg \Delta, \quad m_2 \gg 1. \tag{4.2}$$

These super-monomers form a polymer chain with positions $\{\boldsymbol{r}_0, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_n\}$.

The end-to-end vector $\boldsymbol{r}_j - \boldsymbol{r}_{j-1}$ of super-monomers $\boldsymbol{c}_j$ is such that

$$(\boldsymbol{r}_j - \boldsymbol{r}_{j-1})_x = \sum_{i=(j-1)m}^{jm} (\boldsymbol{b}_i)_x = X_{j,1} + \ldots + X_{j,m_2}, \tag{4.3}$$

where each of the m_2 variables $X_{j,k}$ is a sum of m_1 components $(\boldsymbol{b}_i)_x$.

Since $m_1 \gg \Delta$ and the chain is assumed ideal, the $X_{j,k}$ form a set of identical, *effectively independent* variables:

$$\langle X_{j,k} \rangle = 0, \quad \langle X_{j,k} X_{j,k'} \rangle = 0, \quad \langle X_{j,k}^2 \rangle = \sigma^2(T). \tag{4.4}$$

Applying the central limit theorem (since $m_2 \gg 1$), the distribution of $X_j = (\boldsymbol{r}_j - \boldsymbol{r}_{j-1})_x$ is a centered Gaussian of variance $\langle X_j^2 \rangle = m_2\sigma^2$:

$$P(X_j) = \left(2\pi m_2\sigma^2\right)^{-1/2} e^{-\frac{X_j^2}{2m_2\sigma^2}}. \tag{4.5}$$

Since the three space directions are independent, the probability distributions factorize, and with $X_j^2 + Y_j^2 + Z_j^2 = (\boldsymbol{r}_j - \boldsymbol{r}_{j-1})^2$, we have

$$P(\boldsymbol{r}_j - \boldsymbol{r}_{j-1}) = \left(2\pi m_2\sigma^2\right)^{-3/2} e^{-\frac{\left(\boldsymbol{r}_j - \boldsymbol{r}_{j-1}\right)^2}{2m_2\sigma^2}}. \tag{4.6}$$

Finally, since the super-monomers are independent (ideality), we arrive at

$$P(\boldsymbol{r}_0, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_n) = \left(2\pi m_2\sigma^2\right)^{-3n/2} e^{-\frac{1}{2m_2\sigma^2}\sum_{j=1}^{n}(\boldsymbol{r}_j - \boldsymbol{r}_{j-1})^2}, \tag{4.7}$$

which is a Gaussian probability distribution. Note that it ressembles a canonical distribution $\propto \exp(-\beta H_{\text{eff}})$.

2) Radius of gyration (ideal chain)

The radius of gyration, or effective size, R_g, of a polymer chain is defined as the standard deviation of the end-to-end vector $\boldsymbol{R} = \sum_{i=1}^{N} \boldsymbol{b}_i = \sum_{j=1}^{n} \boldsymbol{c}_j$.

Since $\langle \boldsymbol{c}_j^2 \rangle = \langle X_j^2 \rangle + \langle Y_j^2 \rangle + \langle Z_j^2 \rangle = 3m_2\sigma^2$ (in three dimensions) and $\langle \boldsymbol{c}_j \cdot \boldsymbol{c}_{j'} \rangle = 0$, we get

$$R_g^2 = \langle \boldsymbol{R}^2 \rangle = \left\langle \left(\sum_{j=1}^{n} \boldsymbol{c}_j\right)^2 \right\rangle = n \times 3m_2\sigma^2 + \sum_{j}\sum_{j\neq j'}\langle \boldsymbol{c}_j \cdot \boldsymbol{c}_{j'} \rangle = 3N\frac{\sigma^2}{m_1}. \tag{4.8}$$

We may rewrite this as $(d = 3)$

$$R_g^2 = d \times Na^2, \tag{4.9}$$

which defines an effective momomer size $a(T) = \sigma/\sqrt{m_1}$. Note that a is actually independent of our choice of m_1, since it is the ratio of two quantities independent of our description.

