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Gaussian-cluster models of percolation and self-avoiding walks

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Abstract. Continuum models of percolation and self-avoiding walks are introduced with the property that their series expansions are sums over linear graphs with intrinsic combinatorial weights and explicit dimension dependence.

1. Introduction

The importance of dimensionality in statistical mechanics has motivated the study of a number of systems where the dimensionality D is a freely adjustable parameter. Two examples are the D-dependence of momentum (loop) integrals in field-theoretic models (Leibbrandt 1975) and the series expansions for models defined on a D-dimensional hypercubic lattice where D also appears explicitly (Fisher and Gaunt 1964). This paper introduces models of percolation and self-avoiding walks where series expansions exhibit a D-dependence in yet another way.

The basic idea is to exploit a well known property of gaussian integrals (Kirchhoff 1847). Let $x_1, \ldots, x_n$ be D-dimensional cartesian coordinates of n points and let C be a simple connected graph having n vertices labelled $1, 2, \ldots, n$. If we associate each edge of C with the pair of vertices it connects, then

$$\int d^D x_2 \int d^D x_3 \ldots \int d^D x_n \prod_{\substack{\text{edges} \\ (ij)}} \exp[-(x_i - x_j)^2] = \left(\frac{\pi}{\tau(C)}\right)^{D/2}, \qquad (1)$$

where $\tau(C)$ denotes the number of spanning trees of C. Thus, if a problem can be formulated in the continuum in such a way that the cluster integrals appearing in series expansions are always of the above type, the task is reduced to combinatorics. This strategy has been used previously by Uhlenbeck and Ford (1962) in their study of a gas of particles having the pairwise interaction $-\beta V(r) = \log[1 - \exp(-ar^2)]$.

2. Percolation

Consider the percolation problem defined on a set of N points $x_1, \ldots, x_N$ distributed uniformly at random inside a D-dimensional volume V. Clusters are defined by establishing connections (adjacency) between certain pairs of points. Specifically, points x_i and x_j are connected by an 'edge' with probability $\exp[-a(x_i - x_j)^2]$. Here a plays

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the role of the bond probability and controls the size of clusters when one maintains a fixed density $\rho = N/V$. Equivalently, fixing a and varying ρ reproduces the site-type problem.

Our approach to analysing this model will be to obtain the so-called 'cluster numbers' (Stauffer 1979). A k-cluster is defined to be an edge-connected set of k points having no edge connections with any of the other $N-k$ points. Dividing the average number of k-clusters present in the volume by N gives the cluster numbers $\bar{n}_k(x_1, \ldots, x_N)$. Averaging this quantity over all ensembles of points gives the cluster numbers appropriate to a uniform random distribution of points:

$$n_k = \frac{1}{V^N} \int \mathrm{d}^D x_1 \ldots \int \mathrm{d}^D x_N \bar{n}_k(x_1, \ldots, x_N).$$

We will obtain n_k by considering p_k, the probability that a given point, call it y_1, belongs to a k-cluster (again, averaged over ensembles). The cluster numbers then follow from $n_k = p_k/k$. There are

$$\binom{N-1}{k-1} \tag{2}$$

ways of choosing the other $k-1$ points of the cluster, call them $y_2, \ldots, y_k$. Once chosen, the set of possible k-clusters that can be formed fall into a one–one correspondence with the set of simple connected graphs on k (labelled) vertices, $\mathscr{C}_k$. For a particular graph $C \in \mathscr{C}_k$ with vertices labelled $1, \ldots, k$, one associates the following probability factor with each pair of vertices $1 \leqslant i < j \leqslant k$:

$$P_{ij}(C) = \begin{cases} \exp[-a(y_i - y_j)^2] & \text{if } i \text{ and } j \text{ are adjacent;} \quad (3a) \\ 1 - \exp[-a(y_i - y_j)^2] & \text{otherwise.} \quad (3b) \end{cases}$$

