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Combinatorics and cluster expansions*

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Abstract: This article is about the connection between enumerative combinatorics and equilibrium statistical mechanics. The combinatorics side concerns species of combinatorial structures and the associated exponential generating functions. The passage from species to generating functions is a combinatorial analog of the Fourier transform. Indeed, there is a convolution multiplication on species that is mapped to a pointwise multiplication of the exponential generating functions. The statistical mechanics side deals with a probability model of an equilibrium gas. The cluster expansion that gives the density of the gas is the exponential generating function for the species of rooted connected graphs. The main results of the theory are simple criteria that guarantee the convergence of this expansion. It turns out that other problems in combinatorics and statistical mechanics can be translated to this gas setting, so it is a universal prescription for dealing with systems of high dimension.

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Contents

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1. Introduction

The Rosetta Stone has text carved on its surface with the same passage in two Egyptian language scripts and in classical Greek. One version aids the comprehension of the other. Something like that can happen in mathematics, when ideas turn out to be common to more than one subject. In the case at hand, enumerative combinatorics has a substantial overlap with cluster expansions in statistical mechanics. These expansions themselves come in more than one variant; a particle picture gives rise to a rather different polymer representation. The theory of species of structures is a Rosetta Stone that translates between the combinatorics and the two versions of the cluster expansion.

The first main subject, enumerative combinatorics, is about how to count combinatorial objects, such as subsets and partitions and graphs. The systematic use of exponential generating functions is a particularly useful device when the objects are built from an underlying set (the label set). This practice has been systemized in the theory of species of structures, for instance as presented in the book of Bergeron, Labelle, and Leroux [2].

The second main subject, cluster expansions in statistical mechanics, arises in classic form in the equilibrium statistical mechanics of particles interacting in pairs. Here for technical simplicity the particles are taken to occupy a discrete set of locations. The fundamental quantity is the power series for the expected

number of particles at a given location as a function of activity parameters associated with the locations. This is one version of the cluster expansion. The main theorem is that for a gas with sufficiently weak interaction or sufficiently small activities the cluster expansion has a non-zero radius of convergence, uniformly in the size of the system.

The equilibrium gas interpretation is just one way of looking at the cluster expansion; its importance is much more general in the study of infinite dimensional systems. The locations in the gas picture play the role of coordinates in the infinite dimensional space, and the assumption is that there is some control over the dependence between the coordinates. The conclusion is the existence of a well-defined probability model that depends on parameters in a nice way. A variety of expansion problems in statistical mechanics and combinatorics may treated in such a framework via a polymer representation. An overview of some of these ideas may be found in the book of Malyshev and Minlos [16].

It is a remarkable fact that these two subjects overlap, and where they overlap their results coincide. This is not so apparent, since they have different histories and have developed diverging terminologies. The plan is give a unified picture in terms of the combinatorial theory of species of structures. Thus, the first part of this discussion is the combinatorics, and the second part deals with statistical mechanics and with the convergence of cluster expansions. Two approaches to the convergence problem are presented. One uses a partition of the set of connected graphs such that each set in the partition has exactly one tree. The other one uses the fixed point equations for the exponential generating functions for rooted connected graphs and for rooted trees.

Most of what is presented in this survey is part of the lore of mathematical physics, but it may be useful to have the perspective that is given by the connection with combinatorics. The aim is not to give the most powerful result, but to present the simplest case and direct the reader to recent literature for improvements.

2. Enumerative combinatorics

2.1. Graphs and connected graphs

In the present context the combinatorial object that is most useful is a *graph*. In most of the following this will denote a set of points together with a set of two-point subsets. The points are the vertices of the graph; the two-point subsets are the edges of the graph. Sometimes this is called a simple graph, to emphasize that there are no loops or multiple edges. A graph with all possible edges is called a complete graph. The opposite extreme is a graph with no edges. A graph can have only one vertex, in which case it has no edges. There is also an empty graph with no vertices and no edges. If U is a finite set, then $G[U]$ will denote all graphs with U as vertex set. Counting graphs is easy. If the set U of vertices has n points, then there are $\binom{n}{2}$ possible edges, so there are a total of

$$|G[U]| = 2^{\binom{n}{2}} \tag{2.1}$$

graphs with this vertex set. Thus the number of graphs on $n = 0, 1, 2, 3, 4, 5, 6$ vertices is $1, 1, 2, 8, 64, 1024, 32768$.

Consider a graph with a non-empty vertex set. There may be a partition of the vertex set into non-empty parts such that every edge of the graph is a subset of some part. A *connected graph* is a graph with non-empty vertex set such that the only such partition has just one part, the vertex set itself. It follows that every vertex is connected to every other vertex by a path of edges. Sometimes a connected graph is called a spanning connected graph, to make the point that no vertex can be omitted. A graph with only one vertex is connected. The empty graph is not connected. This last fact is important for counting purposes. If U is the vertex set, write $C[U]$ for the corresponding set of connected graphs. Counting connected graphs is not so easy. The number of connected graphs on a vertex set with $n = 0, 1, 2, 3, 4, 5, 6$ elements is $0, 1, 1, 4, 38, 728, 26704$. There are many connected graphs, in fact, most graphs are connected. This is confirmed by the following argument. Fix a connected graph with n vertices and $n - 1$ edges (a tree graph). Every graph whose edge set includes the edge set of this particular tree graph is connected. The number of edges that are not in the tree graph is $d_n = \binom{n}{2} - (n - 1)$. So the number of graphs that include the tree is 2^{d_n}. That is,

$$|C[U]| \geq 2^{\binom{n}{2}-(n-1)}. \tag{2.2}$$

This crude lower bound for the number of connected graphs is already huge.

A *tree* is a minimal connected graph with a given vertex set. Sometimes this is called a spanning tree. Each tree on a vertex set U with n points has $n - 1$ edges. Let $T[U]$ denote the set of all trees with vertex set U. A famous theorem of Cayley says that there are

$$|T[U]| = n^{n-2} \tag{2.3}$$

trees. The number of trees on a vertex set with $n = 0, 1, 2, 3, 4, 5, 6$ elements is $0, 1, 1, 3, 16, 125, 1296$. There are many fewer trees than connected graphs.

It is important to distinguish graphs on a set from isomorphism classes of graphs. The number of isomorphism classes of graphs on a vertex set with $n = 0, 1, 2, 3, 4, 5, 6$ elements is $1, 1, 2, 4, 11, 34, 156$. The number of isomorphism classes of connected graphs on a vertex set with $n = 0, 1, 2, 3, 4, 5, 6$ elements is $0, 1, 1, 2, 6, 21, 112$. The number of isomorphism classes of trees on a vertex set with $n = 0, 1, 2, 3, 4, 5, 6$ elements is $0, 1, 1, 1, 2, 3, 6$. The numbers counting isomorphism classes are considerably smaller, but they are harder to calculate. Isomorphism classes will play little or no role in the following. They may show up in examples.

Every graph has a partition of its vertex set into non-empty parts on which there is a connected graph. This is even true of the empty graph, since in that case the partition is itself empty. One can think of a connected graph as a graph on a non-empty vertex set that is minimal under partitioning. Thus connected graphs are the natural constituents of graphs. A tree is a connected graph on a non-empty vertex set with a minimal edge set. The goal in the following is to understand connected graphs in terms of trees.

2.2. Colored sets

In enumerative combinatorics it is common to count a set of structures that are built from an underlying set U, often called the label set. In the following it will be helpful to have a somewhat more general starting point. Fix a set $\mathcal{P}$. This is the palette of colors. Thus, for instance, its elements could be red, blue, green. A *colored set* is given by an underlying finite set U and a function $a : U \to \mathcal{P}$. Thus for each j in U there is a color $a(j)$.

The special case when the color palette $\mathcal{P}$ has only one color is called *monochromatic* or *scalar*. In this situation the colored set may be identified with the label set U.

There are various interpretations of the notion of colored set. In probability the elements in U are called balls, and the elements of $\mathcal{P}$ are called urns. A colored set is a way of placing balls into urns. There is also an important physics interpretation. The set $\mathcal{P}$ is a fixed set of locations. These could be locations in space, but all that is important for many purposes is that each location is a box that can be occupied by particles. The set U is a set of particles, and a function $a : U \to \mathcal{P}$ is a particle configuration, in which particle j is placed at location $a(j)$.

There is a notion of isomorphism for colored sets. An isomorphism from $a : U \to \mathcal{P}$ to $b : V \to \mathcal{P}$ is a bijection $\phi : U \to V$ with $b \circ \phi = a$. One maps colored sets using bijections that preserve the colors. Two colored sets that are related in this way are regarded as the same in all important respects. That is, the identities of the points in the set is not important, but the distribution of colors must be preserved. Colored sets with maps given by this notion of isomorphism form a category.

The most basic operation on colored sets is taking a subset. If $a : U \to \mathcal{P}$ is a colored set, and $V \subseteq U$ is a subset, then it inherits the colors. Thus the restriction $a_V : V \to \mathcal{P}$ is the corresponding colored subset.

Taking subsets is fundamental in combinatorics. Given a set, there is a fundamental combinatorial operation that consists of splitting it into an ordered pair of complementary subsets in all possible ways. Another fundamental operation is to partition it into non-empty subsets in all possible ways. It will turn out that another useful operation is that of adjoining an external point of given color.

The colored set idea applies to graphs, where the set U is the vertex set, and the graph is defined by giving a specified set of edges joining pairs of vertices. Both in combinatorics and in physics one wants to do more than simply count graphs. In many applications there is a given assignment to each pair of colors p, q of a corresponding color pair weight $t(p, q)$. It is assumed symmetric: $t(p, q) = t(q, p)$. Then for a given colored set a and a given edge $\{i, j\}$ with $i \neq j$, there is a edge weight $t(a(i), a(j))$ computed from the colors of the two vertices.

This also has a physics interpretation. For a given particle configuration a and for a given pair i, j of particles, there is an edge weight $t(a(i), a(j))$ computed from the locations of the two particles (which could be the same location). This

is a measure of the interaction between this pair of particles. This picture will be considered in more detail in later sections.

For a graph on a colored set there is a notion of graph weight. Let $a : U \to \mathcal{P}$ be a colored set. Consider a graph g with vertex set U. To each such graph is associated the graph weight given by the product over all edges:

$$\mathrm{wt}(g) = \prod_{\{i,j\}\in g} t(a(i), a(j)). \tag{2.4}$$

The total weight associated with all the graphs associated with the colored set a is

$$\sum_{g\in G[U]} \mathrm{wt}(g) = \sum_{g\in G[U]} \prod_{\{i,j\}\in g} t(a(i), a(j)). \tag{2.5}$$

By the distributive law, this can be expressed in the simple form

$$\sum_{g\in G[U]} \mathrm{wt}(g) = \prod_{\{i,j\}} (1 + t(a(i), a(j))), \tag{2.6}$$

where the product on the right is over all two-element subsets of U.

The total weight associated with the connected graphs g associated with the colored set a is

$$\sum_{g\in C[U]} \mathrm{wt}(g) = \sum_{g\in C[U]} \prod_{\{i,j\}\in g} t(a(i), a(j)). \tag{2.7}$$

Unfortunately, there is no simplification of this sum. Connected graphs are combinatorially difficult.

There is an operation called *combinatorial exponential* that takes the weighted connected graph construction into the weighted graph construction. It works like this. Say that $a : U \to \mathcal{P}$ is a colored set. Consider an arbitrary partition Γ of U into a collection of disjoint non-empty subsets. For each subset V in the partition, consider a connected graph corresponding to this vertex set. These fit together to define a graph with vertex set U whose connected components are precisely the subsets V in the partition. For each such V let $a_V : V \to \mathcal{P}$ be the restriction of a to the subset V. The graph weight given by the coloring a of the graph on U is the product over V in the partition Γ of the graph weights given by the colorings a_V of the connected graphs on V.

If we allow all possible partitions, then we get all graphs in this way. It follows from the distributive law that the total weight given by the coloring $a : U \to \mathcal{P}$ of the graphs with vertex set U is given by

$$\sum_{g\in G[U]} \mathrm{wt}(g) = \sum_{\Gamma} \prod_{V\in\Gamma} \sum_{g\in C[V]} \mathrm{wt}(g), \tag{2.8}$$

where the last sum is the total weight for connected graphs g with vertex set V. This combinatorial operation is based on the simple observation that for each graph on a vertex set there is a unique partition of the vertex set with a connected graph on each set in the partition. It is at the heart of the combinatorics

of equilibrium statistical mechanics. The task ahead is to invert this relation to get information about the total weight for the connected graph construction from information about the total weight for the graph construction.

2.3. Multi-indices

In most of the constructions the specific identity of the points in U is not important; one set with a given number of points is as good as any other. Thus it is often useful to describe the situation via a *multi-index*. A multi-index $N : \mathcal{P} \to \mathbf{N}$ is a function from the set of colors to the natural numbers $\mathbf{N} = \{0, 1, 2, 3, \ldots\}$. The sum of the values of the multi-index N is the *order*

$$|N| = \sum_p N(p). \tag{2.9}$$

There is also the *factorial*

$$N! = \prod_p N(p)! \tag{2.10}$$

which is the product of the factorials of the individual factors. Finally, there is the sum of two multi-indices, defined in the obvious pointwise way.

Given a colored set $a : U \to \mathcal{P}$, there is a corresponding multi-index $\mathrm{count}(a)$ given by

$$\mathrm{count}(a) = N, \text{ where } N(p) = \#\{j \in U \mid a(j) = p\}. \tag{2.11}$$

If a multi-index N comes from a colored set $a : U \to \mathcal{P}$, then the order $|N|$ of the multi-index is just the number of elements n in the set U. The number of colored sets $a : U \to \mathcal{P}$ with given multi-index $\mathrm{count}(a) = N$ is the multinomial coefficient $n!/N!$.

The analog of a splitting of a colored set into a pair of complementary subsets is a decomposition of a multi-index N as a sum $N = K + L$ of multi-indices. A multi-index in this decomposition has multiplicity given by the generalized binomial coefficient

$$\binom{N}{K} = \frac{N!}{K!L!}. \tag{2.12}$$

There is also an operation on multi-indices that corresponds to adjoining an external point of color p. This is simply addition with δ_p, where δ_p is the multi-index that is 1 on p and 0 elsewhere.

2.4. Exponential generating functions

An *exponential generating function* is a formal power series in variables w_p indexed by p in $\mathcal{P}$. It is a way of encoding the information given by coefficients $f(a)$ that depend on a choice of colored set a. The *tensor form* of an exponential generating function is

$$F(w) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{a:U_n \to \mathcal{P}} f(a) \prod_{j \in U_n} w_{a(j)}. \tag{2.13}$$

Here for each n the set U_n is a set with n elements.

Another representation of the exponential generating function is in terms of coefficients $f(N)$ that depend on a choice of multi-index N. The *multi-index form* of an exponential generating function is

$$F(w) = \sum_N \frac{1}{N!} f(N) w^N, \tag{2.14}$$

where $w^N = \prod_{p \in \mathcal{P}} w(p)^{N(p)}$. The general relation between the two representations is

$$f(N) = \frac{N!}{n!} \sum_{a:\mathrm{count}(a)=N} f(a), \tag{2.15}$$

where $n = |N|$ is the order of N.