Freely-jointed chain.—The Freely-jointed chain is a toy model in which the N monomers of length b have full orientational freedom. We have then $R_g^2 = \langle (\sum_{i=1}^{N} \boldsymbol{b}_i)^2 \rangle = Nb^2$, since $\langle \boldsymbol{b}_i \cdot \boldsymbol{b}_j \rangle = 0$ $(j \neq i)$, so that $a(T) = b$.

Hence, $a(T)$ can be seen as the monomer length of an equivalent freely-jointed chain.

Thus, for an ideal chain (whatever the limited flexibility between neighboring monomers), we find

$$R_g \sim N^\nu, \qquad \nu = \frac{1}{2}, \tag{4.10}$$

very much like a diffusion process (monomer index replaces time).

Definition of the Kuhn length. For an ideal chain, the Kuhn length b_{K} and the number N_{K} of Kuhn segments are defined by a mapping to the freely-jointed model, through the two relations: $Nb = N_{\mathrm{K}}b_{\mathrm{K}}$ (equality of the total length of the polymer) and $R_g^2 = N_{\mathrm{K}}b_{\mathrm{K}}^2$ (freely jointed). Thus $R_g^2 = Nb\,b_{\mathrm{K}}$ and the Kuhn length is defined by $b_{\mathrm{K}} = R_g^2/(Nb)$. Using the results above, we find the correspondance $b_{\mathrm{K}} = a^2/b$.

3) Gaussian field theory

For $n \gg 1$, we treat j as a continuous variable $j \in [0, n]$:

$$\boldsymbol{r}_j \to \boldsymbol{r}(j), \tag{4.11}$$

$$\boldsymbol{r}_j - \boldsymbol{r}_{j-1} \to \frac{d\boldsymbol{r}}{dj} = \dot{\boldsymbol{r}}, \tag{4.12}$$

$$\left(2\pi m_2\sigma^2\right)^{-3n/2} d^3r_1 \ldots d^3r_n \to \mathcal{D}[\boldsymbol{r}], \tag{4.13}$$

$$\frac{1}{2m_2\sigma^2} \sum_{j=1}^{n} (\boldsymbol{r}_j - \boldsymbol{r}_{j-1})^2 \to \int_0^n dj\, \frac{1}{2m_2\sigma^2} \dot{\boldsymbol{r}}^2 = \mathcal{H}[\boldsymbol{r}], \tag{4.14}$$

This yields

$$d^3r_1 \ldots d^3r_n P(\boldsymbol{r}_0, \ldots, \boldsymbol{r}_n) \to \mathcal{D}[\boldsymbol{r}]e^{-\mathcal{H}[r]}, \tag{4.15}$$

with the partition function $Z = \int \mathcal{D}[\boldsymbol{r}] \exp(-\mathcal{H}[\boldsymbol{r}]) = 1$ since P is normalized.

It is convenient to rescale j into $s = mj \in [0, N]$, in order to restore the real number N of monomers. Performing this change of variable, we arrive at the following field theory, the "Gaussian chain model":

$$\boldsymbol{r}(s), \quad s \in [0, N], \quad \text{real space cutoff } m, \tag{4.16}$$

$$\mathcal{H}[\boldsymbol{r}] = \int_0^N ds\, \frac{1}{2a^2} \dot{\boldsymbol{r}}^2, \tag{4.17}$$

$$Z = \int \mathcal{D}[\boldsymbol{r}]e^{-\mathcal{H}[\boldsymbol{r}]} = 1, \tag{4.18}$$

with, again, the effective monomer length $a(T) = \sigma(T)/\sqrt{m_1}$.

C)   Real polymer chain

If we lift the ideality assumption, we lose the independence of the portions of the polymer chain and the central limit theorem no longer applies: the polymer is no longer Gaussian.