The probability of the cluster configuration is given by the product of these factors multiplied by

$$\prod_{i=1}^{N-k} \prod_{j=1}^{k} \{1 - \exp[-a(z_i - y_j)^2]\} = \prod_{i=1}^{N-k} (1 + f(z_i)),$$

where $z_1, \ldots, z_{N-k}$ are the points not included in the cluster. In the limit $N \to \infty$ with ρ and k fixed, the integrations over the positions $z_1, z_2, \ldots$ can be evaluated in closed form. However, in following the strategy of utilising expressions involving only gaussian integrals, we will be interested in expanding in powers of the density:

$$\frac{1}{V^{N-k}} \int \mathrm{d}^D z_1 \ldots \int \mathrm{d}^D z_{N-k} \prod_{i=1}^{N-k} (1 + f(z_i)) \to \exp\left(\rho \int \mathrm{d}^D z f(z)\right)$$
$$= 1 + \rho \int \mathrm{d}^D z_1 f(z_1) + \frac{\rho^2}{2!} \int \mathrm{d}^D z_1 \int \mathrm{d}^D z_2 f(z_1) f(z_2) + \ldots . \tag{4}$$

When (4) is multiplied by the factors (3), the binomial coefficient (2) (with $N \to \infty$, k fixed) and averaged over the positions $y_1, \ldots, y_k$, one obtains the probability $p_k(C)$ that y_1 belongs to a k-cluster with topology specified by C. Summing $p_k(C)$ over all possible connected graphs $C \in \mathscr{C}_k$ and taking into account the relationship between n_k

and p_k we arrive at the expansion

$$n_k = \frac{\rho^{k-1}}{k!} \sum_{C \in \mathscr{C}_k} \left\{ \sum_{n=0}^{\infty} \frac{\rho^n}{n!} \int \mathrm{d}^D y_2 \ldots \int \mathrm{d}^D y_k \int \mathrm{d}^D z_1 \cdots \int \mathrm{d}^D z_n \prod_{1 \leq i < j \leq k} P_{ij}(C) \prod_{i=1}^{n} f(z_i) \right\} \tag{5}$$

where

$$f(z) = \prod_{i=1}^{k} \{1 - \exp[-a(z - y_i)^2]\} - 1.$$

We see that (5) is a sum of terms of the form (1); the coefficient of

$$\left[\rho\left(\frac{\pi}{a}\right)^{D/2}\right]^{k+n-1} = x^{k+n-1}$$

involving contributions from connected graphs having $k+n$ vertices. With this in mind, we will consider an expansion of the generating function

$$\mathbf{F}(x, y) = \sum_{k=1}^{\infty} y^k n_k(x)$$

organised in the form

$$\mathbf{F}(x, y) = \sum_{m=1}^{\infty} \frac{x^{m-1}}{m!} \left\{ \sum_{C \in \mathscr{C}_m} \left(\frac{1}{\tau(C)}\right)^{D/2} W(C; y) \right\}, \tag{6}$$

where $W(C; y)$ is a polynomial of degree bounded by the number of vertices of C.

We now turn to the problem of evaluating $W(C; y)$ for some graph $C \in \mathscr{C}_{k+n}$. In particular, consider the contributions to the coefficient of y^k. These are due to various graphs $N \in \mathscr{C}_k$ that characterise k-cluster topologies as well as the different ways these graphs might be embedded in C. To be precise, let N be a subgraph of C (written $N \subseteq C$). Denote by $C - N$ the subset of C where all the vertices of N as well as the edges incident to them have been deleted. If $C - N$ is not empty then $C - N$ is a subgraph of C. A subgraph $N \subseteq C$ that corresponds to an acceptable cluster embedding will be called a *nucleus* and has the properties:

(i) N is connected;

(ii) $C - N$ has no edges. (Equivalently: the vertices of N constitute a *covering* of C; i.e. at least one end of every edge of C is a vertex of N.)

The vertices not in the nucleus should be identified with the points $z_1, \ldots, z_n$ outside the cluster, which by (5) are not mutually interconnected by gaussian factors. In (5), the nucleus belongs to a distinguished subset of the $k+n$ vertices of C. If we relax this condition on the embedding we will be overcounting by the factor $\binom{k+n}{n}$. To compensate for this we divide by the same factor in the end.

For a given cluster embedding or nucleus $N \subseteq C$, there are three types of edges e of C. First, if $e \in N$ then e contributes a gaussian factor with a plus sign according to (3*a*). Second, if the endpoints of e belong to N but $e \notin N$ then (3*b*) applies and the gaussian factor comes with a minus sign. Third, if one of the endpoints of e belongs to $C - N$ then the origin of the relevant gaussian was (4) and also carries a minus sign. The parity of the contribution due to a particular nucleus $N \subseteq C$ is thus

$$(-1)^{\varepsilon(C) - \varepsilon(N)},$$

where $\varepsilon(G)$ denotes the number of edges of G.