An isomorphism of colored sets is obtained by permuting the underlying set while preserving the colors. Suppose that $f(a)$ depends only on the isomorphism class of the colored set $a : U \to \mathcal{P}$. Then $f(a)$ depends only on the corresponding multi-index $N = \mathrm{count}(a)$. All the terms in the sum are the same, and so $f(N) = f(a)$. This is the usual situation in practice, and it is summarized in the *symmetry convention*:

$$\text{If } \mathrm{count}(a) = N, \text{ then } \ f(a) = f(N). \tag{2.16}$$

If one thinks of the set $\mathcal{P}$ as a set of values for tensor indices, then $a : U_n \to \mathcal{P}$ is a listing of indices for a rank n tensor, and the coefficient $f(a)$ is a symmetric rank n tensor, in that a permutation of order in which the indices are listed gives the same value of the coefficient. In the monochromatic case the coefficient may be written $f(U)$; it is a scalar that only depends on the cardinality n of U.

Among the natural operations on exponential generating functions are addition, multiplication, differentiation, Euler differentiation, scalar composition, composition, and Hadamard product. In each case there are corresponding operations on the coefficients, and these operations have a combinatorial interpretation. Here is a description for each operation. We use $F(w)$ and $G(w)$ for the exponential generating functions with tensor form coefficients given by $f(a)$ and $g(a)$ and with multi-index form coefficients given by $f(N)$ and $g(N)$.

Sum The sum $F(w) + G(w)$ has tensor form coefficients $f(a) + g(a)$ and multi-index coefficients $f(N) + g(N)$.

Product The product $H(w) = F(w)G(w)$ has tensor form coefficients

$$h(a) = \sum_{\langle V,W \rangle} f(a_V) g(a_W), \tag{2.17}$$

where $a : U \to \mathcal{P}$ is a colored set, and the ordered pairs $\langle V, W \rangle$ are splittings of U into complementary subsets. The colored sets a_V and a_W are obtained by restricting to the corresponding subsets. The multi-index coefficients are

$$h(N) = \sum_{K+L=N} \binom{N}{K} f(K) g(L). \tag{2.18}$$

Derivative The derivative $G(w) = (\partial/\partial w_p)F(w)$ has tensor coefficients $g(a) = f(a^p)$. For $a : U \to \mathcal{P}$ the corresponding a^p is obtained by adjoining an external point $*$ of color p. Thus a^p is defined on the disjoint union $U + \{*\}$ with $a^p(j) = a(j)$ for $j \in U$ and $a^p(*) = p$. The multi-index coefficients are given by $g(N) = f(N + \delta_p)$.

Euler derivative The Euler derivative $H(w) = w_p(\partial/\partial w_p)F(w)$ has tensor coefficients $h(a) = \#\{j \mid a(j) = p\}f(a)$. The multi-index coefficients are given by $h(N) = N(p)f(N)$.

Scalar composition Suppose $F(z) = \sum_{n=0}^{\infty} \frac{1}{n!} f(U_n) z^n$ is defined for z a scalar variable. Suppose $G(0) = 0$. The composition $H(w) = F(G(w))$ is obtained by replacing z by $G(w)$ in $F(z)$. Then $H(w)$ has tensor coefficients

$$h(a) = \sum_{\Gamma} f(\Gamma) \prod_{V \in \Gamma} g(a_V). \tag{2.19}$$

Here $a : U \to \mathcal{P}$, and Γ ranges over partitions of U into a set of non-empty subsets with union equal to U. The multi-index coefficients are

$$h(N) = \sum_{n=0}^{\infty} \sum_{M_1 + \cdots + M_n = N} \frac{1}{n!} \frac{N!}{M_1! \cdots M_n!} f(n) g(M_1) \cdots g(M_n). \tag{2.20}$$

The inner sum is over sequences $M_1, \ldots, M_n$ of n multi-indices with sum N. Since each multi-index M_i is non-zero, this is a finite sum.

Composition The most general notion of composition requires another palette $\mathcal{Q}$ of colors. Suppose that $F(z)$ is an exponential generating function involving variables z_q indexed by $q \in \mathcal{Q}$. Suppose that for each $q \in \mathcal{Q}$ there is a $G_q(w)$ with variables w_p for $p \in \mathcal{P}$. Suppose each $G_q(0) = 0$. Then $H(w) = F(G(w))$ is obtained by replacing each z_q in $F(z)$ by $G_q(w)$. It has tensor coefficients

$$h(a) = \sum_{\Gamma} \sum_{c : \Gamma \to \mathcal{Q}} f(c) \prod_{V \in \Gamma} g_{c(V)}(a_V). \tag{2.21}$$

Here $a : U \to \mathcal{P}$, Γ ranges over partitions of U into a set of non-empty subsets V with union equal to U, and c ranges over colorings of Γ, so each set V in Γ has a color $c(V)$ in $\mathcal{Q}$. The corresponding multi-index version is too awkward to be of much use.

Hadamard product The Hadamard product of $F(w)$ and $G(w)$ is the exponential generating function $H(w)$ with tensor form coefficients $h(a) = f(a)g(a)$ and multi-index form coefficients $h(N) = f(N)g(N)$.

The Hadamard product on exponential generating functions is not a particularly nice operation. However there is one special case where something useful can be said. Say that there is a value $\lambda(q)$ defined for each color q in $\mathcal{P}$. Consider the *multi-variable exponential function*

$$F(w) = \exp(\lambda \cdot w) = \sum_{N} \frac{1}{N!} (\lambda w)^N. \tag{2.22}$$

Here $\lambda \cdot w$ is the scalar product, while λw is the pointwise product. Then the Hadamard product of $F(w)$ with $G(w)$ is just $G(\lambda w)$. In other words, in this special case the Hadamard product induces a scaling of the variable.

2.5. Cluster expansions

The case of scalar composition with the exponential function is particularly important. Suppose that $C(w)$ is an exponential generating function. Further suppose that $C(0) = 0$. Then $G(w) = \exp(C(w))$ is an exponential generating function with $G(0) = 1$. Typically in combinatorics the $G(w)$ will enumerate some kind of objects, and the $C(w)$ will enumerate corresponding connected objects. For this reason, the exponential generating function $C(w)$ may be called the *connected function* associated with $G(w)$, and the representation of $G(w)$ in terms of $C(w)$ is called the *cluster representation*. Its expansion

$$C(w) = \sum_{N \neq 0} \frac{1}{N!} c_N w^N \tag{2.23}$$

is sometimes called the *cluster expansion* for the connected function. A multi-index N for this expansion is called a *cluster*, and the corresponding c_N is a *cluster coefficient*. The partial derivative $\partial C(w)/\partial w_p$ is the *pinned connected function*. It has the cluster expansion

$$\frac{\partial C(w)}{\partial w_p} = \frac{1}{G(w)} \frac{\partial G(w)}{\partial w_p} = \sum_N \frac{1}{N!} c_{N+\delta_p} w^N. \tag{2.24}$$

This is also a cluster expansion. Similarly, the Euler partial derivative $C_p^\bullet(w) = w_p \partial C(w)/\partial w_p$ is the *rooted connected function*. It has the cluster expansion

$$C_p^\bullet(w) = w_p \frac{\partial C(w)}{\partial w_p} = w_p \frac{1}{G(w)} \frac{\partial G(w)}{\partial w_p} = \sum_{N \neq 0} \frac{1}{N!} N(p) c_N w^N. \tag{2.25}$$

The pinned cluster expansion and the rooted cluster expansion give information about the ratio of $\partial G(w)/\partial w_p$ to $G(w)$. The convergence question for one or the other of these expansions is a major topic in mathematical physics. As we shall see, the challenge is to get results that are independent of the number of colors. This is why it is useful to fix one color and consider the pinned connected function or the rooted connected function with that specified color as a reference point. By contrast, the connected function does not refer to a fixed color. To discuss convergence of the connected function it is thus customary to fix a p and consider only terms with $N(p) \geq 1$. The resulting series is dominated by the series for the rooted connected function.

The expression of the coefficients of $G(w)$ in terms of the coefficients of $C(w)$ will here be called the *cluster coefficient representation*. With tensor coefficients it is

$$g(a) = \sum_\Gamma \prod_{V \in \Gamma} c(a_V). \tag{2.26}$$

Here $a : U \to \mathcal{P}$, and Γ ranges over partitions of U into a set of non-empty subsets with union equal to U. The multi-index form is

$$g(N) = \sum_{n=0}^{\infty} \sum_{M_1+\cdots+M_n=N} \frac{1}{n!} \frac{N!}{M_1! \cdots M_n!} c(M_1) \cdots c(M_n). \tag{2.27}$$

In this expression $M_1, \ldots, M_n$ is a sequence taken in order; this is compensated by the division by $n!$.

An important special case is when $G(w)$ is an *multi-affine generating function*, that is when $g(N) \neq 0$ implies $0 \leq N \leq 1$. In that case N may be identified with its support, and we may write

$$G(w) = \sum_X g(X) w^X, \tag{2.28}$$

where $w^X = \prod_{q \in X} w_q$. In the cluster representation $G(w) = \exp(C(w))$, the exponential generating $C(w)$ will not typically be multi-affine, but $G(w)$ is determined by the multi-affine part of $C(w)$. Thus

$$g(X) = \sum_{\Gamma} \prod_{Y \in \Gamma} c(Y), \tag{2.29}$$

where Γ ranges over partitions of X. In this context a set Y is called a cluster, and $c(Y)$ is a cluster coefficient. This is yet another version of the cluster coefficient representation.

A famous realization of the cluster coefficient representation occurs in probability, statistical mechanics, and random field theory. The original coefficients $g(N)$ are *moments* of random variables. That is, there is a probability space with expectation μ and random variables ϕ_p indexed by p in $\mathcal{P}$. Write $\phi^N = \prod_p \phi_p^{N(p)}$. Then

$$g(N) = \mu(\phi^N) = \mu(\prod_p \phi_p^{N(p)}). \tag{2.30}$$

The corresponding connected cluster coefficients $c(N)$ are called *cumulants* or *semi-invariants* or *Ursell functions* or *truncated functions*. Apparently a good concept deserves many names.

2.6. Weighted sets

The original problem in enumerative combinatorics is this: Given a finite set A, generated in some systematic way, find its cardinal number $|A|$. This problem is too limited for many applications. An obvious generalization is the following: assign a weight to each element of the set, and add the weights. When each weight is equal to one, this addition just gives the cardinal number. If the weights are allowed other values, but in a systematic way, then enough of the properties of counting may be preserved so that the more general problem can be solved with little more effort.

The starting point is an arbitrary assignment of weights on the level of colors. For the applications to graphs the natural starting point is *color pair weights*. Each pair of colors p, q gets a weight $t(p,q) = t(q,p)$. Then the individual graphs each have a *graph weight*. The weight function maps each graph g on the underlying set U of a colored set $a : U \to \mathcal{P}$ to the corresponding graph weight given by the product formula $\mathrm{wt}(g) = \prod_{\{i,j\}\in g} t(a(i), a(j))$. Here is an example of a weighted set that will be of central concern in the following developments. It is given by this graph weighting function restricted to the set $C[U]$ of all connected graphs on the vertex set U. The total weight obtained by summing is then

$$\sum_{g\in C[U]} \mathrm{wt}(g) = \sum_{g\in C[U]} \prod_{\{i,j\}\in g} t(a(i), a(j)). \tag{2.31}$$

In general, when we have a set of objects and a weight for each object, then we have a weighted set. A *weighted set* is a finite set *underlying set* $\mathrm{dom}(A)$ together with a *weight function* $A : \mathrm{dom}(A) \to \mathcal{R}$. The elements of the target $\mathcal{R}$ of this function belong to a ring, typically a number system like $\mathbf{R}$ or $\mathbf{C}$ or perhaps a ring of formal power series. The *total weight* of a weighted set is given by

$$|A|_* = \sum_{\alpha\in \mathrm{dom}(A)} A(\alpha). \tag{2.32}$$

In a given context it is often useful to require that the collection of weighted sets under consideration be closed under the operations of disjoint union and Cartesian product. They should obey the following rules. Say that $A : \mathrm{dom}(A) \to \mathcal{R}$ and $B : \mathrm{dom}(B) \to \mathcal{R}$ are weighted sets.

Disjoint union Let $\mathrm{dom}(A) + \mathrm{dom}(B)$ be the usual disjoint union of the sets $\mathrm{dom}(A)$ and $\mathrm{dom}(B)$. Then the disjoint union weighted set $A + B$ is the function $A + B : \mathrm{dom}(A) + \mathrm{dom}(B) \to \mathcal{R}$ given by $(A + B)(\alpha) = A(\alpha)$ if $\alpha \in \mathrm{dom}(A)$ and $(A + B)(\beta) = B(\beta)$ if $\beta \in \mathrm{dom}(B)$.

Cartesian product Let $\mathrm{dom}(A) \times \mathrm{dom}(B)$ be the usual cartesian product of the sets $\mathrm{dom}(A)$ and $\mathrm{dom}(B)$. The Cartesian product weighted set $A \times B$ is the function $(A\times B) : \mathrm{dom}(A)\times\mathrm{dom}(B) \to Rc$ given by $(A\times B)(\alpha,\beta) = A(\alpha)B(\beta)$ for $\alpha \in \mathrm{dom}(A), \beta \in \mathrm{dom}(B)$.

The total weight of a disjoint union is the sum of the total weights, that is, $|A + B|_* = |A|_* + |B|_*$. What is more interesting is that the total weight of a Cartesian product is the product of the total weights, which is expressed by $|A \times B|_* = |A|_*|B|_*$. The reason for this is the distributive law:

$$|A \times B|_* = \sum_\alpha \sum_\beta A(\alpha)B(\beta) = \left(\sum_\alpha A(\alpha)\right)\left(\sum_\beta B(\beta)\right) = |A|_*|B|_*. \tag{2.33}$$

There is a notion of isomorphism for weighted sets. An isomorphism h from $A : \mathrm{dom}(A) \to \mathcal{R}$ to $B : \mathrm{dom}(B) \to \mathcal{R}$ is a bijection $h : \mathrm{dom}(A) \to \mathrm{dom}(B)$ such that $B \circ h = A$. Weighted sets with maps that are isomorphisms form a category.

The advantage of the weighted set concept is that the same constructions work on the level of the underlying sets and on the level of the weighted sets. One could even write $\alpha \in A$ to mean that α is in the underlying set of A, while at the same time writing $A(\alpha)$ for the weight of α. In the following identities involving sum and cartesian product for weighted sets will always accompany corresponding identities for the underlying sets of combinatorial objects.

Weighted set identities generalize those of ordinary enumerative combinatorics. This is because they include the degenerate situation in which the weight function assigns to each element of the underlying set the number 1. In this case giving a weighted set simply amounts to specifying the underlying set. The total weight of such a set is simply the number of points in it. This is the most classic form of combinatorics: counting.

2.7. A species example

The concept of species of combinatorial structures was introduced by André Joyal in 1980. A species assigns to each label set a set of combinatorial structures. In the book of Bergeron, Labelle, and Leroux [2] there is an appendix that gives a table of many common species. These include permutations, subsets, set partitions, trees, graphs, and many others. If the label set U has n elements, then the corresponding number of permutations, subsets, set partitions, trees, graphs constructed from U are $n!$, 2^n, B_n, n^{n-2}, $2^{\binom{n}{2}}$. (Here B_n is the Bell number, the number of partitions of a set with n elements into disjoint non-empty subsets.) These sequences are invariants of the corresponding species. The purpose of species theory is to give a systematic way of constructing such invariants.

