CHAPTER 4

Cluster expansions

The method of cluster expansions allows to write the grand-canonical thermodynamic potential as a convergent perturbation series, where the small parameter is related to the temperature (usually high), the chemical potential (usually low — small densities), and the interactions (small). It was pioneered by Mayer in the 1930's, and made rigorous both by Penrose and Ruelle in 1963. Subsequent works, especially by Kotecký and Preiss, have simplified the method, allowing many generalizations.

We introduce the method in the context of the classical gas in Section 1. We explain the combinatorics, and give the result. We ignore the problems of convergence of various series, until Section 2, where a theorem is provided that rigorizes the computations of Section 1. This theorem applies to a very broad class of physical systems, including lattice spin systems where it helps proving the occurrence of phase transitions, and quantum systems. Assumptions involve the "Kotecký-Preiss criterion", a condition that has proved convenient and rather optimal in many situations.

1. Weakly interacting classical gas

The method is very general and is actually an intriguing piece of combinatorics. Roughly summarized, a sum over arbitrary graphs can be written as the *exponential* of a sum over *connected* graphs. The interactions in the partition functions can be expressed using graphs; the logarithm of the partition function involves a sum over connected graphs.

Recall that the Hamiltonian of the classical gas is $H(\{p_i, q_i\}) = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i<j} U(|q_i - q_j|)$. We work in the grand-canonical ensemble and compute the pressure. Notice that all momenta can be integrated independently. Introducing

$$\lambda = \Big(\frac{2m\pi}{\beta h^2}\Big)^{3/2} \mathrm{e}^{\beta\mu}\,, \tag{4.1}$$

the grand-canonical partition function is given by

$$Z(\beta, V, \mu) = 1 + \sum_{N \geqslant 1} \frac{\lambda^N}{N!} \int_D \mathrm{d}q_1 \dots \int_D \mathrm{d}q_N \exp\Big\{-\beta \sum_{1 \leqslant i<j \leqslant N} U(|q_i - q_j|)\Big\}.$$

We now express the interactions in terms of graphs. Let $\mathcal{G}_N$ denote the set of graphs with N vertices (with unoriented edges, no loops). Then

$$\begin{aligned} \mathrm{e}^{-\beta \sum_{i<j} U(|q_i - q_j|)} &= \prod_{i<j} \Big[\mathrm{e}^{-\beta U(|q_i - q_j|)} - 1 + 1 \Big] \\ &= \sum_{G \in \mathcal{G}_N} \prod_{(i,j) \in G} \Big[\mathrm{e}^{-\beta U(|q_i - q_j|)} - 1 \Big]. \end{aligned}$$

The last product is over edges of the graph G. Let us use the shortcut

$$\zeta(q_i - q_j) = \mathrm{e}^{-\beta U(|q_i - q_j|)} - 1.$$

We now have

$$Z(\beta, V, \mu) = 1 + \sum_{N \geqslant 1} \frac{\lambda^N}{N!} \int_D \mathrm{d}q_1 \dots \int_D \mathrm{d}q_N \sum_{G \in \mathcal{G}_N} \prod_{(i,j) \in G} \zeta(q_i - q_j).$$

A graph can be decomposed into connected graphs $(G_1, \dots, G_k)$. Here, each G_i is a connected graph with set of vertices V_i, and the V_i's form a partition of $\{1, \dots, N\}$: $V_1 \cup \dots \cup V_k = \{1, \dots, N\}$, and $V_i \cap V_j = \varnothing$ if $i \neq j$. There are $k!$ such sequences for each G, since the order of the G_i's does not matter. The sum over G can thus be realized by first summing over k, then over partitions $V_1, \dots, V_k$, and then over connected graphs on the V_i's. Namely,

$$\sum_{G \in \mathcal{G}_N} \prod_{(i,j) \in G} \zeta(q_i - q_j) = \sum_{k=1}^{N} \frac{1}{k!} \sum_{V_1, \dots, V_k} \sum_{\substack{G_1, \dots, G_k \\ G_i \in \mathcal{C}_{V_i}}} \prod_{\ell=1}^{k} \prod_{(i,j) \in G_\ell} \zeta(q_i - q_j).$$

Here, $\mathcal{C}_{V_i}$ denotes the set of connected graphs with vertices V_i. We obtain

$$Z(\beta, V, \mu) = 1 + \sum_{N \geqslant 1} \frac{\lambda^N}{N!} \sum_{k=1}^{N} \frac{1}{k!} \sum_{V_1, \dots, V_k} \sum_{\substack{G_1, \dots, G_k \\ G_i \in \mathcal{C}_{V_i}}} \prod_{\ell=1}^{k} \Big[\Big(\prod_{i \in V_i} \int_D \mathrm{d}q_i \Big) \prod_{(i,j) \in G_\ell} \zeta(q_i - q_j) \Big].$$