In addition to a term proportional to $\dot{\boldsymbol{r}}^2$ (allowed by symmetry), $\mathcal{H}[\boldsymbol{r}]$ should contain terms proportional to $\dot{\boldsymbol{r}}^4$, $\ddot{\boldsymbol{r}}^2$, etc. Furthermore, because of the large loop interactions, it should contain couplings between points far apart along the chain:

$$\mathcal{H}[\boldsymbol{r}] = \int_0^N ds \left(\frac{1}{2a^2} \dot{\boldsymbol{r}}^2 + \dots \right) + \iint_0^N ds_1 \, ds_2 \dots . \qquad (4.19)$$

This is actually a big difficulty: effectively a long-range interaction in term of the field $\boldsymbol{r}(s)$ (unlike the $O(n)$ models).
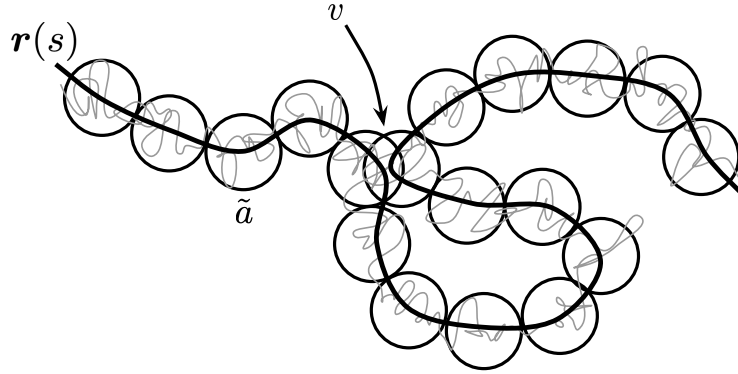
1)   The Edwards model

Figure 4.5: A real polymer chain, in gray, and its coarse-grained description $\boldsymbol{r}(s)$, a necklace of super-monomers containing $\Delta s = m$ monomers. The super-monomer width is $\tilde{a} \simeq a\sqrt{m}$ (Gaussian behavior), with a the effective monomer size, since the non-Gaussian character comes only from the large loop interactions (parameter v indicated).

The simplest model that takes into account the effect of the large loop interactions is Edwards' model:

$$\mathcal{H}_{\mathrm{E}}[\boldsymbol{r}] = \int_0^N ds \, \frac{1}{2a^2} \dot{\boldsymbol{r}}^2 + \iint_0^N ds_1 \, ds_2 \, v \, \delta(\boldsymbol{r}(s_1) - \boldsymbol{r}(s_2)). \qquad (4.20)$$

Critical exponents.—Just as the Ising models predicts exactly the critical exponents of the $O(1)$ model, the Edwards model predicts exaclty the critical exponents of polymers. This is because the two terms above are the relevant terms in the sense of the renormalization group. Actually (see **tutorials**), the Edwards model can be mapped onto the ϕ^4 model in the formal limit $n \to 0$ (de Gennes' theorem).

Justification and physical meaning of the terms of the Edwards model

- The first term, $\propto \dot{\boldsymbol{r}}^2$, would be present in the freely jointed chain. This means that it contains the loss of entropy (free energy cost) associated with the stretching of the coarse-grained chain $\boldsymbol{r}(s)$. Indeed, a chain with a large $\dot{\boldsymbol{r}}$ has, locally, less conformations of the real monomers.

- We neglect higher-order non-Gaussian terms ($\dot{\boldsymbol{r}}^4$, $\ddot{\boldsymbol{r}}^2$, ...), meaning that in this model we treat the chains within the super-monomers as ideal. The non-ideality enters only at a larger scale from the large loop interactions.

- The n super-monomers have large loop interactions. The Edwards term (with coefficient v) is the simplest term that associates a free energy to the crossings: a pointlike interaction.

If $v < 0$, crossings are favored and the chain will collapse (larger entropy, lower free energy). If $v > 0$, crossings are penalized and the chain will swell (good solvent conditions). Since the dimension of $\delta(\boldsymbol{r})$ is the inverse of a volume, $[v] = L^d$. As $[a] = L$, the combination

$$u = \frac{v}{a^d} \tag{4.21}$$

is dimensionless. It is called the *excluded volume parameter*.

2) Simplified renormalization group (RG) analysis

The Edwards model is too difficult to solve exactly. We will discuss de Gennes' renormalization group approach.