A classical example is the power set species P, the species that assigns to a set U the set $P[U]$ of its subsets. As noted above, if U has n elements, then the number of sets in $P[U]$ is 2^n. This number alone does not give a particularly detailed description of the subsets. A first refinement of the species concept is to go beyond counting to adding weights. Assign to each subset V with k elements the weight λ^k. The total weight of $P[U]$ is the polynomial

$$\sum_{k=0}^{n} \binom{n}{k} \lambda^k = (1+\lambda)^n. \tag{2.34}$$

This is a more interesting combinatorial invariant. It includes counting subsets as a special case by setting λ equal to one. On the other hand, setting λ to -1 produces a remarkable cancelation.

Much of classical combinatorics may be done in this framework, with an unstructured label set U. However, for many applications it is useful to allow the weights to depend on additional structure. A particularly natural structure is a given classification of the set U into categories. That is, there is a fixed set $\mathcal{P}$ and a function $a : U \to \mathcal{P}$. There are various interpretations of this kind of structure. For example, if $\mathcal{P}$ is a set of political parties, then each set U of individuals has political preferences $a : U \to \mathcal{P}$. A relatively neutral interpretation is to take $\mathcal{P}$ to be a set of colors; in that case $a : U \to \mathcal{P}$ is a colored set.

Say that each p in $\mathcal{P}$ has an attached weight $\lambda(p)$. Assign to each subset V the product $\prod_{i\in V}\lambda(a(i))$. Then the equation for the total weight of $P[U]$ is

$$\sum_{V\subseteq U}\prod_{i\in V}\lambda(a(i)) = \prod_{i\in U}(1+\lambda(a(i))). \tag{2.35}$$

This formula includes the previous total weight formula as a special case by taking all the weights to be the same. It has many consequences. Here is one. Let X be a set, and let $\mathcal{P}$ be the collection of all subsets of X. For p in $\mathcal{P}$, define $\lambda(p) = -1_p$, the negative of the indicator function of p. For a family $a(i), i \in U$ of subsets of X the formula gives

$$\sum_{V\subseteq U}(-1)^{|V|}1_{\bigcap_{i\in V}a(i)} = 1_{\bigcap_{i\in U}a(i)^c}. \tag{2.36}$$

This is algebraically equivalent to

$$\sum_{\emptyset\neq V\subseteq U}(-1)^{|V|-1}1_{\bigcap_{i\in V}a(i)} = 1_{\bigcup_{i\in U}a(i)}, \tag{2.37}$$

which is the inclusion-exclusion principle.

If we think of the species as assigning to each colored set $a : U \to \mathcal{P}$ the set $P[U]$ together with the weight function, then it is natural to denote the weight function itself by $P[a]$. Thus $P[a]$ is an example of what we have called a weighted set; it is a function $P[a] : P[U] \to \mathcal{R}$ that assigns to each subset $V \subseteq U$ the weight

$$P[a](V) = \prod_{i\in V}\lambda(a(i)). \tag{2.38}$$

This example illustrates the general notion of species. The motivation for species theory, however, cannot be captured by a single example. Instead, the power of the theory is that it gives a systematic theory of operations that build new species from old ones. Some of these operations have nice properties that lead to relatively easy computations. Other constructions are relatively nasty. This taxonomy of operations on species does much to illuminate the workings of combinatorics.

2.8. Combinatorial species

Fix the set $\mathcal{P}$, regarded as a palette of colors, or a set of locations. As before, a colored set $a : U \to \mathcal{P}$ assigns to each label a color, or to each particle a location. A *species* associates to each colored set $a : U \to \mathcal{P}$ a weighted set $F[a] : \mathrm{dom}(F[a]) \to \mathcal{R}$. Here the underlying domain set $\mathrm{dom}(F[a])$ is a set of combinatorial objects, and $F[a]$ is a function that assigns a weight to each of these objects.

The species must also associate to each colored set map from $a : U \to \mathcal{P}$ to $b : V \to \mathcal{P}$ a corresponding map of weighted sets. This correspondence is required

to send identity maps to identity maps. Also, the image of the composition of two maps should be the composition of the two images. In brief, it is a functor from the category of colored sets to the category of weighted sets.

In a specific situation the functor property should be apparent. Thus typically we shall place emphasis on the combinatorial construction as an operation that associates to a colored set a corresponding weighted set. There is a much more extensive discussion of the theory of species of structures in the book [2]. The formal definition above is merely designed to capture the idea that relabeling the elements of the label set U (preserving the colors) must induce a corresponding relabeling of the set of combinatorial objects $\mathrm{dom}(F[a])$ (preserving the weights).

In at least some cases one only needs to know the underlying set U of the colored set $a : U \to \mathcal{P}$ in order to determine the underlying domain set $\mathrm{dom}(F[a])$ of the weighted set $F[a]$. In this case it is reasonable to denote this underlying set by $F[U]$. The weights of the elements of $F[U]$ may of course depend on the coloring a, so we might then write $F[a] : F[U] \to \mathcal{R}$.

An important special case is when a species is defined for sets U without any choice of color (a monochromatic set). There can be a weighting, but the weighting cannot depend on the color. In this case $F[U]$ could denote either the weighted set or its underlying domain set. In the extreme case when the weighting is the default weighting that assigns 1 to each element, the underlying set is $F[U]$. Its total weight is just its cardinality.

Consider a species F. For each colored set a there is a corresponding weighted set $F[a] : \mathrm{dom}(F[a]) \to \mathcal{R}$, and for each such weighted set there is a corresponding total weight

$$f(a) = |F[a]|_* = \sum_{\alpha \in \mathrm{dom}(F[a])} F[a](\alpha) \tag{2.39}$$

belonging to the ring $\mathcal{R}$. This is often the quantity of ultimate interest, since it translates combinatorics into algebra. So we have yet another notion of weight, one that attaches to a colored set a the total weight of the structure associated by F to a.

Each species defines a corresponding exponential generating function whose coefficients are $f(a) = |F(a)|_*$. Explicitly,

$$F(w) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{a:U_n \to \mathcal{P}} \left[\sum_{\alpha \in \mathrm{dom}(F[a])} F[a](\alpha) \right] \prod_{i \in U_n} w_{a(i)}. \tag{2.40}$$

Here are some examples. The graph species and the connected graph species are of course just the formal specification of the graph constructions presented before.

Graph species G There is a given function $t : \mathcal{P} \times \mathcal{P} \to \mathcal{R}$ that is symmetric: $t(p,q) = t(q,p)$. The *graph species* G associates to each colored set $a : U \to \mathcal{P}$ the set $G[U]$ of all graphs g on U. The weight of each graph g is

$$G[a](g) = \prod_{\{i,j\} \in g} t(a(i), a(j)). \tag{2.41}$$

The total weight is then

$$g(a) = |G[a]|_* = \sum_{g \in G[U]} \prod_{\{i,j\} \in g} t(a(i), a(j)) = \prod_{\{i,j\}} (1 + t(a(i), a(j)). \quad (2.42)$$

Connected graph species C The *connected graph species* C associates to each colored set $a : U \to \mathcal{P}$ the set $C[U]$ of all connected graphs g on U. The weight of each connected graph g is

$$C[a](g) = \prod_{\{i,j\} \in g} t(a(i), a(j)). \quad (2.43)$$

The total weight is then

$$c(a) = |C[a]|_* = \sum_{g \in C[U]} \prod_{\{i,j\} \in g} t(a(i), a(j)). \quad (2.44)$$

This time there is no simplification.

Power set with edges species P^p Sometimes it is helpful to consider a set of edges from an external point to an arbitrary subset of the vertex set. Say that the external point has color p. The *power set with edges species* P^p assigns to each colored set $a : U \to \mathcal{P}$ the weighted set $P[a] : P[U] \to \mathcal{R}$ defined by

$$P[a](S) = \prod_{j \in S} t(p, a(j)) \quad (2.45)$$

for each subset $S \subseteq U$. Here $P[U]$ is the set of all subsets of U. The total weight is

$$|P^p[a]|_* = \sum_{S \in P[U]} \prod_{j \in S} t(p, a(j)) = \prod_{j \in U} (1 + t(p, a(j))). \quad (2.46)$$

2.9. Operations on species

There are various operations on species. Here are some basic ones. Let F be a species that associates to each colored set $a : U \to \mathcal{P}$ a weighted set $F[a] : A \to \mathcal{R}$. Similarly, let G be a species that associates to each colored set $a : U \to \mathcal{P}$ a weighted set $G[a] : B \to \mathcal{R}$.

Sum The sum $F + G$ assigns to the colored set a the disjoint union weighted set

$$(F + G)[a] = F[a] + G[a] : A + B \to \mathcal{R}. \quad (2.47)$$

Convolution product The convolution product $F * G$ assigns to the colored set $a : U \to \mathcal{P}$ the weighted set given as a disjoint union of Cartesian products of the form

$$(F * G)[a] = \sum_{\langle V,W \rangle} F[a_V] \times G[a_W]. \quad (2.48)$$

Here $\langle V, W \rangle$ denotes an ordered pair of complementary subsets of U.

External point Let p be in $\mathcal{P}$. Then the external point species F'_p assigns to the colored set a the weighted set

$$F'_p[a] = F[a^p], \tag{2.49}$$

where $a^p : U \cup \{*\} \to \mathcal{P}$ agrees with a on U and sends the extra point $*$ to p. In effect, all that has been done is to add an external point of color p.

Internal point Let p be in $\mathcal{P}$. Then the internal point species $F^\bullet_p$ assigns to the colored set a the weighted set

$$F^\bullet_p[a] = \sum_{\{j \in U | a(j)=p\}} F[a]. \tag{2.50}$$

Thus one has disjoint copies of the construction indexed by the elements of U of color p. One can think of the underlying set of the weighted set as consisting of all ordered pairs j, α, where $a(j) = p$ and α is in the underlying set of the original construction. The weight attached to a pair j, α is just the weight attached to α. In effect, all that has been done is to distinguish a point of color p internal to the underlying set, in all possible ways.

Scalar partitional composition Let F be a species that associates to each (uncolored) set U a weighted set $F[U]$. Suppose that $G[\emptyset]$ is empty. Then $F \circ G$ assigns to the colored set a the weighted set

$$(F \circ G)[a] = \sum_{\Gamma} F[\Gamma] \times \prod_{V \in \Gamma} G[a_V]. \tag{2.51}$$

Here Γ ranges over partitions of U. The resulting value of $F \circ G$ is thus the disjoint union over such Γ of weighted sets, each of which is itself a product of weighted sets given by appropriate values of F and G.

Partitional composition Let F be a species that associates to each colored set $c : U \to \mathcal{Q}$ a weighted set $F[a] : A \to \mathcal{R}$. Similarly, for each $q \in \mathcal{Q}$ let G_q be a species that associates to each colored set $a : U \to \mathcal{P}$ a weighted set $G_q[a] : B \to \mathcal{R}$. Suppose that $G_q[\emptyset]$ is empty. Then $F \circ G$ assigns to the colored set a the weighted set

$$(F \circ G)[a] = \sum_{\Gamma} \sum_{c} F[c] \times \prod_{V \in \Gamma} G_{c(V)}[a_V]. \tag{2.52}$$

Here $c : \Gamma \to \mathcal{Q}$ ranges over colorings of partitions Γ of U.

Cartesian product The Cartesian product $F \times G$ assigns to the colored set a the weighted set

$$(F \times G)[a] = F[a] \times G[a]. \tag{2.53}$$

One can consider the passage from species to exponential generating functions as a combinatorial transform.

Theorem 2.1 (Combinatorial transform)**.** *The combinatorial transform takes the operations on species to the corresponding operations on exponential generating functions.*

In this theorem the operations on the level of species are sum, convolution product, external point, internal point, scalar partitional composition, partitional composition, and Cartesian product. The corresponding operations on exponential generating functions are sum, product, derivative, Euler derivative, scalar composition, composition, and Hadamard product.

2.10. Indicator species

Here are indicator species that are used as building blocks. They are called indicator species because the set of combinatorial structures that they produce is either the empty set or a one-point set.

The empty species 0 The empty species 0 assigns to each colored set the empty set of structures. The exponential generating function is 0.

The empty set indicator species 1 The empty set indicator species 1 assigns to each non-empty colored set the empty set of structures, but it assigns to the empty set a single point with weight one. The exponential generating function is 1.

The one-point colored set of designated color indicator species X_p The one-point set indicator species X_p assigns to each colored set $a : U \to \mathcal{P}$ the empty set of structures, with the exception of the case when $U = \{j\}$ consists of precisely one point with $a(j) = p$. In that case it assigns to a a single point with weight one. The exponential generating function is w_p.

The one-point colored set indicator species X The one-point set indicator species X assigns to each colored set $a : U \to \mathcal{P}$ the empty set of structures, with the exception of the case when $U = \{j\}$ consists of precisely one point. In that case it assigns a single point with weight one. The exponential generating function is $1 \cdot w = \sum_q w_q$.

The set indicator species E The set indicator species (or ensemble species) E assigns to each set U a single point of weight one. The exponential generating function is the exponential function $\exp(z)$, where z is a scalar variable.

The colored set indicator species $\hat{E}$ The colored set indicator species (or ensemble species) is the composition $\hat{E} = E \circ X$. It assigns to each colored set $a : U \to \mathcal{P}$ a single point with weight one. The exponential generating function is the multi-variable exponential function $\exp(1 \cdot w) = \exp(\sum_q w_q)$.

Here are some weighted indicator species examples. The color weight function $t(p, q)$ is defined on pairs of colors, with the symmetry condition $t(p, q) = t(q, p)$. The species can return the empty set or a single point with a weight computed from the color weight function.

The edge indicator species E_2 The edge indicator species E_2 assigns to each colored set $a : U \to \mathcal{P}$ with a two-element set $U = \{i, j\}$ a single point with weight $t(a(i), a(j))$. It assigns the empty set to all other colored sets. The exponential generating function is $\frac{1}{2}\sum_p \sum_q t(p, q)w_p w_q$.

The edge to one colored point indicator species E'_{2p} This species is derived from the edge indicator species. It represents an edge from an external point of color p. It assigns to each colored set $a : U \to \mathcal{P}$ with a one-element set $U = \{j\}$ a single point with weight $t(p, a(j))$. It assigns the empty set to all other colored sets. The exponential generating function is $t_p \cdot w = \sum_q t(p, q)w_q$.

The edges to colored set indicator species $\hat{E}^p$ This species is the composition $\hat{E}^p = E \circ E'_{2p}$. It indicates a set of edges from an external point of color p. It assigns to each colored set $a : U \to \mathcal{P}$ a single point with weight $\prod_{j\in U} t(p, a(j))$. The exponential generating function is $\exp(t_p \cdot w) = \exp(\sum_q t(p, q)w_q)$.

Here are some examples of this apparatus at work, using these set indicator species as a starting point.

Power set with edges Take the convolution product $P^p = \hat{E} * \hat{E}^p$. By the definition of the combinatorial convolution product, the value of this on a colored set $a : U \to \mathcal{P}$ is the disjoint union over all subsets W of U of a single point with weight $\prod_{j\in W} t(p, a(j))$. In other words, $P^p[a]$ consists of all subsets W of U; each subset W determines a set of edges from an external point of color p to the vertices in W. Its exponential generating function is the product $\exp(\sum_q w_p) \exp(\sum_q t(p, q)w_q) = \exp(\sum_q (1 + t(p, q))w_q)$.