The bracket depends on the cardinalities of the V_i's, but not on their actual elements. We therefore sum over the cardinalities $N_1, \dots, N_k \geqslant 1$ with $N_1 + \dots + N_k = N$. The number of partitions of N elements into k subsets with $N_1, \dots, N_k$ elements is given by the multinomial coefficient

$$\frac{N!}{N_1! \dots N_k!}.$$

We then obtain

$$Z(\beta, V, \mu) = 1 + \sum_{N \geqslant 1} \frac{\lambda^N}{N!} \sum_{k \geqslant 1} \frac{1}{k!} \sum_{\substack{N_1, \dots, N_k \geqslant 1 \\ N_1 + \dots + N_k = N}} \frac{N!}{N_1! \dots N_k!} \prod_{\ell=1}^{k} \Big[\sum_{G_\ell \in \mathcal{C}_{N_\ell}} \int_D \mathrm{d}q_1 \dots \mathrm{d}q_{N_\ell} \prod_{(i,j) \in G_\ell} \zeta(q_i - q_j) \Big]$$

In the next section we shall provide sufficient conditions allowing to interchange the sums over N and over k. We then obtain

$$Z(\beta, V, \mu) = 1 + \sum_{k=1}^{N} \frac{1}{k!} \Big[\sum_{N \geqslant 1} \frac{\lambda^N}{N!} \sum_{G \in \mathcal{C}_N} \int_D \mathrm{d}q_1 \dots \mathrm{d}q_N \prod_{(i,j) \in G} \zeta(q_i - q_j) \Big]^k.$$

We see that the partition function is given by the exponential of the bracket. The pressure is then given by

$$p(\beta,\mu) = \lim_{V\to\infty} \frac{1}{\beta V} \sum_{N\geqslant 1} \frac{\lambda^N}{N!} \sum_{G\in\mathcal{C}_N} \int_D \mathrm{d}q_1 \dots \mathrm{d}q_N \prod_{(i,j)\in G} \Big[\mathrm{e}^{-\beta U(|q_i-q_j|)} - 1 \Big].$$

In the case where the potential has finite range, i.e. $U(|q|) = 0$ for $|q|$ bigger than some finite number R, the contribution of positions that are too far apart is zero: The product always vanishes when $|q_i - q_j| > NR$ for some i, j. This justifies the name "cluster expansion", since the pressure is given in terms of integrals involving "clusters" of particles. The behavior of potentials with fast decay at infinity (faster than a suitable power of $|q|$) is similar to that of finite range potentials. We also see that, for given N, the contribution of the integrals is of order of the volume: The integral over q_1 is of order of V, while the integrals over $q_2, \dots, q_N$ are restricted to an area around q_1. Using the rigorous estimates stated in the next section, one can show that the pressure is given by the following expression, where we have set $q_1 = 0$,

$$p(\beta,\mu) = \frac{1}{\beta} \sum_{N\geqslant 1} \frac{\lambda^N}{N!} \sum_{G\in\mathcal{C}_N} \int_{\mathbb{R}^3} \mathrm{d}q_2 \dots \mathrm{d}q_N \prod_{(i,j)\in G} \Big[\mathrm{e}^{-\beta U(|q_i-q_j|)} - 1 \Big]. \tag{4.2}$$

The expression above can be viewed as an expansion with respect to interactions. The term $N = 1$ does not involve the potential $U(|q|)$ and yields

$$p_1(\beta,\mu) = \frac{\lambda}{\beta} = \frac{1}{\beta} \Big(\frac{2m\pi}{\beta h^2} \Big)^{3/2} \mathrm{e}^{\beta\mu} .$$

Recall that the density is given by $n = \frac{\partial p}{\partial\mu}|_\beta$. To lowest order we find $n = \beta p$, or equivalently $p = nk_\mathrm{B}T$. This is the ideal gas law, as it should be!