One step of the renormalization group is carried out by performing three transformations:

$$\boldsymbol{r}(s) \longrightarrow \boldsymbol{r}'(s') = g^D \bar{\boldsymbol{r}}(gs'), \quad s' = s/g. \tag{4.22}$$

1. Coarse-graining by a factor $g > 1$, i.e., transformation of the path $\boldsymbol{r}(s)$ into a smoother path $\bar{\boldsymbol{r}}(s)$. In practice, this is done by removing the high Fourier components in $\boldsymbol{r}(s)$:

Field	$\boldsymbol{r}(s)$	$\boldsymbol{r}(q)$	$\bar{\boldsymbol{r}}(q)$	$\bar{\boldsymbol{r}}(s)$
cutoff	m	$\Lambda \simeq \pi/m$	Λ/g	$m \times g$

with

$$\bar{\boldsymbol{r}}(q) = \begin{cases} \boldsymbol{r}(q) & \text{if } |q| < \Lambda/g, \\ 0 & \text{if } \Lambda/g < |q| < \Lambda. \end{cases} \tag{4.23}$$
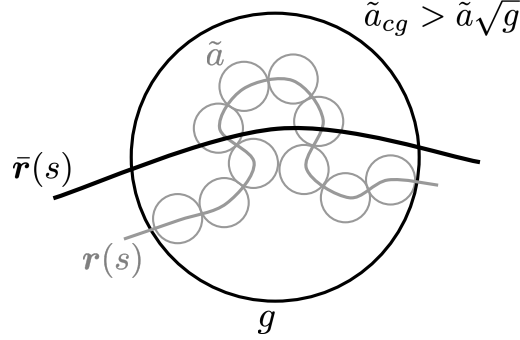
Figure 4.6: Grouping of g super-monomers (gray) into a coarse-grained super-monomer (black). This procedures defines a coarse-grained chain $\bar{r}(s)$. The size of the coarse-grained super-monomers is $\tilde{a}_{cg}$, larger than $\tilde{a}\sqrt{g}$ due to the repulsion between the super-monomers.

2. Rescaling of the parameter: $s' = s/g$. The first two transformations amount to grouping together g super-monomers into a larger super-monomer with again $\Delta s' = m$ (Fig. 4.6). This step conveniently restores the cutoff to its previous value m.

3. Rescaling of the field: $\boldsymbol{r}' = g^D \bar{\boldsymbol{r}}$. The coarse-grained field is multiplied by a power-law factor g^D. The exponent D will be adjusted for the recursion of RG steps to lead to a fixed point (revealing a scale-invariance property).

Recursive projection onto Edwards' model.—During the renormalization procedure, all the terms authorized by symmetry would appear. This is prohibitive. To simplify, at each renormalization step, we are going "project" the effective Hamiltonian onto Edwards' model. In other words, at each step, we will replace the new Hamiltonian by the closest Edwards model[1]. This will yield a series in the parameters:

$$\begin{cases} a_n \to a_{n+1}, \\ v_n \to v_{n+1}, \\ N_n \to N_{n+1} = N_n/g, \\ \Lambda_n \to \Lambda_{n+1} = \Lambda_n. \end{cases} \tag{4.24}$$

3) One renormalization step

Let us assume that at some point during the renormalization process, the Hamiltonian of the polymer is given by

$$\mathcal{H}[\boldsymbol{r}] = \int_0^N ds\, \frac{1}{2a^2}\dot{\boldsymbol{r}}^2 + \iint_0^N ds_1\, ds_2\, v\, \delta(\boldsymbol{r}(s_1) - \boldsymbol{r}(s_2))$$
$$:= H_{\mathrm{E}}[\boldsymbol{r}; a, v, N]. \tag{4.25}$$

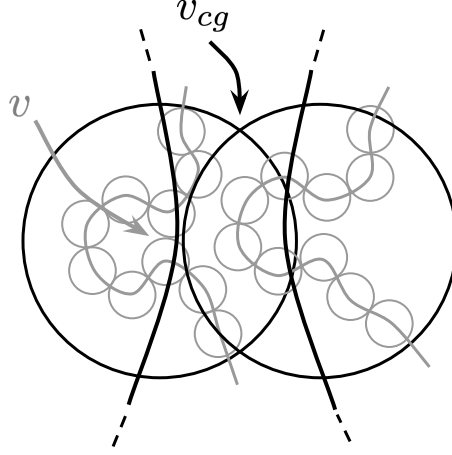[1] There are formal ways to give a precise meaning to this.