Cluster expansion as scalar composition Let C be a species that associates to each colored set $a : U \to \mathcal{P}$ a weighted set $C[a] : C[U] \to \mathcal{R}$. Suppose that $C[\emptyset]$ is empty. Then the scalar partitional composition $G = E \circ C$ assigns to the colored set a the weighted set

$$G[a] = (E \circ C)[a] = \sum_{\Gamma} \prod_{V\in\Gamma} C[a_V]. \tag{2.54}$$

Here Γ ranges over partitions of U. The corresponding transform is $G(w) = \exp(C(w))$.

3. Combinatorial fixed point equations

3.1. The rooted tree fixed point equation

In the following constructions there is always a function $t(p, q)$ defined for colors p, q. It is required that $t(p, q) = t(q, p)$. Let $T_p^\bullet$ be the species of rooted trees with root of color p. To find a combinatorial equation, let X_p be the one-point colored set of designated color indicator species, with weight one. Let $\hat{E}^p = E \circ E'_{2p}$ be the edges to colored set indicator species that assigns to a colored set a the

product $\prod_j t(p, a(j))$. The equation is

$$T_p^\bullet = X_p * (\hat{E}^p \circ T^\bullet). \tag{3.1}$$

This says that a rooted tree on U is given by choosing a root point and partitioning the complement, with a rooted tree on each set in the partition, and with edges from the original root to the new roots. In more detail, a rooted tree on U with root of color p is obtained by splitting U into one point with color p, recognized by X_p, and by doing a construction on the complement, namely $\hat{E}^p \circ T^\bullet$. This in turn is obtained by partitioning the complement and doing the construction $T_q^\bullet$, for some q, on each set in the partition. Each set in the partition gets a corresponding weight factor $t(p, q)$ from the edge.

The exponential generating function for rooted trees thus satisfies

$$T_p^\bullet(w) = w_p \exp(\sum_q t(p, q) T_q^\bullet(w)). \tag{3.2}$$

This is because X_p has exponential generating function w_p and $\hat{E}^p \circ T^\bullet$ has exponential generating function that is the composition of $\exp(\sum_q t(p, q) z_q)$ with $z_q = T_q^\bullet(w)$.

Set $z_p = T_p^\bullet(w)$. Then this is a fixed point equation

$$z_p = w_p \exp(\sum_q t(p, q) z_q). \tag{3.3}$$

This equation is of the form $z = \phi(z)$. It has a unique formal power series solution in which z is expressed as a formal power series in w. Furthermore, this solution is given by iteration starting with 0. Let $z^{(0)} = 0$, and define the sequence $z^{(k)}$ inductively by $z^{(k+1)} = \phi(z^{(k)})$. Then for $k \geq 1$ the term $z^{(k)}$ gives the contribution of all trees of depth $\leq k-1$. Furthermore, $z^{(k)}$ converges to z, in the sense that the each coefficient of the power series expansion of z is achieved at some k. To see this, consider a tree on a set with n points. Then the depth of this tree is at most $n-1$. If $k \geq n$ the term $z^{(k)}$ includes the contribution of all trees of depth at most $n-1$ and so includes the contribution of this particular tree. In other words, for $k \geq n$ the term $z^{(k)}$ includes all contributions of trees with n vertices.

Let us take $t(p, q) \geq 0$ and $w_p \geq 0$. Then the formal power series has only positive terms. We would like to find a hypothesis that guarantees that the formal power series converges. The correct hypothesis was found by Kotecký and Preiss [14], working in the context of statistical mechanics.

Theorem 3.1 (Tree convergence)**.** *Consider the tree exponential generating function with color pair weight factors $t(p, q) \geq 0$, and take the variables $w_q \geq 0$. Suppose the Kotecký-Preiss condition is satisfied, that is, there exists a finite vector $x \geq 0$ such that*

$$w_p \exp(\sum_q |t(p, q)| x_q) \leq x_p. \tag{3.4}$$

Then the power series expansion of $T_p^\bullet(w)$ converges for the given w and has absolute value bounded by x_p.

The inequality in the hypothesis is of the form $\phi(x) \leq x$ with $0 \leq x$. The proof of the theorem is via fixed point iteration. It uses the fact that ϕ is an increasing function, in the sense that $x' \leq x''$ implies $\phi(x') \leq \phi(x'')$. Let $z^{(k)}$ be the kth iterate of ϕ applied to 0. Suppose that $z^{(k)} \leq x$. Then $z^{(k+1)} = \phi(z^{(k)}) \leq \phi(x) \leq x$. By induction it follows that $z^{(k)} \leq x$ for all k. It follows that the limiting power series z for the given value of w also satisfies $z \leq x$. This completes the proof.

There is something mysterious about this argument, since the fixed point equation will in general have several numerical solutions. It may help to look at a more general picture. The natural analysis setting is a complete lattice L, that is, a partially ordered set for which every subset has a supremum and an infimum. There is also a function $\phi : L \to L$ that is increasing, in the sense that $x' \leq x''$ implies $\phi(x') \leq \phi(x'')$. The Knaster-Tarski theorem says that an increasing function ϕ from a complete lattice to itself always has a fixed point. In fact, it has a least fixed point $z = \inf\{y \mid \phi(y) \leq y\}$.

It is perhaps worth recalling the proof of this fact. Let S be the set of y with $\phi(y) \leq y$. Since the lattice is complete, S has an infimum z. Consider arbitrary y in S. Then $z \leq y$, and since ϕ is increasing, $\phi(z) \leq \phi(y) \leq y$. Thus $\phi(z)$ is a lower bound for S. Since z is the greatest lower bound, it follows that $\phi(z) \leq z$. Since ϕ is increasing, $\phi(\phi(z)) \leq \phi(z)$. It follows that $\phi(z)$ is in S. Since z is a lower bound, we have $z \leq \phi(z)$. Hence $\phi(z) = z$.

It is also useful to know when the fixed point equation may be solved by iteration starting with the least element. Let $u^{(k)}$ be the kth iterate. Since ϕ is an increasing function, it follows by induction that the sequence $u^{(k)}$ is increasing. It also follows by induction that each $u^{(k)} \leq z$, where z is the least fixed point. Let $z' = \sup_k u^{(k)}$, so $z' \leq z$. In general z' need not be a fixed point. However, assume the monotone convergence property for increasing sequences: $\sup_k \phi(u^{(k)}) = \phi(\sup_k u^{(k)})$. This says that $z' = \sup_k u^{(k+1)} = \sup_k \phi(u^{(k)}) = \phi(z')$, so z' is indeed a fixed point. It follows that the limit z' of the sequence is the least fixed point z.

In the present context the natural choice of complete lattice is $L = [0, +\infty]^{\mathcal{P}}$. This is just the set of positive vectors indexed by color. The value $+\infty$ is allowed in order to ensure that L is a complete lattice. The condition $\phi(x) \leq x$ with x finite simply guarantees that the fixed point z is itself finite, with $z \leq x$.

When the iteration argument is applied to the tree fixed point, it shows that the least fixed point is given by a convergent power series in powers of w. Even though the fixed point equation can have several solutions, there is just one that has such a convergent power series.

3.2. The connected graph fixed point equation

Trees are relatively easy to treat, because of the nice fixed point equation. Connected graphs present more difficulties. The relation between graphs and

connected graphs is given by the species equation with the scalar partitional composition

$$G = E \circ C. \tag{3.5}$$

This says that one gets graphs by partitioning the vertex set and putting a connected graph on each set in the partition. The corresponding equation for exponential generating functions is the usual cluster representation $G(w) = \exp(C(w))$.

Similarly, the relation between graphs with root of color p and connected graphs with root of color p is given by

$$G_p^\bullet = C_p^\bullet * G. \tag{3.6}$$

This works because a rooted graph is given by a rooted connected graph on a subset and a graph on the complement. The exponential generating function equation is

$$G_p^\bullet(w) = C_p^\bullet(w) G(w). \tag{3.7}$$

Let $\hat{E} = E \circ X$ be the colored set indicator species with weight one for every colored set. Let $\hat{E}^p = E \circ E'_{2p}$ be the colored set indicator species with weight $\prod_{j \in U} t(p, a(j))$ for every colored set $a : U \to \mathcal{P}$. One can consider this as a construction that produces the set of all edges from some external point with color p to a point in U. Consider the convolution product

$$P^p = \hat{E} * \hat{E}^p. \tag{3.8}$$

This power set construction assigns to each colored set $a : U \to \mathcal{P}$ the set of all subsets $W \subseteq U$, where each such W has weight $\prod_{j \in W} t(p, a(j))$. One can consider it as a construction that assigns to each colored set $a : U \to \mathcal{P}$ the set of all possible edge sets from an external point of color p to some subset of U. If U has n points, then there are 2^n such possible edge sets. The exponential generating function for the power set is

$$P^p(w) = \exp(1 \cdot w) \exp(t_p \cdot w) = \exp((1 + t_p) \cdot w). \tag{3.9}$$

Let $G_p^\bullet$ be the species of rooted graphs with root of color p. This satisfies the combinatorial equation

$$G_p^\bullet = X_p * (P^p \times G). \tag{3.10}$$

This says that a graph with root of color p is obtained by taking a root of color p and an ordered pair consisting of a graph on the complement and a subset of the complement. This subset represents the vertices of the graph that are directly connected to the root. The weight of this subset is the product of $t(p, q)$, where q is the color of a point in the subset. The Cartesian product of species translates to the Hadamard product of exponential generating functions. The exponential generating function for rooted graphs thus satisfies

$$G_p^\bullet(w) = w_p G((1 + t_p)w) \tag{3.11}$$

This is unfortunately not a closed equation for the quantity of interest. Also, it involves a nasty scaling operation.

Let $C_p^\bullet$ be the species of rooted connected graphs with root of color p. This satisfies the combinatorial equation

$$C_p^\bullet = X_p * (E \circ (P_+^p \times C)). \tag{3.12}$$

This says that a connected graph is obtained by choosing a root, partitioning the complement, and then on each set in the partition picking a non-empty subset and a connected graph. The vertices in such a non-empty subset are connected by edges to the original root, thus producing the original connected graph.

The exponential generating function for non-empty subsets is

$$P_+^p(w) = \exp(1 \cdot w)(\exp(t_p \cdot w) - 1) = \sum_N \frac{1}{N!}[(1 + t_p)^N - 1]w^N. \tag{3.13}$$

The exponential generating function for the Cartesian product is given by the Hadamard product of $P_+^p(w)$ with $C(w)$, giving $C((1 + t_p)w) - C(w)$. The exponential generating function for rooted connected graphs thus satisfies

$$C_p^\bullet(w) = w_p \exp(C((1 + t_p)w) - C(w)). \tag{3.14}$$

It can be made into a closed equation, in fact, a fixed point equation. However, this comes at a price. By the fundamental theorem of calculus

$$C_p^\bullet(w) = w_p \exp(\sum_q t(p, q) \int_0^1 C_q^\bullet((1 + st_p)w)\, ds). \tag{3.15}$$

The unpleasant feature of this equation is that it involves a scaling factor $1+st_p$. There is also an integral over the s parameter to add to the complication.

4. The equilibrium gas

4.1. Equilibrium statistical mechanics

Mathematicians may appreciate a few words about the terminology of equilibrium statistical mechanics. There are several different probability models; the ones that occur most frequently are the canonical ensemble and the grand canonical ensemble.

In the *canonical ensemble* the volume V and the number of particles n is fixed. The energy value is not fixed; it is tuned by a parameter β, the *inverse temperature*. This parameter is measured in inverse energy units. The Hamiltonian function that expresses the energy of a configuration is denoted H. The temperature and energy enter together via the *Boltzmann factor* $e^{-\beta H}$. There is also a given reference measure μ_0. In all the following we use the same notation for measure and for integral, and in particular for probability measure and expectation. The model is given by the probability measure with expectation

$$\mu(f) = \frac{1}{Z}\mu_0(fe^{-\beta H}). \tag{4.1}$$

Here

$$Z = \mu_0(e^{-\beta H}) \tag{4.2}$$

is the *partition function*. The *free energy* F is defined via the logarithm of the partition function as $-\beta F = \log(Z)$, so

$$Z = e^{-\beta F}. \tag{4.3}$$

The free energy is an example of a thermodynamic potential. The logarithm of the partition function can enter into important calculations. For instance,

$$-\frac{\partial \log Z}{\partial \beta} = \mu(H) \tag{4.4}$$

is the energy of the system.

In the *grand canonical ensemble* the volume V is fixed. The energy is tuned by the inverse temperature parameter β, and the density of particles is tuned by the the activity parameter w. (This is usually called z in the physics literature). The reference measure for an arbitrary number of particles is given by

$$\mu_0^w(f) = \sum_{n=0}^{\infty} \frac{1}{n!} \mu_0^n(f) w^n, \tag{4.5}$$

where μ_0^n is the reference measure for n particles. (In the physics literature the $1/n!$ factor is sometimes included in the reference measures μ_0^n.) The probability model is given by

$$\mu(f) = \frac{1}{\Xi} \mu_0^w(f e^{-\beta H}). \tag{4.6}$$

Here

$$\Xi = \mu_0^w(e^{-\beta H}) \tag{4.7}$$

is the *grand partition function*. The *grand potential* Ω is defined in terms of the logarithm of the grand partition function by $-\beta\Omega = \log(\Xi)$, so

$$\Xi = e^{-\beta \Omega}. \tag{4.8}$$

In physics there is often an identification $\Omega = -PV$, where PV is the pressure-volume work. Thus we can also write

$$\Xi = e^{\beta PV}. \tag{4.9}$$

Sometimes one says, somewhat carelessly, that the thermodynamic potential for the grand canonical ensemble is the *pressure* P. The logarithm of the grand partition function is also important. For instance,

$$w \frac{\partial \log \Xi}{\partial w} = \mu(n), \tag{4.10}$$

the expected number of particles of the system.

In the end, one wants to take the *thermodynamic limit* in which the volume V becomes infinite. In the canonical ensemble the density needs to be fixed, that is, the number of particles is taken proportional to the volume. The grand canonical ensemble is simpler; all that needs to be done is to fix the activity parameter, which controls the density.

4.2. Particles and locations

Here is a particular example of a model in equilibrium statistical mechanics, a gas consisting of a variable number of interacting particles in a discrete space. The discrete space is modeled by a set $\mathcal{P}$ of *locations*. For technical simplicity we shall think of it as finite, but potentially very large. All estimates should be independent of the number of points in this set. This treatment is in the spirit of the thermodynamic limit, that is, the idea that an arbitrarily large region of space might as well be modeled by a space that is of infinite extent in all directions. If we are mainly interested in what is happening deep in the interior of the region, then we may wish to disregard boundary effects. So we try to find quantities that have limits as the boundary becomes arbitrarily remote. In the present framework, the goal is to get results that do not depend on the size of the set $\mathcal{P}$.

Associated with each location $p \in \mathcal{P}$ there is an activity parameter w_p that gives a prior weight for a particle being at site p. In the case of no interaction it will turn out that w_p is the expected number of particles at p, but in general it should be thought of as a parameter that influences the expected number off particles at p in some indirect way. It is natural in this context to take $w_p \geq 0$. However, we shall see that there are important applications where the w_p can take either sign. In these applications there is no direct probabilistic interpretation, but the same formulas work.