The next term, $N = 2$, is especially interesting because it gives the first corrections due to the interactions. There is only one connected graph with two vertices and it contains one edge. We obtain

$$p_2(\beta,\mu) = -\frac{\lambda^2}{2\beta} \int_{\mathbb{R}^3} \Big(1 - \mathrm{e}^{-\beta U(|q|)} \Big) \mathrm{d}q.$$

Standard potentials have a hard-core and a small attractive part. With r the radius of the hard-core, we have

$$\int_{\mathbb{R}^3} \Big(1 - \mathrm{e}^{-\beta U(|q|)} \Big) \mathrm{d}q \approx 2b - 2\beta a,$$

with $b = \frac{2}{3}\pi r^3$, and

$$a = \tfrac{1}{2\beta} \int_{|q|>r} \Big(\mathrm{e}^{-\beta U(|q|)} - 1 \Big) \mathrm{d}q.$$

Notice that a is approximately equal to a constant when β is small. Recall the definition of the fugacity λ, Eq. (4.1); since $n = \frac{\partial p}{\partial\mu}|_\beta$, we have

$$\begin{aligned} p &\approx p_1 + p_2, \\ n &\approx \beta p_1 + 2\beta p_2. \end{aligned}$$

We then have $\beta p \approx n - \beta p_2$. Using $\lambda \approx n$, we have $\beta p_2 \approx -n^2(b - \beta a)$. Since $\beta = 1/k_\mathrm{B}T$, we find

$$p \approx nk_\mathrm{B}T(1 + nb) - n^2 a.$$

Let us use the variable $v = \frac{1}{n}$. To second order, the equation above can be rewritten as

$$\boxed{p = \frac{k_{\rm B} T}{v - b} - \frac{a}{v^2}.}$$

This is **van der Waals equation of state** for interacting gases. It generalizes the ideal gas law, which can be recovered by taking $a, b \to 0$. Parameters a, b are usually determined experimentally, and they give information on the potential.

2. General cluster expansion

Cluster expansion is also useful in mathematical physics because the absolute convergence of the series can be rigorously established. This section proposes a general theorem, and it discusses its application to the classical gas. Further applications include the Ising model and quantum systems, to be considered in later chapters.

Let (X, Σ, μ) be a measure space, where μ is a possibly complex measure. We let $|\mu|$ denote the total variation of μ ($|\mu|$ is essentially the absolute value of μ; in the case where $\mathrm{d}\mu(x) = g(x)\,\mathrm{d}\nu(x)$ with ν a positive measure, then $\mathrm{d}|\mu|(x) = |g(x)|\,\mathrm{d}\nu(x)$). Given a complex measurable symmetric function ζ on $X \times X$, we introduce the partition function by

$$Z = \sum_{n \geqslant 0} \frac{1}{n!} \int \mathrm{d}\mu(x_1) \dots \int \mathrm{d}\mu(x_n) \prod_{1 \leqslant i < j \leqslant n} \bigl(1 + \zeta(x_i, x_j)\bigr). \tag{4.3}$$

The term $n = 0$ of the sum is understood to be 1.

In the case of the classical gas, n represents the number of particles, X is the domain D, $\mathrm{d}\mu(x) = \lambda \mathrm{d}q$ with λ the fugacity of (4.1), $\mathrm{d}q$ is the Lebesgue measure on D, and $\zeta(x_i, x_j) = \mathrm{e}^{-\beta U(|q_i - q_j|)} - 1$.

We denote by $\mathcal{G}_n$ the set of all (unoriented, no loops) graphs with n vertices, and $\mathcal{C}_n \subset \mathcal{G}_n$ the set of connected graphs of n vertices. We introduce the following combinatorial function on finite sequences $(x_1, \dots, x_n)$ in X:

$$\varphi(x_1, \dots, x_n) = \begin{cases} 1 & \text{if } n = 1 \\ \frac{1}{n!} \sum_{G \in \mathcal{C}_n} \prod_{(i,j) \in G} \zeta(x_i, x_j) & \text{if } n \geqslant 2. \end{cases} \tag{4.4}$$

The product is over edges of G. A sequence $(x_1, \dots, x_n)$ is a *cluster* if the graph with n vertices and an edge between i and j whenever $\zeta(x_i, x_j) \neq 0$, is connected.

The cluster expansion allows to express the logarithm of the partition function as a sum (or an integral) over clusters.