Figure 4.7: Large loop interaction between the coarse-grained super-monomers. Due to their hollowness it is easier for them to interpenetrate, therefore the coarse-grained interaction parameter v_{cg} is less that v.

In the transformation $\boldsymbol{r}'(s') = g^D \bar{\boldsymbol{r}}(gs')$, with $s' = s/g$, the coarse-graining is the difficult part. For the moment let us simply assume that it yields for the field $\bar{r}(s)$ an Edwards model $\bar{\mathcal{H}}[\bar{r}]$ with parameters a_{cg} and v_{cg} (together with N and Λ that are not changed by the coarse-graining procedure). Performing then the two rescaling transformations yields[2]

$$\mathcal{H}'[\boldsymbol{r}'] = \bar{\mathcal{H}}[\bar{r}] = \int_0^{N/g} g\, ds' \, \frac{1}{2a_{cg}^2} \left(\frac{d\boldsymbol{r}'}{ds'} \right)^2 g^{-2D} \frac{1}{g^2}$$
$$+ \iint_0^{N/g} g^2 \, ds_1 \, ds_2 \, v_{cg} \, g^{Dd} \, \delta(\boldsymbol{r}'(s_1') - \boldsymbol{r}'(s_2'))$$
$$= H_{\mathrm{E}}[\boldsymbol{r}'; a', v', N/g], \tag{4.26}$$

with

$$\begin{cases} a' = a_{cg} \, g^{1/2} \, g^D, \\ v' = v_{cg} \, g^2 \, g^{Dd}, \end{cases} \tag{4.27}$$

where the three transformation can be seen in order.

Buckingham's π theorem (1914).—A dimensionless function can depend only on the independent dimensionless power-law combinations of its variables.

How does this work? Take the example of a ball of mass m, thrown vertically in presence of gravity g with a velocity v_0 at a height H. What is the time T that it takes to reach the ground? Extracting the combination $\sqrt{H/g}$ which is a time (any choice will lead correct equivalent results

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[2]Recall the property $\delta(\alpha x) = |\alpha|^{-1}\delta(x)$. Applying it d times for $\delta(g^{-D}\boldsymbol{r}')$ yields the factor g^{Dd}.

eventually), it is a function

$$T(v_0, m, g, H) = \sqrt{\frac{H}{g}} f(v_0, m, g, H), \tag{4.28}$$

The dimensionless function f is a pure number, so its value does not change if we change the mass unit from kilograms to grams, while m changes by a factor 1000. Therefore f can only depend on the few dimensionless combinations of the variables. Rewrite (4.28) equivalently as

$$T = \sqrt{\frac{H}{g}} \phi\left(\frac{v_0}{\sqrt{gH}}; \cancel{m, g, H}\right) = \sqrt{\frac{H}{g}} \phi\left(\frac{v_0}{\sqrt{gH}}\right). \tag{4.29}$$

There is no possibility to form dimensionless combinations with (m, g, H), so the function ϕ is a "constant" function of them, hence the result. Note that the exact solution complies with the π theorem, giving $\phi(x) = x + \sqrt{x^2 + 2}$.

By virtue of Buckingham's theorem, we can write without loss of generality:

$$a_{cg}(a, v, N, g) = a\, H(u, g) = a\,(1 + h(u, g)),$$
$$v_{cg}(a, v, N, g) = v\, K(u, g) = v\,(1 - k(u, g)) \tag{4.30}$$

where h and k are dimensionless functions (of unknown sign, for the moment), and $u = v/a^d$. We have taken into account that a_{cg} and v_{cg} cannot depend on N since the coarse-graining is a local procedure, and we did not write explicitly the cutoff m and the space dimension d.