For each ordered pair of points p, q there is a *potential energy* $v(p, q)$, assumed throughout to satisfy $0 \leq v(p, q) \leq +\infty$. There is a corresponding Boltzmann factor $\exp(-\beta v(p, q))$ with $0 \leq \exp(-\beta v(p, q)) \leq 1$. Here $\beta > 0$ is the inverse temperature parameter, measured in energy units. In the following we shall often write the Boltzmann factor as $1 + t(p, q)$, so that the *interaction factor*

$$t(p, q) = \exp(-\beta v(p, q)) - 1 \tag{4.11}$$

is negative, satisfying $-1 \leq t(p, q) \leq 0$. The reason for doing this will be evident in the next section.

A *particle configuration* is a function $a : U_n \to \mathcal{P}$. Here U_n is a set considered as consisting of n *particles*. The corresponding multi-index N that counts the number of particles at each location is called an *occupation number function*. The potential energy $V(a)$ of a particle configuration is

$$V(a) = \sum_{\{i,j\}} v(a(i), a(j)), \tag{4.12}$$

where the sum is over subsets consisting of exactly two particles. The corresponding Boltzmann factor is $\exp(-\beta V(a))$. It weights particle configurations in such a way that higher energy gives lower weight.

The inverse temperature and the energy occur in the dimensionless Boltzmann factor $\exp(-\beta V(a))$. The activities w_p are also dimensionless. For the development of the theory and for flexibility in applications it is helpful to have a separate activity parameter w_p for each location p. Of course there is nothing

to prevent each w_p from being set equal to the same number. On the other hand, it can be useful to have certain locations that are reluctant to have particles, and this can be achieved by taking the corresponding activities to be small.

We begin with the situation that is easiest to interpret, where the activities w_p are all positive. In this situation there is an elegant probability model. The fundamental postulate for the equilibrium gas is that the probability measure is defined by a discrete probability density defined for each particle configuration $a : U_n \to \mathcal{P}$. The number of particles can be any finite number $n = 0, 1, 2, 3, \ldots$. The formula for the probability of having the n particles that constitute U_n in the locations specified by a is

$$\mu(\{a\}) = \frac{1}{\Xi} \frac{1}{n!} \exp(-\beta V(a)) \prod_{k \in U_n} w_{a(k)}. \tag{4.13}$$

Here

$$\Xi = \sum_{n=0}^{\infty} \sum_{a: U_n \to \mathcal{P}} \frac{1}{n!} \exp(-\beta V(a)) \prod_{k \in U_n} w_{a(k)} \tag{4.14}$$

is the normalization needed to make this a discrete probability density. The symbol Ξ is the conventional in physics for the grand partition function, but in much of the following Ξ will be denoted by $G(w)$, since the grand partition function turns out to be the exponential generating function for graphs.

The discrete probability density for particle configurations induces a discrete probability density for occupation number functions. It is given by the formula $\mu(\{N\}) = \sum_{\mathrm{count}(a)=N} \mu(\{a\})$, or

$$\mu(\{N\}) = \frac{1}{\Xi} \frac{1}{N!} \exp(-\beta V(N)) w^N. \tag{4.15}$$

If $V(N) = 0$ for all N, then the probability for k particles at location p is

$$\mu(\{N \mid N(p) = k\}) = \frac{1}{\exp(\sum_q w_q)} \frac{1}{k!} w_p^k \exp(\sum_{q \neq p} w_q) = \frac{1}{k!} w_p^k \exp(-w_p). \tag{4.16}$$

In other words, $N(p)$ has a Poisson distribution with mean w_p. The model describes independent Poisson random variables.

If $V(N) = 0$ for all N with $0 \leq N \leq 1$, and otherwise $V(N) = +\infty$, then for $k = 0, 1$ we get

$$\mu(\{N \mid N(p) = k\}) = \frac{1}{\prod_q (1 + w_q)} w^k \prod_{q \neq p} (1 + w_q) = \frac{w_p}{1 + w_p}. \tag{4.17}$$

This model describes independent Bernoulli random variables.

4.3. Grand potential and density

The grand partition function is given by sums over graphs. To see this, we write $\exp(-\beta v(p, q)) = 1 + t(p, q)$, so $-1 \leq t(p, q) \leq 0$. Thus the deviation of $t(p, q)$

below zero measures the amount of energy interaction between the two sites. It is also the color pair weight that we considered earlier in the context of graphs. In order to make the connection, one may write the grand partition function Ξ as $G(w)$ and recognize it as the exponential generating function for graphs. In the particle notation it is

$$G(w) = \sum_{n=0}^{\infty} \sum_{a:U_n \to \mathcal{P}} \frac{1}{n!} \prod_{\{i,j\}} (1 + t(a(i), a(j))) \prod_j w_{a(j)}. \tag{4.18}$$

In the occupation number notation it takes the simple form

$$G(w) = \sum_N \frac{1}{N!} (1+t)^{\mathrm{Pair}(N)} w^N. \tag{4.19}$$

Here $\mathrm{Pair}(N)$ is a multi-index defined for pairs $\{p, q\}$ of locations. If $p \neq q$ its value is $N(p)N(q)$, while if $p = q$ its value is the binomial coefficient $\binom{N(p)}{2}$. Thus $(1+t)^{\mathrm{Pair}(N)}$ is the product of the Boltzmann factors $1 + t(p, q)$ for all the pairs of particles at various locations described by N. The most immediately useful consequence of this equation is the identity

$$\frac{\partial G(w)}{\partial w_p} = G((1 + t_p)w). \tag{4.20}$$

At this point it is convenient to introduce the exponential generating function $C(w) = \log G(w)$ for connected graphs. This is an important thermodynamic quantity related to the grand potential or the pressure-volume work. In combinatorics it is natural to call it the connected function. The grand partition function is the exponential of the connected function:

$$G(w) = \exp(C(w)). \tag{4.21}$$

The connected function has the cluster expansion

$$C(w) = \sum_{N \neq 0} \frac{1}{N!} c(N) w^n. \tag{4.22}$$

The probabilities of particular configurations will typically be tiny. What one wants to calculate are expectations of random variables, such as the number of particles $N(p) = \#\{i \mid a(i) = p\}$ at a given point p. Such expectations may not have a strong dependence on the total number of locations, so they have a more robust physical significance. In particular, it is reasonable to hope that they may have thermodynamic limits.

The first expectation to be considered is the pinned connected function

$$\frac{\partial C(w)}{\partial w_p} = \frac{1}{G(w)} \frac{\partial G(w)}{\partial w_p} = \frac{1}{G(w)} G((1 + t_p)w) = \exp(C((1 + t_p)w) - C(w)). \tag{4.23}$$

This is the expectation of the random variable

$$(1+t_p)^N = \prod_q (1+t(p,q))^{N(q)} = \exp(-\beta \sum_q v(p,q)N(q)). \tag{4.24}$$

This random variable has the value 1 for occupation number functions N such that $N(q) \geq 1$ implies $v(p,q) = 0$. On the other hand, it is small for occupation numbers N for which there exists a q with $N(q) \geq 1$ and a large value of $\beta v(p,q)$. So, roughly speaking, it is a random variable that indicates avoidance of interaction with location p. Thus, though this is not standard terminology, the pinned connected function could be called the *expected avoidance* at location p. In the graphical interpretation the expected avoidance at location p is the exponential generating function for connected graphs on a set with an external point of color p.

Perhaps the most physically natural expectation is the expectation of the number $N(p)$ of particles at location p given by

$$\mu(N(p)) = \frac{1}{G(w)} G_p^\bullet(w) = C_p^\bullet(w) = w_p \frac{\partial C(w)}{\partial w_p}. \tag{4.25}$$

This has a cluster expansion

$$C_p^\bullet(w) = \sum_{N \neq 0} \frac{1}{N!} N(p) c(N) w^N. \tag{4.26}$$

It will be convenient to refer to the expected number of particles at a point as the *density* of the gas. Thus the density at p is the rooted connected function, which is the exponential generating function for rooted connected graphs with root of color p.

The expression of the density in terms of the connected function can be quite convenient. For instance, in the Poisson model $C(w) = \sum_q w_q$, so $C_p^\bullet(w) = w_p$, as expected. Similarly, in the Bernoulli model $C(w) = \sum_q \log(1+w_q)$, so in this case $C_p^\bullet(w) = w_p/(1+w_p)$.

It is extraordinarily convenient how the cancelation between numerator and denominator is expressed by merely replacing rooted graphs by rooted connected graphs. If the connected function $C(w)$ has coefficients $c(N)$, then the derivative $\partial C(w)/\partial w_p$ has coefficients $c(N+\delta_p)$, and the density $C_p^\bullet(w)$ has coefficients $N(p)c(N)$. Thus the only coefficients $c(N)$ that matter for the density at p are those for which $N(p) > 0$. Each particle configuration that contributes is not only connected but has at least one particle at the root location p.

In the cluster expansion for the density $C_p^\bullet(w)$ the particle configurations that matter are all connected by a chain of interactions to a particle at location p. Remote particles have little effect on the density at p. This suggests why the density might have a thermodynamic limit as the number of locations approaches infinity.

Yet another quantity of interest is the probability of finding no particle at p. Write w_Λ for the variables equal to w_q for q in Λ and to zero elsewhere. The

probability is

$$\mu(\{N \mid N(p) = 0\}) = \frac{G(w_{\mathcal{P}\setminus\{p\}})}{G(w)} = \exp(C(w_{\mathcal{P}\setminus\{p\}}) - C(w)). \tag{4.27}$$

One sees again how convenient it is to have the connected function $C(w)$ to make explicit the cancelation between numerator and denominator. The coefficients $c(N)$ that enter into the difference $C(w) - C(w_{\mathcal{P}\setminus\{p\}})$ are those with $N(p) > 0$. This quantity should also make sense in the thermodynamic limit.

The quantities that describe the equilibrium gas are identical to those that arise in the combinatorial constructions. Only the names have changed. Here is a dictionary that gives the translation.

- The color palette is the set of locations.
- A label set is a set of particles.
- A colored set is a particle configuration.
- A multi-index is a particle occupation number function.
- A color variable is an activity parameter.
- An color pair weight is an interaction factor.
- The graph exponential generating function is the grand partition function.
- The connected graph exponential generating function is the connected function (related to pressure).
- The pinned connected graph exponential generating function is the expected avoidance.
- The rooted connected graph exponential generating function is the density.

4.4. Convergence of the cluster expansion

The next topic is a version of the cluster expansion called the *Mayer expansion*. This refers to the expansion of the pressure or the density of an equilibrium gas in powers of the activity. There is another closely related *virial expansion* that expresses the pressure in terms of the density. Combinatorial aspects of the virial expansion are discussed in an paper of Leroux [15].

The goal here is to present a standard theorem on convergence of the cluster expansion for the rooted connected function (the density) as a function of activity parameters. It says that if the equilibrium gas has sufficiently weak interaction or sufficiently small activity values, then the cluster expansion for the density converges, with a radius of convergence independent of the number of locations. This is a standard result, the work of many authors; see the references in [10, 13, 22]; also consult [4, 5, 6, 9, 17]. In one version, that of Kotecký-Preiss [14], the condition for convergence is precisely the condition for convergence of a certain tree expansion.

Theorem 4.1 (Cluster expansion convergence)**.** *Consider the equilibrium gas system with interactions* $-1 \le t(p,q) \le 0$ *and activities* w_p *satisfying* $|w_p| \le w_p^*$. *Suppose there are finite* $x_p \ge 0$ *such that Kotecký-Preiss condition*

$$w_p^* \exp(\sum_q |t(p,q)| x_q) \le x_p \tag{4.28}$$

is satisfied, so that the corresponding rooted tree series $T_p^\bullet(w^*)$ *(defined with weights* $0 \le |t(p,q)| \le 1$*) converges to a value bounded by* x_p*. Then the series* $C_p^\bullet(w)$ *for the expected number of particles at a site* p *converges absolutely for* $|w| \le w^*$*, and its value satisfies*

$$|C_p^\bullet(w)| \le x_p < +\infty. \tag{4.29}$$

Sometimes the Kotecký-Preiss criterion and similar results are stated in terms of the pinned connected function. As argued before, this function could also be called the expected avoidance for location p. For this reformulation it is natural to make the change of variable $x_p = w_p^* e^{a_p}$.

Theorem 4.2 (Cluster expansion convergence)**.** *Consider the equilibrium gas system with interactions* $-1 \le t(p,q) \le 0$ *and activities* w_p *satisfying* $|w_p| \le w_p^*$*. Suppose there are finite* $a_p \ge 0$ *such that Kotecký-Preiss condition*

$$\sum_q |t(p,q)| w_q^* e^{a_q} \le a_p \tag{4.30}$$

is satisfied. Then the pinned connected function series $\partial C(w)/\partial w_p$ *for the expected avoidance at location* p *converges absolutely, and its value satisfies*

$$\left| \frac{\partial C(w)}{\partial w_p} \right| \le e^{a_p} < +\infty. \tag{4.31}$$

This form of the theorem has the feature that the parameters to be estimated appear together in the combination $|t(p,q)|w_q^*$. For this to be a small parameter either the interaction $t(p,q)$ can be small or the activity bound w_p^* can be small.

The following sections present two proofs of the theorem. One works directly with an equation for the exponential generating function for the rooted connected graphs. The other is via partitioning the set of connected graphs, following the approach of Penrose [18]. These are not the only proof strategies; another particularly powerful technique is the use of Brydges-Kennedy tree identities [7, 6] and the related Abdesselam-Rivasseau forest identities [1]. See [8, Section VIII] for a recent treatment.

Recently Fernández and Procacci [13] used Penrose partitioning to give a new cluster expansion convergence theorem. Let $|t_p|$ be the vector with components $|t(p,q)|$ for q in $\mathcal{P}$. Define the rooted grand partition function by

$$G(|t|_p x) = \sum_N \frac{1}{N!}(1+t)^{\mathrm{Pair}(N)}(|t_p|x)^N = \sum_N \frac{1}{N!}(1+t)^{\mathrm{Pair}(N)}|t_p|^N x^N. \tag{4.32}$$

The quantity $\mathrm{Pair}(N)$ counts the number of pairs of particles at various locations $\{p,q\}$, and $(1+t)^{\mathrm{Pair}(N)}$ is the resulting Boltzmann factor. The quantity $|t_p|^N = \prod_q |t(p,q)|^{N(q)}$ is the product of interaction factors that link p to another location q. The Fernández-Procacci condition is that there is a finite vector $x \ge 0$ such that

$$w_p^* G(|t|_p x) \le x_p. \tag{4.33}$$

Their conclusion is convergence of the cluster expansion for the density with values of w satisfying $|w_p| \leq w_p^*$.

Since $(1+t)^{\mathrm{Pair}(N)} \leq 1$, the Kotecký-Preiss condition

$$w_p^* \sum_N \frac{1}{N!}(|t_p|x)^N = w_p^* \exp(|t_p| \cdot x) \leq x_p \tag{4.34}$$

implies the Fernández-Procacci condition. It follows that the Fernández-Procacci result implies the Kotecký-Preiss result. While it may be difficult to compute $(1+t)^{\mathrm{Pair}(N)}$ exactly, Fernández-Procacci showed that it is possible to estimate this quantity in such as way as get useful results.

It is also possible to get results for the case of negative potential $v(p,q) < 0$ (which corresponds to $t(p,q) > 1$) under a certain positive definiteness condition (stability). Procacci [20] has recently made progress on this. New work of Poghosyan and Ueltschi [19] gives a particularly nice formulation.

Finally, it should be acknowledged that space is not discrete. Fortunately, the entire apparatus of cluster expansions can be carried out in Euclidean space or even on a general measurable space [22]. The role of activity parameters is then played by activity measures.

