Chapter 1

Introduction

The main subject of this course is the study of certain functional integrals arising in statistical mechanics and physics.

1.1 Some motivation: an example of Gibbs measure

Let us consider the atoms in a perfect cristal. At equilibrium the atoms are located at the sites $x \in \Lambda$ where $\Lambda \subset \mathbb{Z}^d$ is a finite set. Thermal fluctuations and other perturbations may cause the atoms to move a bit away from their equilibrium position. The atom at site x is displaced to a postition $x + \vec{\varphi}(x)$, where $\vec{\varphi}(x) \in \mathbb{R}^d$. The collection of all displacements $\{\varphi(x)\}_{x\in\Lambda}$ is called a *field* (vector valued)

$$\begin{aligned} \varphi: \quad & \Lambda \to \mathbb{R}^d \\ & x \to \varphi(x) \end{aligned}$$

Each function $\varphi \in (\mathbb{R}^d)^\Lambda$ is a possible configuration for the deformed cristal. The set of all possible configurations will be denoted by

$$\Omega = (\mathbb{R}^d)^\Lambda.$$

Atoms "prefer" to remain near their equilibrium position so it takes some effort to displace them. This is encoded in the energy functional

$$\begin{aligned} H_\Lambda: \quad & (\mathbb{R}^d)^\Lambda \to \mathbb{R} \\ & \varphi \to H(\varphi) = \tfrac{1}{2} \textstyle\sum_{x\sim y \in\Lambda} \|\vec{\varphi}(x) - \vec{\varphi}(y)\|^2 \end{aligned} \tag{1.1.1}$$

where we use the L_2 norm $\|v\|^2 = \sum_{j=1}^d v_j^2$ and $x \sim y$ denotes a pair of nearest neighbors on the lattice $\|x-y\| = 1$. Note that if we deform each atom by the same amount $\vec{\varphi}(x) = \vec{\varphi}\ \forall x$ then we are doing a global translation of the cristal (no deformation) and the corresponding energy is zero.

We assign to each configuration φ a weight (probability density) proportional to $exp[-\beta H_\Lambda(\varphi)]$ where $\beta = 1/T$ and T is the temperature. Is this choice consistent with our intuition? For a large deformation the energy is large and the corresponding probability is small, as we should expect since it is "hard" to deform a cristal. The insertion of the β parameter is also consistent. Indeed for small temperature the atoms are "frozen" and moving them is "hard": the corresponding β is large thus giving a small probability. For high temperature the atoms are "exited" and move very easily: the corresponding β is small thus giving a large probability.

Boundary conditions The cristal is connected to the external world through the boundary of the volume Λ. This interaction translates into *boundary conditions* on H_Λ. The corresponding energy functional will be denoted by $H_\Lambda^{(bc)}$.

All the above arguments can be made precise by introducing a probability measure on $(\Omega, \mathcal{F})$ defined by

$$d\mu_{\Lambda,\beta}^{(bc)}(\varphi) = \frac{e^{-\beta H_\Lambda^{(bc)}(\varphi)}}{Z_{\Lambda,\beta}} d\varphi \tag{1.1.2}$$

where Ω is the set of all possible configurations (in our case deformations of the cristal), $\mathcal{F}$ is a $\sigma-$algebra on Ω and $d\varphi = \prod_{x\in\Lambda}\prod_{j=1}^{d} d\varphi_j(x)$ is the Lebesgue measure. Finally $Z_{\Lambda,\beta}$ is the normalization constant ensuring that $\mu_{\Lambda,\beta}^{(bc)}(\Omega) = 1$. This constant is called the *partition function*

$$Z_{\Lambda,\beta} = \int_\Omega e^{-\beta H_\Lambda^{(bc)}(\varphi)} d\varphi.$$

Remark 1 If we insert in the definition above the energy functional (1.1.1), the corresponding integral is divergent! The boundary conditions will ensure the integral is finite.

Remark 2 The energy functional (1.1.1), is a quadratic form

$$H_\Lambda(\varphi) = (\varphi, A\varphi) = \sum_{x,y\in\Lambda} \varphi(x) A_{xy} \varphi(y)$$

where for any pair x, y of sites not on the boundary of Λ we have

$$A_{xy} = \begin{cases} -1 & \|x-y\| = 1 \\ 2d & x = y \\ 0 & \|x-y\| > 1 \end{cases}$$

The corresponding measure (1.1.2) is called a *gaussian measure*. Most of the problems we will consider will be given by some form of gaussian measures, or perturbations of gaussian meausures.

1.2 Thermodynamic limit

The measure defined in (1.1.2) is called a *finite volume Gibbs measure.* If now we take a sequence of growing volumes Λ_n with $\Lambda_n \to \mathbb{Z}^d$ we can ask the following quastions

- Does the sequence of measures converge to some infinite volume measure?
- If yes, does the limit depend on the choice of the boundary conditions?

