A LECTURE ON CLUSTER EXPANSIONS

Salvador Miracle-Sole

Centre de Physique Théorique, CNRS Luminy, Case 907,
F-13288 Marseille Cedex 9, France. E-mail: miracle@cpt.univ-mrs.fr

Abstract

A short exposition with complete proofs of the theory of cluster expansions for an abstract polymer system is presented.

Consider a countable set $\mathcal{P}$, whose elements will be called polymers. Let $\mathcal{I}$ be a subset of $\mathrm{P}_2(\mathcal{P})$, the set of all subsets of $\mathcal{P}$ with two elements. We say that two polymers γ and γ' are incompatible if $\{\gamma, \gamma'\} \in \mathcal{I}$ or if $\gamma = \gamma'$, and we will also write $\gamma \not\sim \gamma'$. If $\{\gamma, \gamma'\} \notin \mathcal{I}$ we say that the two polymers are compatible and we write $\gamma \sim \gamma'$.

Assume that a complex valued function $\phi(\gamma)$, $\gamma \in \mathcal{P}$, is given. We call $\phi(\gamma)$ the weight, or the activity, of the polymer γ. For any finite subset $\Lambda \subset \mathcal{P}$, the partition function $Z(\Lambda)$ of the polymer system is defined by

$$Z(\Lambda) = \sum_{\substack{X \subset \Lambda \\ \text{compatible}}} \prod_{\gamma \in X} \phi(\gamma) \tag{1}$$

The sum runs over all subsets X of Λ such that $\gamma \sim \gamma'$ for any two distinct elements of X. If X contains only one element, X is considered a compatible subset, and if $X = \emptyset$, the product is interpreted as the number 1.

We introduce the following function on $\mathcal{P} \times \mathcal{P}$

$$f(\gamma, \gamma') = \begin{cases} -1 & \text{if } \gamma \not\sim \gamma' \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

Let $\mathcal{G}_n$, $n \geq 2$ be the set of connected graphs with n vertices, $1, \ldots, n$. We consider undirected graphs without multiple edges, equivalently defined by a subset of $P_2(\{1,\ldots,n\})$ which determines the edges. Given $g \in \mathcal{G}_n$ we define the value of g on a sequence $(\gamma_1,\ldots,\gamma_n) \in \mathcal{P}^n$ as

$$g(\gamma_1,\ldots,\gamma_n) = \prod_{(i,j)\in g} f(\gamma_i,\gamma_j) \tag{3}$$

where $(i,j) \in g$ means that the graph g has an edge connecting i with j. We also define $\mathcal{G}_1$ as the set containing only one graph g having only one vertex (and no edges) and write

$$g(\gamma) = 1, \quad \gamma \in \mathcal{P} \tag{4}$$

Theorem 1 (Expansion) *Define*

$$a^{\mathrm{T}}(\gamma_1,\ldots,\gamma_n) = \sum_{g\in\mathcal{G}_n} g(\gamma_1,\ldots,\gamma_n) \tag{5}$$

Then, we have

$$\ln Z(\Lambda) = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\in\Lambda^n} a^{\mathrm{T}}(\gamma_1,\ldots,\gamma_n) \prod_{i=1}^{n} \phi(\gamma_i) \tag{6}$$

Proof. The partition function can be written as

$$Z(\Lambda) = 1 + \sum_{\gamma\in\Lambda} \phi(\gamma) + \sum_{n=2}^{\infty} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\in\Lambda^n} \prod_{i=1}^{n} \phi(\gamma_i) \prod_{1\le i<j\le n} (f(\gamma_i,\gamma_j)+1) \tag{7}$$