THEOREM I (Cluster expansion).
Assume that $|1+\zeta(x,y)| \leqslant 1$ *for all* $x, y \in X$, *and that there exists a nonnegative function* a *on* X *such that for all* $x \in X$,

$$\int |\zeta(x,y)| \, \mathrm{e}^{a(y)} \, \mathrm{d}|\mu|(y) \leqslant a(x), \tag{4.5}$$

and $\int \mathrm{e}^{a(x)} \, \mathrm{d}|\mu|(x) < \infty$. *Then we have*

$$Z = \exp\Bigl\{\sum_{n\geqslant 1} \int \mathrm{d}\mu(x_1) \dots \int \mathrm{d}\mu(x_n) \, \varphi(x_1, \dots, x_n)\Bigr\}.$$

Combined sum and integrals converge absolutely. Furthermore, we have for all $x_1 \in X$

$$1 + \sum_{n\geqslant 2} n \int \mathrm{d}|\mu|(x_2) \dots \int \mathrm{d}|\mu|(x_n) \, |\varphi(x_1, \dots, x_n)| \leqslant \mathrm{e}^{a(x_1)}. \tag{4.6}$$

COROLLARY 4.1 (Classical gas). *Suppose that* $U(|q|) \geqslant 0$, *and that*

$$\lambda \int_{\mathbb{R}^3} \Bigl(1 - \mathrm{e}^{-\beta U(|q|)}\Bigr) \mathrm{d}q \leqslant \mathrm{e}^{-1}.$$

The pressure is then given by (4.2), *where the series is absolutely convergent and is analytic in* β *and* μ.

PROOF. Positivity of the potential ensures that $|1+\zeta(q_i, q_j)| \leqslant 1$. The criterion (4.5) holds with $a(q) \equiv 1$. □

Stable potentials with small attractions can also be treated, see Ruelle's book.

The criterion (4.5) first appeared on an article by Kotecký and Preiss. It is usually easy to guess the function a. It is translation invariant whenever the system is translation invariant. Therefore it must be constant in the classical gas. A little calculation shows that $a(x) = 1$ is the optimal choice. Another typical application deals with "polymers", that are represented by connected sets on $\mathbb{Z}^d$. Then a must be at least proportional to the cardinality, because of the left side in (4.5). And a usually cannot be bigger in order for the integral to converge.

PROOF OF THEOREM III. Another inequality turns out to be helpful. Multiplying both sides of (4.6) by $|\zeta(x, x_1)|$ and integrating over x_1, we find using (4.5)

$$\sum_{n\geqslant 1} \int \mathrm{d}|\mu|(x_1) \dots \int \mathrm{d}|\mu|(x_n) \Bigl(\sum_{i=1}^{n} |\zeta(x, x_i)|\Bigr) |\varphi(x_1, \dots, x_n)| \leqslant a(x) \tag{4.7}$$

for all $x \in \mathbb{A}$.

The strategy is to show inductively that (4.5) implies (4.6). Convergence of the cluster expansion follows and allows to prove Theorem III.

We prove that the following holds for all N,

$$1 + \sum_{n=2}^{N} n \int \mathrm{d}|\mu|(x_2) \dots \int \mathrm{d}|\mu|(x_n) |\varphi(x_1, \dots, x_n)| \leqslant \mathrm{e}^{a(x_1)}. \tag{4.8}$$

The case $N=1$ is clear and we consider now any N. The left side is equal to

$$1+\sum_{n=2}^{N}\int \mathrm{d}|\mu|(x_2)\dots\int \mathrm{d}|\mu|(x_n)\frac{1}{(n-1)!}\Big|\sum_{G\in\mathcal{C}_n}\prod_{(i,j)\in G}\zeta(x_i,x_j)\Big|. \tag{4.9}$$

Let us focus on the sum over connected graphs G. Removing all edges of G with one endpoint on 1 yields a possibly disconnected graph G'. Let $(G_1,\dots,G_k)$ be a sequence of connected graphs where G_i has set of vertices V_i, $V_1\cup\dots\cup V_k=\{2,\dots,n\}$, and $V_i\cap V_j=\varnothing$ if $i\neq j$. Each sequence determines a graph G', and to each G' corresponds $k!$ such sequences. See Fig. 4.1 for an illustration. Therefore

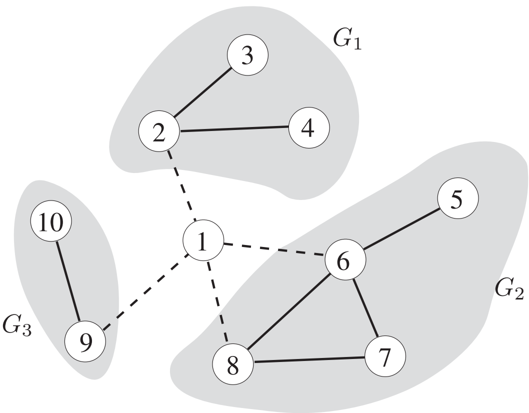

FIGURE 4.1. Illustration for G, G', and $(G_1,\dots,G_k)$.