4.5. Cluster expansion convergence via tree fixed point

This section gives a proof that the cluster expansion converges that is based on a fixed point equation. The idea was inspired by work of Ueltschi [22]. The version of the proof presented here makes no mention of graphs or any other form of combinatorics [10]. Of course the quantities used in the proof do have graphical interpretations; that just adds to their charm.

Here is the result to be proved. Suppose $-1 \leq t(p,q) \leq 0$ and $w_p \geq 0$. Suppose that there are finite $x_p \geq 0$ so that the Kotecký-Preiss condition $w_p \exp(\sum_q |t(p,q)|x_q) \leq x_p$ holds. Then the sum $C_p^\bullet(w)$ for the expected number of particles converges absolutely, and in fact

$$0 \leq C_p^\bullet(w) \leq -C_p^\bullet(-w) \leq x_p < \infty. \tag{4.35}$$

The starting point is the definition of the grand partition function $G(w)$ as a power series with terms $g(N) = (1+t)^{\mathrm{Pair}(N)}$. The fundamental equation (3.11) then follows immediately from the definition.

Once we have the grand partition function, we can define the connected function $C(w)$ by $G(w) = \exp(C(w))$. The corresponding equation (3.7) for the density then follows by differentiating. The fundamental equation may then be reformulated as an equation (3.14) for the density. This in turn gives the fixed point equation (3.15).

One technical problem with the fixed point equation is that the $t(p,q)$ factor is negative. So instead let $\check{C}_p^\bullet(w) = -C_p^\bullet(-w)$. This will be an upper bound for $C_p^\bullet(w)$. It satisfies the equation

$$\check{C}_p^\bullet(w) = w_p \exp(\sum_q |t(p,q)| \int_0^1 \check{C}_q^\bullet((1+st_p)w)\, ds). \tag{4.36}$$

Compare this with the tree equation

$$T_p^\bullet(w) = w_p \exp(\sum_q |t(p,q)| T_q^\bullet(w)). \tag{4.37}$$

These are fixed point equations

$$\check{z} = \psi(\check{z}) \tag{4.38}$$

and

$$z = \phi(z). \tag{4.39}$$

Each of these equations has a solution as an exponential generating function in powers of w for which all Taylor coefficients are positive. While the iteration functions ψ and ϕ are quite different, they have the same value $\psi(x) = \phi(x)$ for an x that does not depend on w.

Consider the iteration $v^{(0)} = 0$ and $v^{(k+1)} = \psi(v^{(k)})$. This generates a sequence of exponential generating functions with positive Taylor coefficients. Furthermore, it increases to the fixed point $\check{z}$. The Kotecký-Preiss condition is that there is a finite vector $x \geq 0$ with $\phi(x) \leq x$. Suppose that for some k we have $v^{(k)} \leq x$. Then $v^{(k+1)} = \psi(v^{(k)}) \leq \psi(x) = \phi(x) \leq x$. It follows by induction that $v^{(k)} \leq x$ for all k. Hence $\check{z} \leq x$. In fact, since we could take $x = z$, we have $\check{z} \leq z$. The density $\check{z}$ is dominated by the tree fixed point z.

4.6. Cluster expansion convergence via partitioning and tree bounds

This section presents a graphical proof of convergence of the cluster expansion. Even though it is possible in some cases to reason without using the graph language, there are other situations where it is much more convenient. In any case, the graph setting gives a picture that is simple and direct.

The starting point is the existence of a Boolean partition of the set of connected graphs. From a Boolean partition one immediately gets an identity that relates connected graphs to trees. This in turn gives a tree bound, from which the cluster expansion convergence theorem is immediate.

Let E be a set. A Boolean interval is a subset of the power set $P(E)$ of the form $[A, B] = \{C \mid A \subseteq C \subseteq B\}$.

Theorem 4.3 (Boolean partition)**.** *Fix a vertex set U. Then there is a map χ from the trees on U to the connected graphs on U such that the set of connected graphs is the disjoint union of the Boolean intervals $[T, \chi(T)]$.*

The map χ and the resulting partitioning is far from unique. As an example, take the case when U has 3 vertices. There are four connected graphs T_1, T_2, T_3, K_3. One way to partition is to take $\chi(T_1) = K_3$, while $\chi(T_2) = T_2$ and $\chi(T_3) = T_3$. Then the set of connected graphs is the disjoint union of the intervals $[T_1, K_3]$, $[T_2, T_2]$, $[T_3, T_3]$, that is, of the sets $\{T_1, K_3\}, \{T_2\}, \{T_3\}$.

There are several ways to construct such a partition into Boolean intervals. Here is the construction due to Penrose. The graph distance between two points

is the minimum number of edges in the graph needed to make a path from one point to the other. Choose a root point r in the vertex set U. Then each connected graph on U defines a finite sequence of disjoint non-empty subsets $L_0, L_1, L_2, \ldots, L_m$ that exhaust U and such that $L_0 = \{r\}$. The set L_k consists of the points in U at graph distance k from the root. Conversely, given such a sequence of L_k, there is a corresponding collection of connected graphs. Thus the set of all connected graphs is partitioned, with the partitions indexed by such sequences. For each sequence, the connected graphs may have arbitrary edges present or absent between vertices in the same L_k. Thus the within-layer edges are arbitrary. Furthermore, for $k \geq 1$ and for each vertex in L_k there are edges going to a non-empty set of vertices in L_{k-1}. All inter-layer edges are of this form.

Linearly order the vertices U starting with r. For each connected graph G on U there will be a corresponding tree $\phi(G)$ on U. A tree is defined by giving a function from U to U with no cycle other than a fixed point at the root. Start with the connected graph G and the corresponding partition of U. Consider i in U, other than the root. Then i belongs to some L_k in the partition with $k \geq 1$. Then the tree maps i to the j in L_{k-1} that is least in the order.

The set of connected graphs with $\phi(G) = T$ consists of all connected graphs inducing the same partition, with some set of within-layer edges and with inter-layer edges from i in L_k to j and to a non-empty set of j' in L_{k-1} with $j' \geq j$. The maximal such graph $\chi(T)$ has all possible within-layer edges and all inter-layer edges from i in L_k to j' in L_{k-1} with $j' \geq j$. Thus the set of graphs with $\phi(G) = T$ is the Boolean interval $[T, \chi(T)]$. This completes the construction.

There are other ways to construct a partition into Boolean intervals [21]. Such constructions always involve arbitrary choices, such as a linear ordering of the vertices or a linear ordering of the edges. A geometric explanation for why partitioning is possible and for why it involves arbitrary choices may be found in [3]. The idea is that for a fixed set of vertices, the complements of the edge sets of connected graphs form a simplicial complex. The complements of the edge sets of trees are the facets of this complex. A topological property of this simplicial complex ensures the partitioning is possible.

Fernández and Procacci [13] found that the particular construction used by Penrose was the appropriate path to their result on the convergence of the cluster expansion. See [11] for an alternative approach to their result using an identity of the type introduced in [6, 7, 1].

Theorem 4.4 (Connected graph identity)**.** *The total weight of the connected graphs is*

$$c(a) = |C(a)|_* = \sum_T \prod_{\{i,j\} \in T} t(a(i), a(j)) \prod_{\{i,j\} \in \chi(T) \setminus T} (1 + t(a(i), a(j))). \quad (4.40)$$

The proof starts with the connected graph sum $c(a) = \sum_{G_c} \prod_{\{i,j\} \in G_c} t(a(i), a(j))$. Each connected graph G_c in a Boolean interval $[T, \chi(T)]$ is the disjoint union of the tree T with a subset H of $\chi(T) \setminus T$. By the Boolean partition

identity the connected graph sum is

$$c(a) = \sum_T \prod_{\{i,j\}\in T} \sum_{H\subseteq\chi(T)\setminus T} \prod_{\{i,j\}\in H} t(a(i), a(j)). \tag{4.41}$$

By the distributive law the sum over subsets H of the products of the $t(a(i), a(j))$ factors gives a single product of $1 + t(a(i), a(j))$ factors.

Corollary 4.5 (Alternating sign property)**.** *Take each $t(p, q)$ with $-1 \le t(p, q) \le 0$. If $a : U \to \mathcal{P}$ with a set U with n elements, then the sign of the total weight $c(a) = |C(a)|_*$ of connected graphs with vertex set U is $(-1)^{n-1}$.*

This is obvious because each tree has $n-1$ edges. The tree factors are negative, and the remaining factors are positive.

Theorem 4.6 (Tree bound)**.** *Let $-1 \le t(p, q) \le 0$ be the edge factor for graphs. For each colored set (particle configuration) the absolute value of the total weight $c(a) = |C(a)|_*$ of connected graphs with the weight factors $t(p, q)$ is bounded by the total weight $t(a) = |T(a)|_*$ of trees taken with the weight factors $|t(p, q)|$. That is,*

$$|c(a)| \le t(a). \tag{4.42}$$

This comes from estimating the tree factors by their absolute values and the remaining factors by one. The explicit form of the tree bound is

$$|\sum_{G_c} \prod_{\{i,j\}\in G_c} t(a(i), a(j))| \le \sum_T \prod_{\{i,j\}\in T} |t(a(i), a(j))|. \tag{4.43}$$

The total weight for connected graphs involves a huge amount of cancelation, due to the fact that the interaction factors are negative. The partitioning identity gives a way of making this cancelation explicit. The conclusion is the remarkable fact that the various series for connected graphs, rooted connected graphs, and so on are bounded term by term by the corresponding series for trees, rooted trees, and so on.

The connected graph identity also gives information about invariants of partitioning. For each partitioning scheme $T \mapsto \chi(T)$, define the corresponding h-polynomial

$$h(s) = \sum_T s^{|\chi(T)\setminus T|}. \tag{4.44}$$

The coefficients of this polynomial describe how many trees give rise to an element of the partition of each fixed size.

Proposition 4.7 (Invariants of partitions)**.** *The h-polynomial that describes the number of sets in the partition of each fixed size is the same for every partition.*

The proof of this proposition follows from the connected graph identity with $t(p, q) = t$. This is

$$\sum_{G_c} t^{|G_c|} = t^{n-1} \sum_T \sum_{T\subseteq H\subseteq\chi(T)} t^{|H\setminus T|} = t^{n-1} \sum_T (1 + t)^{|\chi(T)\setminus T|} = t^{n-1} h(1 + t). \tag{4.45}$$

The left hand side depends only on the number of connected graphs of each size, and so it is independent of the partition. It follows that the same is true for the right hand side. Thus the polynomial $h(1+t)$ is independent of the partition. It follows that the polynomial $h(s)$ is independent of the partition.

Here is an example of an h-polynomial . Take $n = 3$. There are four connected graphs. Their weight is $t^3 + 3t^2 = t^2(t+3) = t^2((1+t)+2) = t^2 h(1+t)$. Thus $h(s) = s+2$. Thus no matter how the partitioning is done, there is one part where $\chi(T) = K_3$ is the complete graph, and there are two parts where $\chi(T) = T$.

5. Hard-core interaction and polymers

5.1. Soft interaction

There are at least four levels at which one can consider the equilibrium particle gas, starting with the most general and ending with the most special. The case considered up to now is that of the soft repulsive interaction, which is the case of a potential $V(p,q)$ satisfying $0 \le V(p,q) \le +\infty$. As we have seen, if $V(p,q) = 0$ for all p, q then the number of particles at each location p is a Poisson random variable with mean w_p. So one might think of the soft case as a situation where one is perturbing Poisson random variables.

Level 1: Soft interaction The function $1 + t(p,q) = \exp(-\beta V(p,q))$ has values in the interval $[0,1]$.

Level 2: Hard-core self-repulsion The function $1+t(p,p) = \exp(-\beta V(p,p))$ is restricted to have values 0 or 1. Thus there can be at most one particle at a given location. Particle configurations are sets of locations.

Level 3: Hard-core interaction The function $1 + t(p,q) = \exp(-\beta V(p,q))$ is restricted to have values 0 or 1. Every configuration is either allowed or completely forbidden.

Level 4: Polymer interaction There is a set T such that each p in $\mathcal{P}$ is a non-empty finite subset of T. In this case p is called a polymer. The function $1 + t(p,q) = \exp(-\beta v(p,q))$ is 1 if $p \cap q = \emptyset$ and 0 if $p \cap q \neq \emptyset$. An allowed configuration is a collection of non-intersecting polymers.

5.2. Hard-core self-repulsion

For a hard-core self-repulsion the only particle configurations $a : U_n \to \mathcal{P}$ are those that are injective functions: different particles occupy different locations. The corresponding occupation number function will just be the indicator function of the subset X of occupied locations. For each such subset X there are $n!$ corresponding particle configurations. A particle configuration thus has an alternate description as a finite set $X \subseteq \mathcal{P}$. The grand partition function is an multi-affine generating function. In general, the expected number of particles at location p is just the probability of a particle at p. Otherwise, the formulas are the same.

In the case of hard-core self-repulsion but no other interaction, the probability of a particle at p is

$$\sum_{N(p)=1} p(N) = \frac{1}{\prod_q (1+w_q)} w_p \prod_{q \neq p} (1+w_q) = \frac{w_p}{1+w_p}. \tag{5.1}$$

Therefore the probability distribution for the number of particles at p is Bernoulli with probability $w_p/(1+w_p)$ for one particle and $1/(1+w_p)$ for no particle. The probability model is given by independent Bernoulli distributions for the number of particles at a given locations. So one can think of the general case of hard-core self-repulsion as a perturbation about the Bernoulli distribution.

The fact that the grand partition function $G(w)$ is multi-affine may also be seen from the general formula in terms of sums over graphs. Consider an n and a particle configuration a such that $a(i) = a(j) = p$ for some $i \neq j$. Consider the contribution to the graph sum in

$$g(a) = \sum_G \prod_{\{i,j\} \in G} t(a(i), t(a(j))) \tag{5.2}$$

from this pair. Partition the set of graphs into two parts, depending on whether the pair $\{i,j\}$ is an edge or not. Each graph in the first part has a factor $t(p,p) = -1$, and each graph in the second part has no such factor. There is perfect cancelation, so $g(a) = 0$. This argument does not apply to the connected function, since connected graphs prefer having edges to not having edges. Indeed, the connected function is not multi-affine.

In the case of hard-core self-repulsion Dobrushin [9] proved that if there are finite $x_p \geq 0$ with

$$w_p^* \prod_q (1 + |t(p,q)| x_q) \leq x_p, \tag{5.3}$$

then the cluster expansion for the density converges for w satisfying $|w_p| \leq w_p^*$. This is yet one more finite fixed point condition. The relation to the other conditions is the following. It is clear that

$$w_p^* \prod_q (1 + |t(p,q)| x_q) \leq w_p^* \prod_q \exp(|t(p,q)| x_q) = w_p^* \exp(\sum_q |t(p,q)| x_q). \tag{5.4}$$

Thus the Kotecký-Preiss condition implies the Dobrushin condition, so for hard-core self-repulsion the Dobrushin result implies the Kotecký-Preiss result. For a comparison with the Fernández-Procacci result, notice that with hard-core self-repulsion $(1+t)^{\mathrm{Pair}(N)} \neq 0$ implies $0 \leq N \leq 1$. So

$$w_p^* G(|t|_p x) \leq w_p^* \sum_{0 \leq N \leq 1} |t_p|^N x^N = w_p^* \prod_q (1 + t(p,q) x_q). \tag{5.5}$$

It follows that for hard-core self-repulsion the Dobrushin condition implies the Fernández-Procacci condition. Turning this around, the Fernández-Procacci result implies the Dobrushin result.