and developing the second product

$$\begin{aligned} Z(\Lambda) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{\substack{k_1,\ldots,k_m \\ \sum_i k_i = n}} \sum_{g_1\in\mathcal{G}_{k_1}} \sum_{g_2\in\mathcal{G}_{k_2}} \cdots \sum_{g_m\in\mathcal{G}_{k_m}} \frac{n!}{k_1!k_2!\ldots k_m!} \\ \sum_{(\gamma_1,\ldots,\gamma_n)\in\Lambda^n} g_1(\gamma_1,\ldots,\gamma_{k_1}) g_2(\gamma_{k_1+1},\ldots,\gamma_{k_1+k_2}) \ldots \\ \ldots g_m(\gamma_{k_1+\ldots+k_{m-1}+1},\ldots,\gamma_n) \prod_{i=1}^{n} \phi(\gamma_i) \\ = 1 + \sum_{m=1}^{\infty} \frac{1}{m!} \left(\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{g\in\mathcal{G}_k} \sum_{(\gamma_1,\ldots,\gamma_k)\in\Lambda^k} g(\gamma_1,\ldots,\gamma_k) \prod_{i=1}^{k} \phi(\gamma_i) \right)^m \end{aligned}$$

$$= \exp\left(\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{g\in\mathcal{G}_k} \sum_{(\gamma_1,\ldots,\gamma_k)\in\Lambda^k} g(\gamma_1,\ldots,\gamma_k) \prod_{i=1}^{k} \phi(\gamma_i) \right) \tag{8}$$

The theorem is proved.

With any finite sequence $\Gamma = (\gamma_1,\ldots,\gamma_n) \in \mathcal{P}^n$ we associate the graph $\theta(\Gamma)$ with vertices $\{1,\ldots,n\}$ obtained by drawing an edge between the vertices i and j if $\gamma_i \not\sim \gamma_j$. We observe that $g(\Gamma) \neq 0$ only if $\theta(\Gamma)$ is a connected graph (i.e., if $\theta(\Gamma) \in \mathcal{G}_n$) and $g \in \mathcal{G}_n$ is a subgraph of $\theta(\Gamma)$. Then

$$a^{\mathrm{T}}(\Gamma) = \sum_{g\in\mathcal{G}_n} g(\Gamma) = \sum_{\substack{g\subset\theta(\Gamma)\\ g\in\mathcal{G}_n}} (-1)^{|g|} \tag{9}$$

where $|g|$ is the number of edges of the graph g. In other words, $a^{\mathrm{T}}(\Gamma)$ is equal to the number of connected subgraphs of $\theta(\Gamma)$ with an even number of edges minus the number of connected subgraphs with an odd number of edges. If the graph $\theta(\Gamma)$ is not connected, $a^{\mathrm{T}}(\Gamma) = 0$.

We observe that the $a^{\mathrm{T}}(\gamma_1,\ldots,\gamma_n)$, $n = 1, 2, \ldots$, are symmetric functions. Thus, we can write the considered expansions also in terms of multi-indices instead of finite sequences. A multi-index X on a set $\mathcal{P}$ is a function $X(\gamma)$, $\gamma \in \mathcal{P}$, taking non-negative integer values and such that $\operatorname{supp} X = \{\gamma \in \mathcal{P} : X(\gamma) \geq 1\}$ is a finite set or, equivalently, such that $|X| = \sum_{\gamma\in\mathcal{P}} X(\gamma)$ is a finite number. We denote by $\mathrm{M}(\Lambda)$ the set of multi-indices defined on Λ.

If X is a given multi-index and $\Gamma = (\gamma_1,\ldots,\gamma_n)$, $n = |X|$, one of the sequences corresponding to X, we define $a^{\mathrm{T}}(X) = a^{\mathrm{T}}(\Gamma)$, and a new function

$$\phi^{\mathrm{T}}(X) = \Big(\prod_{\gamma\in\mathcal{P}} X(\gamma)! \Big)^{-1} a^{\mathrm{T}}(X) \prod_{\gamma\in\mathcal{P}} \phi(\gamma)^{X(\gamma)} \tag{10}$$

Taking into account that the number of different sequences Γ associated to X is $n!/\prod_{\gamma\in\mathcal{P}} X(\gamma)!$, the statement in theorem 1 can be written as

$$\ln Z(\Lambda) = \sum_{X\in\mathrm{M}(\Lambda)} \phi^{\mathrm{T}}(X) \tag{11}$$

The multi-indices such that $a^{\mathrm{T}}(X) \neq 0$ (i.e., whose associated graph $\theta(\Gamma)$ is connected) will be called clusters.