We now assume that $g \approx 1$ is a small number (like 3, 5 or 7, even 10). Note that if we chain 25 steps with $g = 3$, the result is a huge coarse-graining or ratio $G = 3^{25} \approx 10^{12}$. Since for $g = 1$ the coarse-graining step is ineffective (it does nothing) we expect to have $|h| \ll 1$ and $|k| \ll 1$ for $g \approx 1$.

Indeed, if v was zero, the coarse-graining would change nothing because the model would be Gaussian[3]. So the change is only caused by v, by the large loop interactions. But the latter are scarce within the new super-monomers if g is small, so we expect that if $g \approx 1$, the coarse-graining will change very little.

Putting together Eqs. (4.27) and (4.30), we obtain the equations describing one renormalization step:

$$\begin{cases} a' = a\,[1 + h(u, g)]\, g^{\frac{1}{2} + D}, \\ v' = v\,[1 - k(u, g)]\, g^{2 + Dd}. \end{cases} \tag{4.32}$$

---

[3]If $\mathcal{H}[\boldsymbol{r}]$ is Gaussian, with $\boldsymbol{r}(s) = N^{-1}\sum_q \boldsymbol{r}_q e^{iqs}$, one gets

$$\mathcal{H}[\boldsymbol{r}] = \int_0^N ds\, \frac{1}{2a^2}\dot{\boldsymbol{r}}^2 = \frac{1}{N}\sum_q \frac{q^2}{2a^2}\boldsymbol{r}_q \cdot \boldsymbol{r}_q^\star. \tag{4.31}$$

Modes with different q are uncoupled, therefore integrating out, in a coarse-graining, the modes with $|q| > \Lambda/g$ leaves $\mathcal{H}$ unchanged for the modes with $|q| < \Lambda/g$.

Properties of the functions h and k.—As explained in Fig. 4.6, we have $\tilde{a}_{cg} > \tilde{a}\sqrt{g}$ due to the repulsion between the super-monomers. This implies $a_{cg} > a$, hence $h > 0$. Actually, we have

$$\begin{cases} h > 0, \\ k > 0, \end{cases} \tag{4.33}$$

Since as explained in Fig. 4.7, we expect $v_{cg} < v$ due to the hollowness of the coarse-grained super-monomers[4], so $k > 0$.

For $u \to 0$, we have also $h \to 0$ and $k \to 0$, since the model is Gaussian and the coarse-graining has no effect. Hence

$$\begin{cases} h(0, g) = 0, \\ k(0, h) = 0. \end{cases} \tag{4.34}$$

There is also an important property that derives from the group structure of the renormalization group. Performing successively two coarse-grainings of amount g is equivalent[5] to performing one coarse-graining of amount $g \times g = g^2$, so the following property holds:

$$\begin{cases} 1 + h(u, g^p) = [1 + h(u, g)]^p, \\ 1 - k(u, g^p) = [1 - k(u, g)]^p. \end{cases} \tag{4.35}$$

4) Renormalization flow and fixed points

Chaining renormalization steps[6], we obtain the renormalization flow equations:

$$\begin{cases} a_{n+1} = a_n \left[1 + h(u_n, g)\right] g^{\frac{1}{2}+D}, \\ v_{n+1} = v_n \left[1 - k(u_n, g)\right] g^{2+Dd}, \end{cases} \tag{4.36}$$

with $u_n = v_n/a_n^d$. In addition, we have $N_{n+1} = N_n/g$ and the cutoff $\Lambda_n = \pi/m$ remains constant.

Equivalently, we can keep track of a_n and u_n, yielding

$$\begin{cases} a_{n+1} = a_n \left[1 + h(u_n, g)\right] g^{\frac{1}{2}+D}, \\ u_{n+1} = u_n \dfrac{1 - k(u_n, g)}{[1 + h(u_n, g)]^d} g^{2-\frac{d}{2}} = f(u_n). \end{cases} \tag{4.37}$$

Note that D has disappeared in the recursion for u_n.