5.3. Hard-core interaction

An even more special case is the hard-core interaction gas. This is a hard core gas for which the potential for locations p, q satisfies $v(p,q) = 0$ or $v(p,q) = +\infty$. The corresponding Boltzmann factor $1 + t(p,q) = \exp(-\beta v(p,q))$ takes the value either 1 or 0. Thus $t(p,q)$ takes the value 0 or -1. Two points $p \neq q$ are compatible if $1 + t(p,q) = 1$, incompatible if $1 + t(p,q) = 0$. This defines a graph structure H with vertex set $\mathcal{P}$, where an edge is present between p, q whenever $t(p,q) = -1$. This is a more general kind of graph, since it has a loop at every vertex.

A *graph homomorphism* is a map from the vertices of a graph G to the vertices of another graph H that sends edges to edges. The formula for the grand partition function is

$$G(w) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{G} \sum_{a:U_n \to \mathcal{P}} (-1)^{|G|} \prod_{j \in U_n} w_{a(j)}, \tag{5.6}$$

where the sum is over graphs G with vertex set U_n and over functions $a : U_n \to \mathcal{P}$ that are graph homomorphisms from G to H. However, as we have seen, the contribution of the particle configurations that are not injective sums to zero. So we may instead write this as the sum over graphs G with vertex set U_n and over injective functions $a : U_n \to \mathcal{P}$ that are graph homomorphisms from G to H. Finally, we may identify the graph G with its image in H and write this as

$$G(w) = \sum_{X} \sum_{G} (-1)^{|G|} w^X, \tag{5.7}$$

where the sum is over graphs G on $X \subseteq \mathcal{P}$ that are subgraphs of H.

For the connected function the corresponding representation is

$$C(w) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{G_c} \sum_{a:U_n \to \mathcal{P}} (-1)^{|G_c|} \prod_{j \in U_n} w_{a(j)}, \tag{5.8}$$

where the sum is over connected graphs G_c with vertex set U_n and over functions $a : U_n \to \mathcal{P}$ that are graph homomorphisms from G_c to H. Notice that the subgraph of H whose vertices are the image of a and whose edges are the images of the edges of G is connected.

The general formula for the cluster coefficient is

$$c(a) = \sum_{G_c} (-1)^{|G_c|} \tag{5.9}$$

when a is a graph homomorphism from G to H and is zero otherwise. We can represent the coefficients of the grand partition function in terms of the first order coefficients of the connected function. These coefficients are given by

$$c(Y) = \sum_{G_c} (-1)^{|G_c|}, \tag{5.10}$$

where G_c ranges over connected graphs with vertex set Y that are subgraphs of H. The contribution of a connected graph is $+1$ if it has an even number of edges and -1 if it has an odd number of edges. This explicit representation is a good reminder that such graph expressions involve rather large cancelations.

In the hard-core interaction case it is interesting to contrast various probability expressions. The *avoidance probability* is

$$\frac{\partial C(w)}{\partial w_p} = \frac{G(w_{\mathcal{P}\setminus\bar{p}})}{G(w)} = \exp(C(w_{\mathcal{P}\setminus\bar{p}}) - C(w)), \tag{5.11}$$

where $\bar{p}$ denotes the set of q such that are not compatible with p. This will be automatically bounded above by one in the case when the weights w_p are positive and there is a genuine probability interpretation. The sum in the exponential is over connected graphs such that $N(q) \geq 1$ for some q with $t(p,q) = 1$. The probability of a particle at p has just one more factor of w_p, so it is given by

$$P_p^1 = C_p^\bullet(w) = w_p \frac{\partial C(w)}{\partial w_p}, \tag{5.12}$$

while the probability for no particle at p is

$$P_p^0 = \frac{G(w_{\mathcal{P}\setminus\{p\}})}{G(w)} = \exp(C(w_{\mathcal{P}\setminus\{p\}}) - C(w)). \tag{5.13}$$

In the latter case the sum in the exponential is over connected graphs such that $N(p) \geq 1$.

5.4. Polymer systems

In a polymer system there is a set T, finite or countably infinite. A point t in T will be called a *site*. Each element A in $\mathcal{P}$ is a non-empty finite subset of T. Before such an object was called a color or a location, but in this context it is called a *polymer*. The constraint is that polymers cannot overlap. Typically only certain kinds of sets A are admissible as polymers. This can be ensured by requiring that the corresponding weights w_A are fixed with value zero, or one can simply restrict the set $\mathcal{P}$. In order for the formulas to make sense, it is customary to work within finite subsets $\Lambda \subseteq T$ with coefficients w_A that vanish unless $A \subseteq \Lambda$. The idea is that the results should be uniform in Λ.

The grand partition function for a polymer system will be written as $Z(w)$. If Λ is a given finite subset of T, we can write $Z(w_{P(\Lambda)})$ for the value when w is set zero except for polymers A that belong to $P(\Lambda)$. Of course $A \in P(\Lambda)$ is equivalent to $A \subseteq \Lambda$. It is convenient to denote this instead by $Z_\Lambda(w)$.

The grand partition function for a polymer is thus of the form

$$Z_\Lambda(w) = \sum_\Gamma \prod_{A\in\Gamma} w_A, \tag{5.14}$$

where Γ ranges over finite sets of non-overlapping admissible subsets of Λ. Because of the way it arises in applications, we shall refer to $Z_\Lambda(w)$ as the partition function. In fact, it often arises as a partition function for a statistical mechanical system whose underlying space is the set T of sites. This makes it natural to define the free energy F_Λ by

$$Z_\Lambda = \exp(-\beta F_\Lambda). \tag{5.15}$$

It is perhaps confusing that the particle location language has been replaced by the polymer language. Here is a dictionary that may be helpful.

- A particle location is a polymer (a subset of the set of sites).
- A particle occupation number function (for hard-core interaction) is a set of polymers that are present (occupied).
- An activity parameter is a polymer weight (not necessarily positive).
- The interaction factor (for hard-core interaction) is exclusion (non-overlap) of polymers.
- The grand partition function is the partition function.
- The connected function is (a multiple of) the free energy.
- The pinned connected function is the avoidance probability (not necessarily bounded above by one).

Proposition 5.1 (Convergence of cluster expansion for polymers)**.** *Let the partition function Z_Λ have a polymer representation in terms of coefficients w_A, with no restriction on sign, but satisfying a bound $|w_A| \leq w_A^*$. Suppose the Kotecký-Preiss condition is satisfied in the following form: there is a constant $c \geq 0$ such that for each B we have*

$$\sum_{A \cap B \neq \emptyset} w_A^* e^{c|A|} \leq c|B|. \tag{5.16}$$

Then for each $A \subseteq \Lambda$ the avoidance probability has a convergent power series expansion in powers of the w_A, and the sum satisfies

$$\frac{\partial C_\Lambda(w)}{\partial w_A} = \frac{Z_{\Lambda \setminus A}(w)}{Z_\Lambda(w)} = \exp(C_{\Lambda \setminus A}(w) - C_\Lambda(w)) \leq e^{|A|}. \tag{5.17}$$

There is a somewhat sharper criterion for the convergence in the polymer case due to Gruber and Kunz. Fernández-Procacci show that in the polymer context their result implies the Gruber-Kunz result which implies the Dobrushin result which implies the Kotecký-Preiss result. The stronger results give a somewhat better radius of convergence in specific examples. The book [16, Chapter 3] works with the Gruber-Kunz framework. The article [12] presents a typical application.

5.5. Cluster representations as polymer partition functions

It is remarkable that this polymer structure arises naturally in the context of combinatorics, namely in the situation when there is a cluster representation.

Proposition 5.2 (Cluster representation as polymer system)**.** *For $\Lambda \subseteq T$ consider the cluster representation representing combinatorial coefficients Z_Λ by cluster coefficients w_A in the form*

$$Z_\Lambda = \sum_\Gamma \prod_{A \in \Gamma} w_A. \tag{5.18}$$

Here Γ ranges over partitions of X into non-empty pairwise disjoint subsets with union X. Suppose that $w_A = 1$ for each A that is a one-point subset. Then the cluster representation is the partition function for a polymer.

It may be that the condition on one-point subsets is not satisfied, but then it is often possible to get a partition function for a polymer by dividing both sides by the product of the $w_{\{t\}}$ for t in Λ. This amounts to dividing each w_A by the product of the $w_{\{t\}}$ for $t \in A$, so one just works with these modified activities.

We shall see that the cluster representation often arises in a context where the Z_Λ is related to a graph sum associated with the set Λ of sites, while the w_A is a corresponding quantity related to a connected graph sum associated with the subsets A. The partition Γ then arises from the decomposition of graphs into connected subgraphs. Either the contributions of the one-point connected graphs are already equal to one, or one takes care of the problem by division.

The terminology is inherently confusing, since when the cluster representation is interpreted as a grand partition function, then it is possible to do a cluster expansion of the cluster representation. That is, the cluster representation represents combinatorial coefficients in terms of cluster coefficients associated with connected clusters of sites. Then this representation is reinterpreted as a grand partition function, which has a cluster expansion indexed by connected clusters of polymers. The activity parameters in the grand partition function are the cluster coefficients in the cluster representation. Again a dictionary that may be helpful.

- A particle location is a polymer which is a cluster of sites.
- A particle occupation number function is a set of polymers which in turn is a partition into clusters of sites.
- An activity parameter is a polymer weight which is a cluster coefficient.
- The grand partition function is the partition function which is a combinatorial coefficient.

6. Random fields

6.1. Gibbs measures

Cluster expansion ideas are important for understanding an equilibrium gas system, but their importance is much more general. In other physical systems it is often possible to introduce a cluster representation in a more or less natural way, most often in the framework of a polymer system. One such example is that

of a random field defined by a Gibbs measure. Here is the general framework; a particular application will follow.

Let T be a countable set, and consider the product space $\Omega = \mathbf{R}^T$. In physics a real function ϕ on T is often called a scalar field. This is of course just an element of the product space Ω. A *random field* is given by specifying a probability measure μ on Ω. Thus ϕ may be considered as a random function, and its values ϕ_t for $t \in T$ form a collection of random variables.

In physics the usual procedure is to start with a random field μ_0 that is well-understood and to use this to build another random field μ that has more significant interactions. The same general strategy applies both to systems from classical and quantum statistical mechanics and from Euclidean quantum field theory. Here are two examples of random fields μ_0 that make good starting points.

Independent random variables This is the case when the measure μ_0 is a product measure μ_0. The random variables ϕ_t for t in T are independent. Once the distribution of each ϕ_t is known, the distribution of the entire random field is determined by product property for independent random variables.

Gaussian random variables This is the case when the measure μ_0 is Gaussian. The random variables ϕ_t for t in T have a joint Gaussian distribution. Their distribution is thus determined by the means $m(t) = \mu_0(\phi_t)$ and the covariances

$$C(s,t) = \mu_0((\phi_s - m_s)(\phi_t - m_t)). \tag{6.1}$$

The goal is to define another probability measure μ on Ω that gives a random field that describes the state of a interacting system at a given temperature. This measure should be formally defined by a factor that depends on the energy H of the infinite system. The problem is that the energy for an infinite system is given by a divergent series. The solution is to deal with an approximate expression H_Λ for the energy, obtained by restricting the interactions to sites in a finite subset $\Lambda \subseteq T$. This in turn defines an approximate measure μ_Λ. Then estimates are derived that show that these measures converge to a limit μ as Λ gets large.

Thus suppose that H_Λ is a measurable function on Ω, bounded below, depending only on the coordinates ϕ_t for t in Λ. This represents the approximate version of the energy. Let β be the inverse temperature, measured in inverse energy units. Then $W_\Lambda = \exp(-\beta H_\Lambda)$ is a Boltzmann weight factor that is used to define the approximate probability model μ_Λ corresponding to the subset Λ. Define the partition function

$$Z_\Lambda = \mu_0(W_\Lambda) \tag{6.2}$$

and the probability measure whose expectation is given by

$$\mu_\Lambda(f) = \frac{1}{Z_\Lambda} \mu_0(f W_\Lambda). \tag{6.3}$$

This defines a new random field μ_Λ that has non-trivial interactions in Λ. The

corresponding *free energy* F_Λ is then defined by

$$Z_\Lambda = \exp(-\beta F_\Lambda). \tag{6.4}$$

In general it is difficult to control the limit of large Λ. In order to have some hope of this the reference measure μ_0 and the energy functions H_Λ cannot depend too strongly on too many coordinates. When this is the case, there is an extensive theory of the resulting interacting measures μ_Λ and of their large Λ limits. A probability measure μ on Ω that arises in this way as a large Λ limit is called a *Gibbs measure*. There are elegant characterizations of such measures, but, as always, getting control of specific examples can involve some effort. An introduction to Gibbs measures may be found in [16, Chapter 1].

The situation is quite different from that of the equilibrium gas of particles, since there is no activity parameter. However, in some cases it is possible to construct a polymer cluster representation, where the role of the activity parameter is played by a cluster coefficient representing the size of the interaction. This cluster coefficient may have either sign. With suitable estimates it is then possible to show that the cluster expansion converges and hence that the ratio has a large Λ limit.

The procedure is in several steps. The first is to find a cluster representation

$$Z_\Lambda = \mu_0(W_\Lambda) = \sum_\Gamma \prod_{A\in\Gamma} w_A \tag{6.5}$$

for the denominator. Here the w_A are cluster coefficients associated to certain polymers A. The second step is to find a similar representation for the numerator

$$\mu_0(fW_\Lambda) = \sum_{R,\Gamma} \tilde{w}_R \prod_{A\in\Gamma} w_A, \tag{6.6}$$

where f only depends on the ϕ_t for $t \in B$, the subset R is $R = \emptyset$ or satisfies $R \cap B \neq \emptyset$, and where $A \in \Gamma$ implies $A \cap (B \cup R) = \emptyset$. Once this is accomplished, one has a representation

$$\mu(f) = \sum_R \tilde{w}_R \frac{Z_{\Lambda\setminus(B\cup R)}}{Z_\Lambda}. \tag{6.7}$$

As is shown in [16, Chapter 3] the main difficulty in taking the limit of large Λ is to control the ratio

$$\frac{Z_{\Lambda\setminus A}}{Z_\Lambda} = \exp(\beta(F_\Lambda - F_{\Lambda\setminus A})) \tag{6.8}$$

uniformly in Λ for fixed A. This is the avoidance probability, so this is just another instance of the need to control the convergence of the cluster expansion.

The following subsections treat the cluster representation for the situation when the reference measure μ_0 describes independent random variables. The discussion is confined to the situation where the interactions are weak or the

temperature is high. It is also possible to find a cluster representation at low temperature perturbing around a ground state.

The case where μ_0 is a Gaussian measure is also of great importance. In this case there is a graphical structure that arises from the combinatorics of Gaussian random variables. The cluster representations relates moments (sums over graphs) to cumulants (sums over connected graphs). See [5] or [6] or [16, Chapter 2, Sections 1,2, 3; Chapter 4, Section 6] for a more complete account of cluster representations for perturbations of Gaussian measures.

6.2. Cluster expansion for perturbations of a product measure

One important type of Gibbs measure arises from perturbing a product probability measure. In physics these are often called spin systems, but their importance is more general. Here it is shown that a polymer cluster representation arises rather naturally in this application.