Theorem 2 (Convergence) *Assume that there is a positive function $\mu(\gamma)$, $\gamma \in \mathcal{P}$, such that, for all $\gamma_0 \in \mathcal{P}$,*

$$|\phi(\gamma_0)| \leq (e^{\mu(\gamma_0)} - 1) \exp\Big(- \sum_{\gamma \not\sim \gamma_0} \mu(\gamma)\Big) \tag{12}$$

Then, for all $\gamma_1 \in \mathcal{P}$, we have

$$\sum_{X \in \mathrm{M}(\mathcal{P}),\, X(\gamma_1) \geq 1} |\phi^{\mathrm{T}}(X)| \leq \mu(\gamma_1) \tag{13}$$

$$\sum_{X \in \mathrm{M}(\mathcal{P})} X(\gamma_1) |\phi^{\mathrm{T}}(X)| \leq e^{\mu(\gamma_1)} - 1 \tag{14}$$

We first prove the following lemma.

Lemma 1 *For any $X \in \mathrm{M}(\mathcal{P})$, we have*

$$(-1)^{|X|+1} a^{\mathrm{T}}(X) \geq 0 \tag{15}$$

Proof of lemma 1. We introduce the partition function

$$Z^*(\Lambda) = \sum_{\substack{X \subset \Lambda \\ \text{compatible}}} \prod_{\gamma \in X} \Big(- |\phi(\gamma)|\Big) \tag{16}$$

for which

$$- \ln Z^*(\Lambda) = \sum_{X \in \mathrm{M}(\Lambda)} - \Big(\prod_{\gamma \in \mathcal{P}} X(\gamma)!\Big)^{-1} a^{\mathrm{T}}(X) \prod_{\gamma} \Big(- |\phi(\gamma)|\Big)^{X(\gamma)} \tag{17}$$

If inequality (15) is satisfied, we have

$$- \ln Z^*(\Lambda) = \sum_{X \in \mathrm{M}(\Lambda)} |\phi^{\mathrm{T}}(X)| \tag{18}$$

showing that lemma 1 is equivalent to the fact that all terms in the expansion of $- \ln Z^*(\Lambda)$ are positive. This fact will be proved by an induction argument on the subsets Λ. It certainly holds when Λ contains only one polymer. Assume that it holds for a given Λ and let $\gamma_0 \in \mathcal{P} \backslash \Lambda$. ¿From the definition of Z^* we see that

$$Z^*(\Lambda \cup \{\gamma_0\}) = Z^*(\Lambda) - |\phi(\gamma_0)| Z^*(\Lambda_0) \tag{19}$$

with $\Lambda_0 = \{\gamma \in \Lambda : \gamma \sim \gamma_0\}$, and

$$-\ln\, Z^*(\Lambda \cup \{\gamma_0\}) = -\ln\, Z^*(\Lambda) - \ln\left(1 - \frac{|\phi(\gamma_0)|Z^*(\Lambda_0)}{Z^*(\Lambda)}\right) \tag{20}$$

On the other hand, we have

$$Z^*(\Lambda_0)/Z^*(\Lambda) = \exp \sum_{X\in \mathrm{M}(\Lambda)\backslash \mathrm{M}(\Lambda_0)} |\phi^{\mathrm{T}}(X)| \tag{21}$$

This shows the positivity of all the terms in the expansion of the second term in the right hand side of equation (20) (remark that the series expansions of the functions $\exp x$ and $-\ln(1-x)$ have only positive terms for $x \geq 0$). Since, by assumption, this is also the case for the first term, it follows that also $-\ln\, Z^*(\Lambda \cup \{\gamma_0\})$ satisfies the induction hypothesis. The lemma is proved.