The answer to this question gives informations on the existence of a phase transition in the model (ex: liquid/gas or cristal/liquid).

1.3 Functional integrals

The object of this course if the study of a class of *functional integrals* of the type (1.1.2) . These are integrals over spaces of *functions.*

Going back to our initial example, cristal deformations, let us consider $d = 1$ and $\Lambda = (1, 2, \ldots, N)$. An element of the space of configurations $\varphi \in \Omega$ is a function *function* $\varphi : \Lambda \to \mathbb{R}$, but we can see it also a set on N real numbers $\varphi = (\varphi(1), \ldots, \varphi(N))$ corresponding to the values of the function at each point. Any function

$$\begin{aligned} F: \quad & \Omega \to \mathbb{R} \\ & \varphi \to F(\varphi) \end{aligned}$$

can be seen as a function on N real variables $F(\varphi) = F(\varphi(1), \ldots, \varphi(N))$. The Lebesgue measure on Ω is then the Lebesgue measure on the product space $\mathbb{R}^N$.

$$d\varphi = \prod_{j=1}^{N} d\varphi(j).$$

Using Fubini's theorem we can define the integral

$$\int f(x_1, \ldots, x_N) dx_1 \cdots dx_N$$

indipendently of the integration order, for any integrable function $f : \mathbb{R}^N \to \mathbb{R}$ ($\int |f|$ is finite). This construction can be generalized to a *countable* set of variables.

When $d > 1$, let Λ a *finite* set of sites in $\mathbb{Z}^d$. At each site we have d variables $\varphi_1(x), \ldots .\varphi_d(x)$. Since Λ is finite we can define the product Lebesgue measure on the $d|\Lambda|$ variables corresponding to a cristal deformation φ. The thermodynamic limit then can be seen as the problem of defining the integral over an infinite number of variables.

Functions in the continuum . The arguments above concern only spaces of discrete functions $\varphi = \{\varphi(x)\}_{x\in\Lambda}$, where Λ is a set of lattice sites. Let us suppose now that the atoms are not in a solid phase but rather in a gas state. Then each atom could be anywhere in a region $\Lambda \subset \mathbb{R}^d$ of finite volume. The function $\varphi(x) \in \mathbb{R}^+$ may represent the number of particles in a small neighborhood of x. Then a configuration of the system is given by $\varphi = \{\varphi(x)\}_{x\in\Lambda}$ an *uncountable* set of real variables. Measure theory teaches us how to construct sigma-algebras out of countable products. In order to make sense of a measure on a uncountable product space we introduce spaces of distributions.

1.4 Role of the boundary conditions

Boundary conditions fix how the region Λ we are studying is connected to the outside. In our example we could say that on the boundary of our cristal we are attached to a very stable material where atoms are practically frozen. Then we have $\varphi(x) = 0$ for all sites x on the boundary of Λ (Dirichlet type b.c.)

The role of b.c. in the measure $d\mu_\Lambda^{(b.c)}$ when Λ gets big is analog to the initial conditions in a PDE. let us consider two famous PDEs: the heat and wave equations in one dimension:

$$\begin{aligned} &\partial_t u(x,t) = \alpha^2 \partial_x^2 u(x,t), \qquad u(x,0) = u_0(x), \quad x \in \mathbb{R}, t \geq 0, \\ &\partial_{tt} u(x,t) = v^2 \partial_x^2 u(x,t), \qquad u(x,0) = \phi(x),\ u_t(x,t) = \psi(x) \quad x \in \mathbb{R}, t \geq 0. \end{aligned}$$

The solution for the first (heat) equation is independent of the details of the initial condition $u_0(x)$: in particular any irregularities of u_0 are instantaneously smoothed out. This means we loose information. On the contrary, the solution of the second (wave) equation depends very strongly from the initial conditions. Actually, in this case the initial profile ϕ travels without ever changing shape. This means information is transferred without losses.

In the language of measures, the independence of the limit from the boundary conditions means there is only one possible measure describing our system at very large volume (one possible phase) , the dependence means that there are several possible measures at large volume (hence several possible phases).

1.5 Multiscale analysis

Let us look again at the cristal energy $H_\Lambda^{(b.c)}(\varphi) = \frac{1}{2}\sum_{x\sim y\in\Lambda} \|\vec{\varphi}(x) - \vec{\varphi}(y)\|^2$ with $\varphi(x) = 0$ for all x on the boundary, meaning that $x \in \Lambda$ but there exists at least one site $y \in \Lambda^c$ with $x \sim y$. In this functions only nearest neighbor sites $x \sim y$ interact. Then the corresponding density $e^{-\beta H_\Lambda^{(bc)}}$ is maximal when the variables φ are approximately constant on small regions (otherwise the probability is small). In other words the integral over $d\mu$ is concentrated around regions in Ω corresponding to configurations that are "locally constant".