Consider a product probability measure μ_0 indexed by $t \in T$. One perturbs this by a Boltzmann factor $W_\Lambda = \exp(-\beta H_\Lambda)$, where $\Lambda \subseteq T$, and W_Λ only depends on the coordinates ϕ_t for t in Λ. For simplicity consider only the case when $H_{\{t\}} = 0$, so $W_{\{t\}} = 1$. This will mean that there will be no headaches about one-point subsets.

A classic example is when the Hamiltonian is $H_\Lambda = \sum_Y U_Y$, where Y ranges over subsets of Λ with two or more points. The term U_Y is supposed to depend only on the coordinates ϕ_t with t in Y. The the Boltzmann factor W_Λ has the product structure $W_\Lambda = \prod_Y \exp(-\beta U_Y)$.

Theorem 6.1. *The system with product probability measure μ_0 and Hamiltonian $H_\Lambda = \sum_Y U_Y$ admits a polymer cluster representation.*

To obtain the cluster representation, write the Boltzmann factor as

$$W_\Lambda = \prod_Y \exp(-\beta U_Y) = \prod_Y (1 + \chi_Y), \tag{6.9}$$

where $\chi_Y = \exp(-\beta U_Y) - 1$. The distributive law then gives

$$W_\Lambda = \sum_\Delta \prod_{Y \in \Delta} \chi_Y, \tag{6.10}$$

where Δ ranges over hypergraphs on Λ. The $\Delta = \emptyset$ term is 1.

A *hypergraph* is a set Λ of vertices together with a collection Δ of non-empty subsets. Such a non-empty subset is a hyper-edge or *link*. (In our case each link has two or more points.) The *support* of a hypergraph is the subset $\bigcup \Delta$ of vertices that belong to some set in Δ. A hypergraph Δ is *connected* if the support of Δ is non-empty and cannot be partitioned into non-empty sets with no links joining the parts. (Thus in the present context a connected hypergraph is only required to connect the vertices in its support.) If Δ is a hypergraph, then the support of Δ may be partitioned into non-empty subsets on each of which there is a connected hypergraph.

If $A \subset \Lambda$, define

$$\alpha_A = \sum_{\Delta_c} \prod_{Y \in \Delta_c} \chi_A, \tag{6.11}$$

where Δ_c ranges over connected hypergraphs with support A.

Lemma 6.2. *The Boltzmann factor may be written as sum over products of independent factors in the form*

$$W_\Lambda = \sum_{\Gamma} \prod_{A \in \Gamma} \alpha_Y, \tag{6.12}$$

where Γ ranges over collections of disjoint subsets of Λ, where each subset has two or more points.

In the representation given by the lemma the $\Gamma = \emptyset$ contribution is 1. The proof of the lemma begins by breaking hypergraphs into connected parts. The sum over hypergraphs Δ is then a sum over collections Γ of disjoint sets and over assignments S of connected hypergraphs to these sets. The S range over functions from Γ to connected hypergraphs with the property that $S(A)$ is a connected hypergraph with support A. The product over Δ is equivalent to the product over A in Γ and the links in the corresponding $S(A)$. Hence

$$W_\Lambda = \sum_{\Gamma} \sum_{S} \prod_{A \in \Gamma} \prod_{Y \in S(A)} \chi_Y. \tag{6.13}$$

Apply the distributive law. This gives

$$W_\Lambda = \sum_{\Gamma} \prod_{A \in \Gamma} \sum_{\Delta_c} \prod_{Y \in \Delta_c} \chi_Y, \tag{6.14}$$

where Δ_c ranges over connected hypergraphs with support A. This proves the lemma.

The advantage of the representation in the lemma is that the α_A are independent with respect to the product measure μ_0. It follows that the partition function is also a sum over a product, in the form

$$Z_\Lambda = \mu_0(W_\Lambda) = \sum_{\Gamma} \prod_{A \in \Gamma} w_A, \tag{6.15}$$

where the cluster coefficient

$$w_A = \mu_0(\alpha_A) = \sum_{\Delta_c} \mu_0 \left(\prod_{Y \in \Delta_c} \chi_Y \right) \tag{6.16}$$

plays the role of an activity parameter.

The numerator may be handled in a similar way. Say that f only depends on the coordinates corresponding to the set B. Then there are two kinds of terms in the expansion of fW_Λ in hypergraphs on the sets A in Γ. In some

of these none of the connected components intersect B. For these one gets a product of f with a product of independent random variables α_A. For the other terms one decomposes the hypergraph into one connected component that is connected to B and remaining connected components that are not. The result is the representation

$$fW_\Lambda = \sum_{R,\Gamma} \tilde{\alpha}_R \prod_{A\in\Gamma} \alpha_A, \tag{6.17}$$

where $R = \emptyset$ or $R \cap B \neq \emptyset$, and where $A \in \Gamma$ implies $A \cap (B \cup R) = \emptyset$. Taking expectations and using independence gives a representation

$$\mu_0(fW_\Lambda) = \sum_{R,\Gamma} \tilde{w}_R \prod_{A\in\Gamma} w_A. \tag{6.18}$$

6.3. Convergence of the cluster expansion

The cluster representation must be accompanied by estimates in order to be able to prove anything about convergence. What follows is a derivation of such estimates.

Theorem 6.3. *Consider finite subsets Λ of the set T of sites. Consider a product probability measure μ_0 on the fields indexed by T. Let*

$$H_\Lambda = \sum_Y U_Y, \tag{6.19}$$

where the interactions U_Y depend only on the fields indexed by $Y \subseteq \Lambda$ with $|Y| \geq 2$. Let $u_Y = \sup|U_Y|$, and suppose that for some $a > 0$ and $b > 0$

$$\sup_t \sum_{t\in Y} u_Y e^{a|Y|} \leq b. \tag{6.20}$$

Let f be a bounded function depending on the fields indexed by $B \subseteq \Lambda$. Define the expectation

$$\mu_\Lambda(f) = \frac{\mu_0(fe^{-\beta H_\Lambda})}{\mu_0(e^{-\beta H_\Lambda})}. \tag{6.21}$$

If βb is sufficiently small, then the cluster expansion for $\mu_\Lambda(f)$ converges, and the estimates are uniform in Λ.

The remainder of this section outlines the proof of this theorem. The hypothesis of the theorem describes a reasonable Banach space for describing the interactions, and the condition of small norm indicates a regime of high temperature or weak interaction. The main task is to obtain an estimate of the Kotecký-Preiss type. A more detailed account may be found in [16, Chapter 4, Sections 1,2].

Recall that $\chi_Y = \exp(-\beta U_Y) - 1$. Let $v_Y = \sup|\chi_Y|$. The main hypothesis of the theorem is that βb is small. In the following we consider a small constant

$x > 0$ that is controlled by βb. The new starting point is then

$$\sup_t \sum_{t \in Y} v_Y e^{a|Y|} \leq x. \tag{6.22}$$

This condition says that the total interaction with a given point is small. Actually what is used is the consequence

$$\sup_t \sum_{|Y|=m, t \in Y} v_Y \leq x e^{-am}. \tag{6.23}$$

The quantity to be estimated is the cluster coefficient

$$|w_A| \leq \sum_{\Delta_c} \prod_{Y \in \Delta_c} v_Y, \tag{6.24}$$

where Δ_c ranges over connected hypergraphs on A.

Lemma 6.4. *For each c with $0 < c < a$ there is a sufficiently small x such that the cluster coefficients satisfy a Kotecký-Preiss bound*

$$\sup_t \sum_{t \in A} |w_A| e^{c|A|} \leq c. \tag{6.25}$$

The proof of this lemma will require two more lemmas. The plan is to use an inductive argument that involves removing one link of size m from a connected hypergraph with n links, so that the remaining links comprise a collection of r connected hypergraphs, for some $r \leq m$. Here are the details.

Consider the sum over connected hypergraphs with root t given by

$$s = \sum_{t \in \bigcup \Delta_c} \prod_{Y \in \Delta_c} v_Y e^{c|Y|}. \tag{6.26}$$

Since $A = \bigcup \Delta_c$ implies $|A| \leq \sum_{Y \in \Delta_c} |Y|$, we have

$$\sum_{t \in A} |w_A| e^{c|A|} \leq s. \tag{6.27}$$

All that is required is to show that if the parameter x that controls the size of the v_Y is sufficiently small, then s also becomes arbitrarily small. The following lemma shows that the contributions of these connected hypergraphs satisfies a recursive estimate such as one would find in a tree structure.

Lemma 6.5. *For $n \geq 1$ let*

$$s_n = \sup_t \sum_{|\Delta_c|=n : t \in \bigcup \Delta_c} \prod_{Y \in \Delta_c} v_Y e^{c|Y|}. \tag{6.28}$$

be the contribution of all rooted connected hypergraphs with n links. Set $s_0 = 0$. Take $0 < c < a$, so that $\epsilon = e^{(c-a)} < 1$. Then for $n \geq 1$

$$s_n \leq x \sum_{m=0}^{\infty} \epsilon^m \sum_{r=0}^{m} \binom{m}{r} \sum_{n_1 + \cdots + n_r = n-1} s_{n_1} \cdots s_{n_r}. \tag{6.29}$$

For $n \geq 2$ the right hand side of the inequality only has contributions from $r \geq 1$ and each $n_i \geq 1$. For $n = 1$ only $r = 0$ contributes, and the sum over the empty sequence of the empty product gives 1. So in this case the inequality says that $s_1 \leq x/(1-\epsilon)$. For the inductive step linearly order the points t in T. Also linearly order the finite subsets Y of T. Consider a connected hypergraph Δ_c rooted at t with n links. Consider the least Y in Δ_c with t in Y. Then $\Delta_c \setminus \{Y\}$ has $n-1$ links and is naturally partitioned into connected parts. Let r be the number of such connected parts. Say that Δ'_c is one of these connected parts with underlying set $\bigcup \Delta'_c$. Since Y connects Δ_c, there is a least t' in $Y \cap \bigcup \Delta'_c$. Let $S \subseteq Y$ be the set of such t'. Since the Δ'_c are separate connected components of $\Delta_c \setminus \{Y\}$, the points t' corresponding to distinct Δ'_c are distinct. So S has r points. Let m be the number of points in Y. Sum over m and over the corresponding links Y rooted at t. Also sum over the r element subsets $S \subseteq Y$. These subsets correspond to the r connected parts of $\Delta_c \setminus \{Y\}$. Then sum over the number of links in each part. The contributions factor, and the result is the recursive estimate

$$s_n \leq \sum_{m=0}^{\infty} \sum_{|Y|=m, t \in Y} v_Y e^{cm} \sum_{r=0}^{m} \binom{m}{r} \sum_{n_1+\cdots+n_r=n-1} s_{n_1} \cdots s_{n_r} \tag{6.30}$$

where the sum is over all $n_1, \ldots, n_r$ constrained by $n_1 + \cdots + n_r = n-1$. Estimate the sum over Y via the parameter x. This immediately gives the lemma.

Lemma 6.6. *If x is sufficiently small, then the sum $s = \sum_{n=1}^{\infty} s_n$ representing the contributions of all rooted connected hypergraphs converges, and the sum approaches zero as x approaches zero.*

Majorize the s_n by a sequence $\bar{s}_n$ obtained by fixed point iteration, where $\bar{s}_0 = 0$ and for $n \geq 1$

$$\bar{s}_n = x \sum_{m=0}^{\infty} \epsilon^m \sum_{r=0}^{m} \binom{m}{r} \sum_{n_1+\cdots+n_r=n-1} \bar{s}_{n_1} \cdots \bar{s}_{n_r}. \tag{6.31}$$

We can write this via an index shift

$$\bar{s}_n = x \sum_{m=0}^{\infty} \epsilon^m \sum_{r=0}^{m} \binom{m}{r} \bar{t}_{n-1}, \tag{6.32}$$

on a convolution sum

$$\bar{t}_n = \sum_{n_1+\cdots+n_r=n} \bar{s}_{n_1} \cdots \bar{s}_{n_r}. \tag{6.33}$$

Consider the generating function $p = \sum_{n=1}^{\infty} \bar{s}_n q^n$. For the generating function the convolution sum becomes a product p^r, and the shift of index corresponds to multiplication by q. Therefor p satisfies a fixed point equation

$$p = x \sum_{m=0}^{\infty} \epsilon^m \sum_{r=0}^{m} \binom{m}{r} q p^r = qx \sum_{m=0}^{\infty} \epsilon^m (1+p)^m = qx \frac{1}{1-\epsilon(1+p)}. \tag{6.34}$$

This fixed point equation has solution

$$p = \frac{2qx}{(1-\epsilon) + \sqrt{(1-\epsilon)^2 - 4\epsilon qx}}. \tag{6.35}$$

For $q = 1$ and x sufficiently small the fixed point p is small and is given by $\bar{s} = \sum_n \bar{s}_n$. Therefore $s = \sum_n s_n$ is also small. This proves the bound on the sum over rooted connected hypergraphs, which establishes the lemma.

The last two lemmas finish the proof that the Kotecký-Preiss condition is satisfied. The cluster expansion theorem then gives the bound $|Z_{\Lambda\setminus A}/Z_\Lambda| \leq e^{c|A|}$. The next task is to use this to estimate the expansion of

$$\mu_\Lambda(f) = \sum_R \tilde{w}_R \frac{Z_{\Lambda\setminus(B\cup R)}}{Z_\Lambda}, \tag{6.36}$$

where $R = \emptyset$ or $R \cap B \neq \emptyset$. Then $\tilde{w}_R$ is a sum over hypergraphs Δ with $\bigcup \Delta = R$ such that B, Δ is connected. As a consequence

$$|\tilde{w}_R| \leq \sum_\Delta \|f\| \prod_{Y\in\Delta} v_Y. \tag{6.37}$$

We need to estimate

$$\sum_R |\tilde{w}_R| e^{c|B\cup R|} \leq \sum_\Delta \|f\| e^{c|B|} \prod_{Y\in\Delta} v_Y e^{c|Y|}. \tag{6.38}$$

Here the hypergraphs Δ are such that B, Δ is connected.

Remove B; the remaining hypergraph breaks up into r connected components, with $0 \leq r \leq |B|$. So the last quantity is bounded by

$$\|f\| e^{c|B|} \sum_{r=0}^{|B|} \binom{|B|}{r} s^r = \|f\| e^{c|B|} (1+s)^{|B|}. \tag{6.39}$$

Since this is finite, the conclusion is that the expansion for $\mu_\Lambda(f)$ is convergent. The fact that this is taking place in the finite set Λ plays no role in the estimates, so the result applies to arbitrarily large systems.

7. Conclusion

The combinatorial mathematics of exponential generating functions is closely related to the grand partition function for the equilibrium gas. A ratio related to this grand partition function gives the density of the gas. This quantity has a cluster expansion that has a radius of convergence that is independent of the size of the system.

The classic criterion for the radius of convergence uses a reduction of a sum over connected graphs to a sum over tree graphs. The sum over rooted tree graphs has a recursive structure that is well-known in combinatorics, and the convergence criterion is the condition for the finiteness of the exponential generating function for rooted tree graphs. The entire story provides a remarkable

connection between the science of enumerative combinatorics and the physics of equilibrium statistical mechanics.

There is another surprise. The gas picture may be specialized to a situation where, instead of describing a particle at a location, it describes the presence of a polymer, a composite object. These polymers arise in the description of interaction terms in the physics of random fields. The cluster expansion thus gives results in areas of physics that have little to do with the equilibrium gas.

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