$$\Big|\sum_{G\in\mathcal{C}_n}\prod_{(i,j)\in G}\zeta(x_i,x_j)\Big|\leqslant\sum_{k\geqslant1}\frac{1}{k!}\Big|\sum_{(G_1,\dots,G_k)}\prod_{\ell=1}^{k}\Big\{\prod_{(i,j)\in G_\ell}\zeta(x_i,x_j)\sum_{G'_\ell}\prod_{(i,j)\in G'_\ell}\zeta(x_i,x_j)\Big\}\Big|. \tag{4.10}$$

The sum over G'_ℓ runs over nonempty sets of edges with one endpoint on 1 and one endpoint in V_ℓ ($i=1$ in the last product). We have

$$\begin{aligned}\sum_{G'_\ell}\prod_{(i,j)\in G'_\ell}\zeta(x_i,x_j)&=\prod_{i\in V_\ell}\big(1+\zeta(x_1,x_i)\big)-1\\&=\sum_{i\in V_\ell}\zeta(x_1,x_i)\prod_{\substack{j\in V_\ell\\ j\neq i}}\big(1+\zeta(x_1,x_j)\big).\end{aligned}$$

This shows that the absolute value of the left side is bounded by $\sum_{i\in V_\ell}|\zeta(x_1,x_i)|$.

The sum over sequences $(G_1,\dots,G_k)$ can be done by first choosing the respective numbers of vertices $m_1,\dots,m_k$ whose sum is $n-1$, then by summing over partitions of $\{2,\dots,n\}$ in sets $V_1,\dots,V_k$ with $|V_i|=m_i$, and finally by choosing connected graphs for each set of vertices. The number of partitions is $\frac{(n-1)!}{m_1!\dots m_k!}$.

Then (4.9) can be bounded by

$$1 + \sum_{n=2}^{N} \sum_{k \geqslant 1} \frac{1}{k!} \sum_{\substack{m_1,\dots,m_k \geqslant 1 \\ m_1+\dots+m_k=n-1}} \prod_{\ell=1}^{k} \Big[\int \mathrm{d}|\mu|(y_1) \dots \int \mathrm{d}|\mu|(y_{m_\ell}) \\ |\varphi(y_1,\dots,y_{m_\ell})| \sum_{i=1}^{m_\ell} |\zeta(x_1,y_i)| \Big].$$

We can sum over n; the constraint $m_1 + \dots + m_k \leqslant N-1$ can be relaxed into $m_\ell \leqslant N-1$ for all ℓ. Using (4.7) with $n \leqslant N-1$, we obtain the bound

$$1 + \sum_{k \geqslant 1} \frac{1}{k!} [a(x_1)]^k = \mathrm{e}^{a(x_1)}. \tag{4.11}$$

This proves inequality (4.6). Absolute convergence of the cluster expansion follows from (4.6) and summability of $\mathrm{e}^{a(x)}$.

We now use this bound to prove that the partition function is given by the exponential of the sum of connected graphs. The product in (4.3) is less than one, so the sum over N is absolutely convergent. Retracing the developments of Section 1, we obtain

$$Z = 1 + \lim_{N\to\infty} \sum_{n=1}^{N} \sum_{k\geqslant 1} \frac{1}{k!} \sum_{\substack{m_1,\dots,m_k \geqslant 1 \\ m_1+\dots+m_k=n}} \frac{1}{m_1! \dots m_k!} \\ \prod_{\ell=1}^{k} \Big\{ \int \mathrm{d}\mu(x_1) \dots \int \mathrm{d}\mu(x_{m_\ell}) \sum_{G \in \mathcal{C}_{m_\ell}} \prod_{(i,j)\in G} \zeta(x_i,x_j) \Big\} \tag{4.12}$$

This expression has the structure $\lim_{N\to\infty} \sum_k A_N(k)$, and we need to take the limit under the sum. By the estimate of the theorem, we have that

$$|A_N(k)| \leqslant \frac{1}{k!} \Big[\sum_{n \geqslant 1} \int \mathrm{d}|\mu|(x_1) \dots \int \mathrm{d}|\mu|(x_n) \, |\varphi(x_1,\dots,x_n)| \Big]^k$$

for all N. The bracket is less than $\int \mathrm{e}^{a(x_1)} \, \mathrm{d}\mu(x_1)$ by (4.6), and this is finite by assumption. This allows to use the dominated convergence theorem. As $N \to \infty$, we obtain the exponential stated in the theorem. □