---

[4]Even if the super-monomers cannot interpenetrate, the new super-monomers can, so $v_{cg} < v$.

[5]This would be exact if we were not projecting on Edwards' model. Here it is actually an approximation.

[6]The transformation $a_n \to a_{n+1}$ and $v_n \to v_{n+1}$ is independent of n thanks to the fact that the cutoff does not evolve (and the length of the polymer does not appear in the relations).
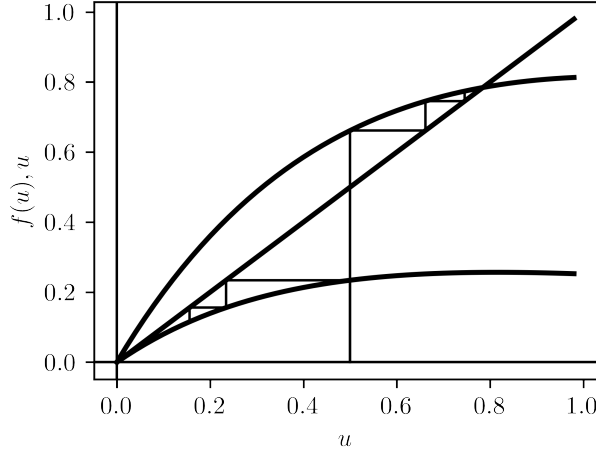
Figure 4.8: Renormalization flow $u_{n+1} = f(u_n)$ starting from u_0. For $d > 4$ the flow converges towards the Gaussian point $u_G^\star$. For $d < 4$ it converges towards the Edwards fixed point $u_E^\star$.

Fixed points

A fixed point is a solution $u^\star$ of the equation $f(u^\star) = u^\star$. Let us look for a solution $u^\star \neq 0$:

$$\frac{1 - k(u^\star, g)}{[1 + h(u^\star, g)]^d} = g^{\frac{d}{2} - 2} \qquad (u^\star \neq 0). \tag{4.38}$$

This has no solution for $d \geq 4$, since $g^{d/2 - 2} > 1$ while the left-hand side is < 1. Thus, for $d \geq 4$ the only fixed point is the Gaussian point $u_G^\star = 0$.

As can be seen in Fig. 4.8, for $d \geq 4$ the Gaussian fixed point is attractive, while for $d \leq 4$ it becomes repulsive and there is another fixed point, $u_E^\star \neq 0$, the Edwards' fixed point, that becomes attractive[7].

Each fixed point actually corresponds to a particular value $D^\star$. This is because the equation $a_{n+1} = a_n = a^\star$ does depend on D. We are interested in $a^\star \neq 0$ (otherwise the asymptotic monomer size would vanish), so we have from (4.37)

$$D^\star = -\frac{1}{2} - \frac{\ln\left[1 + h(u^\star, g)\right]}{\ln g}. \tag{4.39}$$

Gaussian fixed point.— It corresponds to

$$\begin{cases} u = u_G^\star = 0, \\ D_G^\star = -\frac{1}{2}, \end{cases} \tag{4.40}$$

---

[7]The graph of Fig. 4.8 is obtained for simple monotonic functions $h(u) = \alpha u$ and $k(u) = \beta u$, with $\alpha > 0$ and $\beta > 0$, consistent with the fact that the effect of v on the coarse-graining increases with v.

since $h(0, g) = 0$, and it is actually the Gaussian model.

Edwards' fixed point.—It corresponds to

$$\begin{cases} u = u_{\mathrm{E}}^{\star}, \\ D_{\mathrm{E}}^{\star} = -\frac{1}{2} - \dfrac{\ln\left[1 + h(u_{\mathrm{E}}, g)\right]}{\ln g} < -\frac{1}{2}, \end{cases} \tag{4.41}$$

with $u_{E}^{\star}$ solution of

$$\frac{1 - k(u_{E}^{\star}, g)}{\left[1 + h(u_{E}^{\star}, g)\right]^{d}} = g^{\frac{d}{2} - 2}. \tag{4.42}$$

Universality—It would seem that $u_{\mathrm{E}}^{\star}$ and $D_{\mathrm{E}}^{\star}$ depend on g. Actually they do not. They are pure numbers depending only on the space dimension d. Indeed, changing g, i.e., replacing g by g^{p}, leaves the equations for $u_{E}^{\star}$ and $D_{\mathrm{E}}^{\star}$ unchanged thanks to the group structure (4.35).