We can now put together the total contribution of a term in (5) coming from a particular nucleus $N \subseteq C$:

$$\sum_{k=1}^{\infty} y^k n_k = \ldots + \frac{x^{k+n-1} y^k}{k!n!} \frac{1}{\binom{k+n}{n}} (-1)^{\varepsilon(C)-\varepsilon(N)} \left(\frac{1}{\tau(C)}\right)^{D/2} + \ldots$$

$$= \ldots + \frac{x^{k+n-1}}{(k+n)!} \left(\frac{1}{\tau(C)}\right)^{D/2} (-1)^{\varepsilon(C)-\varepsilon(N)} y^k + \ldots .$$

Summing all those terms involving a particular graph C gives the weight polynomial

$$W(C; y) = \sum_{\substack{\text{nuclei} \\ N \subseteq C}} (-1)^{\varepsilon(C)-\varepsilon(N)} y^{\nu(N)}, \tag{7}$$

where $\nu(G)$ denotes the number of vertices of G.

The generating function (6) may also be expressed as a sum over non-isomorphic connected graphs,

$$\mathbf{F}(x, y) = \sum_{\substack{\text{non-isomorphic} \\ C}} \frac{x^{\nu(C)-1}}{\sigma(C)} \left(\frac{1}{\tau(C)}\right)^{D/2} W(C; y),$$

where $\sigma(G)$ is the order of the symmetry group of G. The first few terms of this sum, up to graphs with four vertices, are given in table 1.

We will now prove two theorems involving the weight polynomial $W(C; y)$. These are simple consequences of the following lemma:

Lemma 1. Let C be any non-trivial, simple, connected graph and let v be any vertex of C. Then,

$$\sum_{\substack{\text{nuclei} \\ \{N \subseteq C | v \in N\}}} (-1)^{\varepsilon(N)} = 0, \tag{8}$$

where the summation is over all nuclei containing v. A proof is given in the appendix.

Theorem 1. Let C be a simple connected graph with at least one cut vertex v. Then $W(C; 1) = 0$.

Proof. Let $N \subseteq C$ be a nucleus of C. Suppose $v \notin N$. Then, since N is a nucleus, v is adjacent only to vertices of N. Now N is connected so we conclude that $C - v$ is connected contrary to the statement that v is a cut vertex. Thus $v \in N$ and the statement of the theorem follows immediately from (7) and Lemma 1.

Theorem 2. Let C be a non-trivial, simple, connected graph. Then

$$\mathrm{d}W(C; 1)/\mathrm{d}y = 0.$$

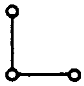
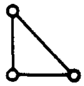
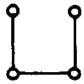
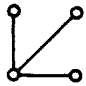
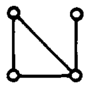
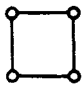
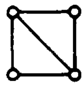
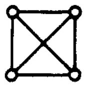
Proof.

$$(-1)^{\varepsilon(C)} \frac{\mathrm{d}}{\mathrm{d}y} W(C; 1) = \sum_{\substack{\text{nuclei} \\ N \subseteq C}} (-1)^{\varepsilon(N)} \nu(N)$$

$$= \sum_{v \in C} \left\{ \sum_{\substack{\text{nuclei} \\ \{N \subseteq C | v \in N\}}} (-1)^{\varepsilon(N)} \right\}$$

$$= 0.$$

Table 1.

C	$\sigma(C)$	$\tau(C)$	$W(C; y)$	$h(C)$
	1	1	y	1
	2	1	y^2-2y	2
	2	1	y^3-2y^2+y	2
	6	3	$-2y^3+3y^2$	6
	2	1	$y^4-2y^3+y^2$	2
	6	1	$y^4-3y^3+3y^2-y$	0
	2	3	$-2y^4+4y^3-2y^2$	4
	8	4	$-3y^4+4y^3$	8
	4	8	$4y^2-6y^3+y^2$	12
	24	16	$-6y^4+8y^3$	24

There is another way of understanding the statement of theorem 2. Let P_{finite} be the probability that a given point in the percolation problem belongs to a finite cluster. Then

$$P_{\text{finite}}(x)=\sum_{k=1}^{\infty} kn_k(x)=\frac{\mathrm{d}}{\mathrm{d}y}\mathbf{F}(x,1)=1,$$

with only the trivial graph contributing to the sum (6). This agrees with our expectation that $P_{\text{finite}}=1$ on the interval $0\leqslant x<x_c$, where x_c is the critical density.