Proof of theorem 2. We use again an induction argument on the subsets Λ. Assume that, for a given Λ and any $\gamma \in \Lambda$, the following estimate holds

$$\sum_{X\in \mathrm{M}(\Lambda),\, X(\gamma)\geq 1} |\phi^{\mathrm{T}}(X)| \leq \mu(\gamma) \tag{22}$$

This inequality can also be written as

$$-\ln Z^*(\Lambda) + \ln Z^*(\Lambda\backslash\{\gamma\}) \leq \mu(\gamma) \tag{23}$$

and, for all $\Lambda' \subset \Lambda$, it implies

$$-\ln Z^*(\Lambda) + \ln Z^*(\Lambda') \leq \sum_{\gamma\in\Lambda\backslash\Lambda'} \mu(\gamma) \tag{24}$$

and, in particular,

$$Z^*(\Lambda_0)/Z^*(\Lambda) \leq \exp\Big(\sum_{\gamma:\gamma\in\Lambda,\gamma\not\sim\gamma_0} \mu(\gamma)\Big) \tag{25}$$

because $\Lambda\backslash\Lambda_0 = \{\gamma \in \Lambda : \gamma \not\sim \gamma_0\}$. Since Λ does not contain γ_0, we get

$$|\phi(\gamma_0)|\frac{Z^*(\Lambda_0)}{Z^*(\Lambda)} \leq |\phi(\gamma_0)| \exp\Big(-\mu(\gamma_0) + \sum_{\gamma:\gamma\in\mathcal{P},\gamma\not\sim\gamma_0} \mu(\gamma)\Big) \tag{26}$$

and, taking the assumption (12) of the theorem into account,

$$\left|\frac{\phi(\gamma_0)Z^*(\Lambda_0)}{Z^*(\Lambda)}\right| \leq e^{-\mu(\gamma_0)}(e^{\mu(\gamma_0)}-1) = 1-e^{-\mu(\gamma_0)} \tag{27}$$

Then, using (20) and the fact that $-\ln(1-x)$ is an increasing function of x, for any real x in the interval $-1<x<1$, we obtain

$$-\ln\frac{Z^*(\Lambda\cup\{\gamma_0\})}{Z^*(\Lambda)} \leq -\ln\Big(1-\Big(1-e^{-\mu(\gamma_0)}\Big)\Big) = \mu(\gamma_0) \tag{28}$$

This proves the induction hypothesis (22) for $\Lambda\cup\{\gamma_0\}$, and therefore for all Λ (being valid when Λ contains only one element). Statement (13) of the theorem is proved.

Finally, if $\gamma_0\in\Lambda$ and Λ_0 is defined as above, we have

$$\sum_{X\in\mathrm{M}(\Lambda)} X(\gamma_0)|\phi^{\mathrm{T}}(X)| = -|\phi(\gamma_0)|\frac{\partial}{\partial|\phi(\gamma_0)|}\ln Z^*(\Lambda) = \frac{|\phi(\gamma_0)|Z^*(\Lambda_0)}{Z^*(\Lambda)} \tag{29}$$

Then, the statement (14) follows from hypothesis (12), taking into account inequality (24) and that now Λ contains γ_0. This ends the proof of the theorem.