We will assume, as we know to be true in the $O(n)$ models, that Hamiltonians more complicated and realistic than Edwards' (i.e., real polymers), would converge to the same fixed points. This amounts to assume that only the two Edwards terms are relevant.

Physical interpretation of the RG fixed point results.—Take a real polymer and look at its statistical features on a very large scale. In other words look at the fluctuations of $\bar{r}(s)$ for a coarse-graining factor $G \gg 1$. Scaling down this smoothed polymer chain by a universal factor $g^{D^{\star}} < 1$ (with $D^{\star} = -1/2$ if $d > 4$ and $D^{\star} = D_{\mathrm{E}}^{\star} < -1/2$ if $d < 4$), i.e., looking at $\boldsymbol{r}' = G^{D^{\star}}\bar{\boldsymbol{r}}$, we see is a *universal polymer object*

If $d > 4$, this object seems to cross itself like a Gaussian, ideal, phantom (irrespective of the u_0 coefficient of the real polymer, even very large). If $d < 4$, this object seems to repel itself with a universal excluded volume parameter $u_{\mathrm{E}}^{\star}$ (irrespective of the u_0 coefficient of the real polymer, even very small).

5) Radius of gyration

The renormalization group allows to demonstrate that the radius of gyration follows a power law (and in principle to calculate the critical exponent).

Megascope.—One can see the renormalization group transformation

$$\boldsymbol{r}(s) \longrightarrow \boldsymbol{r}'(s') = g^{D}\bar{\boldsymbol{r}}(gs') \tag{4.43}$$

as an image processing aparatus, a "megascope" that takes pictures of the real fluctuating polymer and outputs a zoomed-out image ($D < 0$) where the microscopic details are smoothed out. For $g \gg 1$, the megascope thus shows a transformed image of the large-scale behavior of the system.

Within Edwards' model, the radius of gyration of the polymer is a function of (a, v, N). It depends actually also of Λ and d, but we will omit these fixed quantities[8]. Using the π theorem, there exists dimensionless function f such that

$$R_g = af(u, N). \tag{4.44}$$

Since the megascope image is both a scaled/smoothed image of the actual (a, v, N) polymer and a different polymer with parameters $(a', v', N/g)$, we have

$$R_g = g^{-D} a' f(u', N/g). \tag{4.45}$$

Taking $g \gg 1$ (which requires N extremely large) the image reaches practically the fixed point, and we have

$$R_g = g^{-D} a^\star f(u^\star, N/g). \tag{4.46}$$

Let us now choose g such $N/g = N_0$, where $N_0 \gg 1$ is a fixed quantity. We have then

$$R_g = \left(\frac{N}{N_0}\right)^{-D} a^\star f(u^\star, N_0), \tag{4.47}$$

i.e.,

$$R_g \sim N^\nu, \qquad \nu = -D. \tag{4.48}$$

Note that we actually find $R_g = C\, a^\star N^{-D}$, with $C(d)$ a universal constant. Indeed $C = N_0^D f(u^\star, N_0)$ has an apparent dependence on N_0 that is not real, since R_g does not depend on N_0. Therefore C is a universal constant[9], like $u^\star$.

Consequently, for $d > 4$ real polymers have exactly $\nu = 1/2$ (although they self-repel), while they have $\nu > 1/2$ for $d < 4$.

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[8]Note that Λ is a choice we make at the beginning of the description (in the initial coarse-graining). The constants a and v depend on this choice, but not the physics, since the coarse-graining preserves the exact behavior of the system.

[9]The fixed points $a^\star$ and $v^\star$, contrary to $u^\star$, are not universal constants: they depend on the starting a and v.