To obtain a non-trivial series we consider the mean cluster size, $\mathbf{S}(x)$, which is unity at $x=0$ and diverges at $x=x_c$:

$$\mathbf{S}(x)=\sum_{k=1}^{\infty} kn_k\Big/\sum_{k=1}^{\infty} n_k$$

$$=\left\{\sum_{\substack{\text{stars}\\ S}}\frac{x^{\nu(S)-1}}{\nu(S)!}\left(\frac{1}{\tau(S)}\right)^{D/2}W(S;1)\right\}^{-1}.$$

Here the weight $W(S; 1)$ is non-zero only for graphs without cut vertices ('stars') by theorem 1. Below are the first few terms:

$$\mathbf{S}(x)^{-1}=1-\tfrac{1}{2}x+\tfrac{1}{6}(\tfrac{1}{3})^{D/2}x^2+[\tfrac{1}{8}(\tfrac{1}{4})^{D/2}-\tfrac{1}{4}(\tfrac{1}{8})^{D/2}+\tfrac{1}{12}(\tfrac{1}{16})^{D/2}]x^3+\ldots.$$

The formal $D=0$ limit of $\mathbf{S}(x)$ is readily evaluated since now the gaussian integrations do not involve $\tau(S)$ but are simply ± 1. A convenient starting point is (5) where we first argue that the summation over connected graphs $C \in \mathscr{C}_k$ collapses to the single term involving the *complete* graph K_k. Any graph with two non-adjacent vertices would have contained a factor $(3b)$ yielding two equal terms of opposite sign upon integration. Counting up the terms produced by the factors $f(z_i)$ we then have,

$$\begin{aligned} n_k &= \frac{x^{k-1}}{k!}\sum_{n=0}^{\infty}\frac{x^n}{n!}\left\{\sum_{i=1}^{k}(-1)^i\binom{k}{i}\right\}^n \\ &= \frac{x^{k-1}}{k!}e^{-x} \qquad\qquad (D=0) \\ \mathbf{S}(x)^{-1} &= (1-\mathrm{e}^{-x})/x. \end{aligned}$$

While $D=0$ is not a physically interesting case, this result does provide a useful check on the coefficients of $\mathbf{S}(x)^{-1}$ for general D.

3. Self-avoiding walks

Let $x_1, \ldots, x_n$ be a sequence of points in D-dimensional space visited by a self-avoiding walk of $n-1$ steps beginning at the point x_1. As in the percolation problem, we would like to express the idea of a 'chain' as well as the 'excluded volume effect' in terms of gaussian factors. This can be done using the following partition function ($n \geqslant 2$):

$$Z_{n-1}=\left(\frac{1}{\pi^{D/2}}\right)^{n-1}\int \mathrm{d}^D x_2 \ldots \int \mathrm{d}^D x_n \times \prod_{i=1}^{n-1}\exp[-(x_i-x_{i+1})^2]\prod_{|i-j|>1}\{1-\exp[-(x_i-x_j)^2]\}. \tag{9}$$

The first product above realises the chain constraint and by itself reproduces the behaviour of the unrestricted walk if one identifies Z_n with the number of walks of length $n-1$. The second product, over all non-consecutive pairs of points, enforces the excluded volume constraint and renders the problem non-trivial.

Observe that every term of (9) has at most one gaussian factor connecting each pair of points. If we imagine writing out the $n!$ copies of (9) generated by all permutations of the labels on the points and dividing by $n!$, the resulting sum in graphical language becomes:

$$Z_{n-1}=\frac{1}{n!}\sum_{C\in\mathscr{C}_n}(-1)^{\varepsilon(C)-n+1}h(C)\left(\frac{1}{\tau(C)}\right)^{D/2}. \tag{10}$$

Here $h(C)$ counts the number of *Hamiltonian paths* in C, i.e. the number of permutations of the vertices $v(1)v(2)\ldots v(n)$ such that $v(i)$ and $v(i+1)$ are adjacent in C for $1 \leqslant i < n$. We can improve upon (10) by using the fact that a general connected graph can be decomposed into a tree of non-trivial stars connected at cut vertices. Moreover, for *Hamiltonian* connected graphs ($h(C)>0$), such a tree must always be a linear chain. Thus, if we define the generating functions

$$\mathbf{G}(x)=\sum_{n=1}^{\infty} Z_n x^n$$

$$\mathbf{z}(x)=\sum_{\substack{\text{non-trivial}\\ \text{stars}\\ S}} \frac{(-1)^{\varepsilon(S)-\nu(S)+1}}{\nu(S)!} h(S)\left(\frac{1}{\tau(S)}\right)^{D/2} x^{\nu(S)-1}$$

then,

$$\mathbf{G}(x)=\sum_{k=1}^{\infty} \mathbf{z}^k=\frac{\mathbf{z}(x)}{1-\mathbf{z}(x)}. \tag{11}$$