The following consequences of the theorem concern the correlation functions and the truncated correlation functions. Notice that, for Λ finite and $\{\gamma_1,\ldots,\gamma_n\}\subset\Lambda$, these functions can be written as

$$\rho_\Lambda(\gamma_1,\ldots,\gamma_n) = Z(\Lambda)^{-1}\Big(\prod_{i=1}^n\phi(\gamma_i)\Big)Z(\cap_{i=1}^n\Lambda_i) \tag{30}$$

$$= Z(\Lambda)^{-1}\Big(\prod_{i=1}^n(\phi(\gamma_i)\,\partial/\partial\phi(\gamma_i))\Big)Z(\Lambda) \tag{31}$$

$$\rho_\Lambda^{\mathrm{T}}(\gamma_1,\ldots,\gamma_n) = \Big(\prod_{i=1}^n(\phi(\gamma_i)\,\partial/\partial\phi(\gamma_i))\Big)\ln Z(\Lambda) \tag{32}$$

with $\Lambda_i=\{\gamma\in\Lambda:\gamma\sim\gamma_i\}$.

Corollary 1 *Under the hypothesis of theorem 2, the thermodynamic limits ($\Lambda\uparrow\mathcal{P}$) of the correlation functions and the truncated correlation functions, ρ and ρ^{T}, exist. Moreover*

$$|\rho(\gamma_1,\ldots,\gamma_n)| \leq \prod_{i=1}^n(e^{\mu(\gamma_i)}-1) \tag{33}$$

Proof. Expressions (30), (31) and (32) show that the corresponding expansions in terms of the $\phi^{\mathrm{T}}(X)$ are

$$\rho_\Lambda(\gamma_1,\ldots,\gamma_n) = \Big(\prod_{i=1}^{n}\phi(\gamma_i)\Big)\exp\Big(\sum_{X\in Q(\gamma_1,\ldots,\gamma_n)}\phi^{\mathrm{T}}(X)\Big) \tag{34}$$

$$\rho^{\mathrm{T}}(\gamma_1,\ldots,\gamma_n) = \sum_{X\in\mathrm{M}(\mathcal{P})} X(\gamma_1)\ldots X(\gamma_n)\phi^{\mathrm{T}}(X) \tag{35}$$

where $Q(\gamma_1,\ldots,\gamma_n) = \mathrm{M}(\mathcal{P})\backslash\mathrm{M}(\cap_{i=1}^{n}\mathcal{P}_i)$ is the set of X whose support contains a γ incompatible with one of the γ_i, $i=1,\ldots,n$. The corollary follows from the convergence of these expansions stated in theorem 2. A simple extension of the argument leading to inequality (15) proves the inequality stated in the corollary.

Corollary 2 *Assume that, for all* $\gamma_0\in\mathcal{P}$,

$$|\phi(\gamma_0)| \le e^{-t}(e^{\mu(\gamma_0)}-1)\exp\Big(-\sum_{\gamma\not\sim\gamma_0}\mu(\gamma)\Big) \tag{36}$$

where $e^{-t}<1$ *is a uniform factor. Then the following cluster property is satisfied (for all* $\gamma_1\in\mathcal{P}$*)*

$$\sum_{(\gamma_2,\ldots,\gamma_n)\in\mathcal{P}^{n-1}} |\rho_\Lambda^{\mathrm{T}}(\gamma_1,\ldots,\gamma_n)| \le (n-1)!\,t^{-n+1}(e^{\mu(\gamma_1)}-1) \tag{37}$$

Proof. Theorem 2 and assumption (36) imply the bound

$$\sum_{X\in\mathrm{M}(\mathcal{P})} X(\gamma_1)e^{t\,|X|}|\phi^{\mathrm{T}}(X)| \le (e^{\mu(\gamma_1)}-1) \tag{38}$$

Taking into account equation (32) and that

$$e^{t\,|X|} = \sum_{n=0}^{\infty}\frac{t^n}{n!}\Big(\sum_{\gamma\in\mathcal{P}}X(\gamma)\Big)^n \tag{39}$$

we obtain the stated estimate (37) from this bound.

Some comments and references on the subject of this lecture can be found in S. Miracle-Sole, On the convergence of cluster expansions, to appear in Physica A.