In particular the boundary conditions can affect only a small number of sites near to the boundary of Λ. If the fraction of sites on the boundary $|\partial\Lambda|/|\Lambda|$ vanishes as $\Lambda \to \mathbb{Z}^d$, (take for instance a growing sequence of cubes), then it is reasonable to expect that boundary conditions will have no influence on the limit. Boundary conditions may change the limit only if they are able to interact effectively with *all* sites in Λ. When this happends we say that a short range interaction becomes effectively long range.

The analysis of the large volume limit can then be translated in the analysis of multiscale effects (short range interactions becoming effectively long range).

Note that, except in some special cases, we cannot compute the integrals in a closed form! We need tools to get estimates as precise as possible.

1.6 Plan of the course

We will consider some examples of functional integrals arising from statistical mechanics and physics, and learn techniques to construct the limit as the number of variables tends to infinity.

In models coming from statistical mechanics the measure is always a probability measure (real positive and normalized to 1). The field φ may take values in a discrete set (ex: ± 1), in a bounded set (ex: $\varphi(x) = \cos(\theta_x)$, with $\theta \in [0, 2\pi[$), in an unbounded set $\varphi(x) \in \mathbb{R}$.

In models coming from physics, the measure may become complex valued, though still normalized to 1. The field φ may be a real or complex vector, a matrix and some components of φ may even be Grassmann variables (anticommuting numbers $ab = -ba$).

In many cases the energy is of the form

$$H(\varphi) = \sum_{x,y} J_{xy} \|\varphi(x) - \varphi(y)\|^2 + \sum_x V(\varphi(x)),$$

where $J_{xy} = J_{yx} \geq 0$. The first term creates an interaction between different sites, the second term gives a set of independent constraints on each variable (it is called the diagonal term). When $J_{xy} = 0 \; \forall x, y$, the measure $e^{-\beta H}$ factors in a product of measures. When $V = 0$, the integral cannot be factored. Depending on the relative size of the parameters, we will see that the integral is dominated by the interaction term or the diagonal term. These two situations correspond to different physical properties in the underlying model.

Some examples of potential V are

- $V(\varphi) = m^2\|\varphi\|^2 + \lambda\|\varphi\|^4$ (single well)
- $V(\varphi) = \lambda(\|\varphi\|^2 - \mu)^2$ (double well or mexican hat)
- $V(\varphi) = \lambda \ln(1 + \|\varphi\|^2)$ (log potential)

In the first two cases the potential is a convex function, for large $\|\varphi\|$, in the last case, the function becomes concave, adding additional problems.

1.7 Digression: why choosing an exponential weight?

We will motivate the choice of an exponential weight in the simpler case of a *finite* set of possible configurations. On can justify the same arguments in the general case (see for instance the lecture notes by Stefan Adams, chapter 7, http://www.mis.mpg.de/preprints/ln/lecturenote-3006.pdf).

Let Ω_Λ the set of all possible configurations for our finite system (the cristal in our example) and let $H : \Omega \to \mathbb{R}$ be the corresponding energy functional. Since Ω is finite, in order to define a probability measure we only need to give a set of numbers $\{\mu(\omega)\}_{\omega\in\Omega}$ such that $0 \leq \mu(\omega) \leq 1$ and $\sum_\omega \mu(\omega) = 1$. Let us consider how the system is connected to the external world.

Case 1: Isolated system The only way to change the energy of the system is to "give away" some of it or "take in " some of it from outside. But an isolated system has no exchange with the exterior so in this case the energy is fixed $H(\omega) = E \ \forall \omega \in \Omega$. Then there is no way to decide which configuration is preferable (they all have the same energy) and the most reasonable choice for μ is the uniform distribution that assigns the same weight to each configuration:

$$\mu(\omega) = \frac{1}{|\Omega|} \qquad \forall \omega \in \Omega, \quad \text{where}|\Omega| = \text{cardinal of } \Omega.$$

Case 2: system in contact with a reservoir at fixed temperature T In this case the energy can change, but since the temperature outside is fixed the *average energy* of our system is given by

$$\mathbb{E}[H] = \sum_{\omega\in\Omega} \mu(\omega) H(\omega) = E(T). \tag{1.7.3}$$

This time a uniform measure would not work since we expect large deformations (large energies) to be more unlikely than small deformations (small energies). The correct choice is to take a measure "as uniform as possible" under the constraint (1.7.3). To quantify how "uniform" a measure is we use the entropy. Let $\mathcal{M}(\Omega)$ be the set of probability measures on Ω, then the entropy is defined as

$$\begin{aligned} S: \ & \mathcal{M}(\Omega) \to \mathbb{R} \\ & \mu \to S(\mu) = -\textstyle\sum_\omega \mu(\omega) \ln \mu(\omega). \end{aligned}$$

To see the kind of information we obtain from S let us consider two extreme cases:

(a) $\mu(\omega) = 1/|\Omega|$ the uniform measure. Then we have the same propability of being anywhere inside Ω: this means we have as little information as possible. In this case $S(\mu) = \ln(|\Omega|)$, that is a large number when Ω is large.

(b) $\mu(\omega) = \delta_{\omega\omega_0}$ a measure localized on just one element ω_0 of Ω. Then we know (with probability 1) that we must be exactly on the configuration ω_0: this means we have the maximal information. In this case $S(\mu) = -\mu(\omega_0)\ln(\omega_0) = 0$.

In general, the more "uniform" our measure is, the larger S. Therefore we choose the measure μ that maximizes $S(\mu)$, under the constraint (1.7.3).

Lemma 1 *Let* H *be a (non constant) energy functional,*

$$\nu_\beta(\omega) = \frac{e^{-\beta H(\omega)}}{Z_\beta}, \qquad Z_\beta = \sum_\omega e^{-\beta H(\omega)}.$$

a Gibbs measure and set

$$\begin{array}{lll} f: &]0,+\infty] & \to \mathbb{R} \\ & \beta & \to f(\beta) = \mathbb{E}_{\nu_\beta}[H]. \end{array}$$

Then we have the following results.

(a) *For each* $E \in$ *Range*(f) *there exists a parameter* $\bar{\beta}$ *such that for* $\beta = \bar{\beta}$ $\mathbb{E}_{\nu_{\bar{\beta}}}[H] = E$.

(b) *For any probability measure satisfying* $\mathbb{E}_\mu[H] = E$ *we have* $S(\mu) \leq S(\nu_{\bar{\beta}})$. *Equality holds only for* $\mu = \nu_{\bar{\beta}}$.

Remark When H is constant ($H(\omega) = H\ \forall\omega$) then the Gibbs measure ν_β coincides with the uniform measure for any choice of β.

Proof Let $\bar{H}_\beta = \mathbb{E}_{\nu_\beta}[H]$. In order to prove (a) note that

$$f'(\beta) = -\mathbb{E}_{\nu_{\bar{\beta}}}\left[(H - \bar{H}_\beta)^2\right] = -\sum_\omega \nu_\beta(\omega)(H(\omega) - \bar{H}_\beta)^2 < 0,$$

since $\nu_\beta(\omega) > 0\ \forall\omega$ and there is at least one ω where $(H(\omega) - \bar{H}_\beta)^2 > 0$ (otherwise H would be the constant function). Then f is injective, hence (a).

To prove (b), note that

$$S(\mu) = -\sum_\omega \mu(\omega)\ln\mu(\omega) = -\sum_\omega \mu(\omega)\ln\frac{\mu(\omega)}{\nu_{\bar{\beta}}(\omega)} - \sum_\omega \mu(\omega)\ln\nu_{\bar{\beta}}(\omega).$$

Now using the definition of ν_β the second term is

$$-\sum_\omega \mu(\omega)\ln\nu_{\bar{\beta}}(\omega) = \sum_\omega \mu(\omega)\ln Z_{\bar{\beta}} + \bar{\beta}\sum_\omega \mu(\omega)H(\omega) = \ln Z_{\bar{\beta}} + \bar{\beta}E = S(\nu_{\bar{\beta}})$$

Inserting this we have

$$S(\mu) = S(\nu_{\bar{\beta}}) - \sum_\omega \mu(\omega)\ln\frac{\mu(\omega)}{\nu_{\bar{\beta}}(\omega)} = S(\nu_{\bar{\beta}}) - \sum_\omega \nu_{\bar{\beta}}(\omega)\Phi(X(\omega)) = S(\nu_{\bar{\beta}}) - \mathbb{E}_{\nu_{\bar{\beta}}}[\Phi(X(\omega))]$$

where we set

$$\Phi(x) = x\ln x, \qquad X(\omega) = \frac{\mu(\omega)}{\nu_{\bar{\beta}}(\omega)}.$$

Now $\Phi''(x) = 1/x > 0$ so by Jensen's inequality

$$\mathbb{E}_{\nu_{\bar{\beta}}}[\Phi(X(\omega))] \geq \Phi\Big(\mathbb{E}_{\nu_{\bar{\beta}}}[X(\omega)]\Big) = \Phi(1) = 0.$$

Since Φ is strictly convex, equality holds only when $X(w)$ is a constant function, that means there exist a constant K such that $\mu(\omega) = K\nu_{\bar{\beta}}(\omega)\ \forall\omega$. But $\sum_\omega \mu(\omega) = \sum_\omega \nu_{\bar{\beta}}(\omega) = 1$, then $K = 1$. This completes the proof of (b). $\square$