To understand (11), consider a particular sequence of non-trivial Hamiltonian stars $S_1, \ldots, S_k$ and choose Hamiltonian paths for each one with beginning and ending vertices $(v_1, u_1), \ldots, (v_k, u_k)$. In order that $C=S_1S_2\ldots S_k$ has a Hamiltonian path beginning at v_1 and ending at u_k the stars must be glued together in a unique way; namely at the cut vertices $u_1=v_2$, $u_2=v_3, \ldots, u_{k-1}=v_k$. Moreover, it is also clear that $\tau(C)=\tau(S_1)\tau(S_2)\ldots\tau(S_k)$ irrespective of the details of the decomposition. Finally, one can check that the counting of vertices and excess edges (minus signs) is correct.

The series $\mathbf{z}(x)$ begins:

$$\mathbf{z}(x)=x-(\tfrac{1}{3})^{D/2}x^2+[-(\tfrac{1}{4})^{D/2}+3(\tfrac{1}{8})^{D/2}-(\tfrac{1}{16})^{D/2}]x^3+\ldots.$$

Values of $h(C)$ have been included in table 1.

We again observe that the formal $D=0$ limit is easily evaluated. Considering (9) with $D=0$ we see that $Z_n=0$ for $n\geqslant 2$. Thus,

$$\mathbf{G}(x)=x \qquad \mathbf{z}(x)=x/(1+x) \qquad (D=0).$$

4. Conclusion

A particularily interesting question concerns the nature of the singularities of the generating functions discussed above as the dimensionality is varied. If we formally set $D=\infty$, the singularities are simple poles:

$$\mathbf{S}(x)=(1-\tfrac{1}{2}x)^{-1} \qquad \mathbf{G}(x)=x/(1-x) \qquad (D=\infty).$$

This result is not unexpected and indeed the dominant singularity is believed to remain a simple pole provided $D>D_c$. The value of the critical dimension depends on the particular problem and it is believed that $D_c=6$ for percolation (Harris *et al* 1975), and $D_c=4$ for self-avoiding walks (de Gennes 1972). Evidence of such a critical dimensionality might be obtained from numerical work with the series expansions for $\mathbf{S}(x)^{-1}$ and $\mathbf{z}(x)$.

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Appendix

Proof of Lemma 1. We will use induction on $\nu(C)$. There is exactly one simple connected graph with two vertices, C_2. If we take v to be either one of the two vertices then the nuclei that contain v are v itself and C_2 giving $1-1=0$ in (8). Now suppose the statement holds for all C with $\nu(C)=2,3,\ldots,n-1$ for some $n\geq 3$. Let C_n be any simple connected graph with $\nu(C_n)=n$ and let $\{v,u\}\in C_n$ be any two vertices connected by an edge $e\in C_n$. The proof will proceed by decomposing $\mathcal{N}_v$, the set of nuclei $N\subseteq C_n$ that contain v. We begin by defining the sets

$$\mathcal{N}_1=\{N\in\mathcal{N}_v|e\notin N \text{ and } u\in N\}$$
$$\mathcal{N}_2=\{N+e|N\in\mathcal{N}_1\}.$$

Clearly, $\mathcal{N}_2\subseteq\mathcal{N}_v$ and moreover, $\mathcal{N}_1\cap\mathcal{N}_2=\varnothing$. Thus,

$$\begin{aligned}\sum_{N\in\mathcal{N}_1\cup\mathcal{N}_2}(-1)^{\varepsilon(N)}&=\sum_{N\in\mathcal{N}_1}(-1)^{\varepsilon(N)}+\sum_{N\in\mathcal{N}_1}(-1)^{\varepsilon(N)+1}\\&=0.\end{aligned}\tag{12}$$

The set of nuclei in the complement, $\mathcal{N}_v-(\mathcal{N}_1\cup\mathcal{N}_2)$, is decomposed further:

$$\mathcal{N}_3=\{N\in\mathcal{N}_v|u\notin N\}$$
$$\mathcal{N}_4=\{N\in\mathcal{N}_v-\mathcal{N}_2|e\in N\}.$$

For $N\in\mathcal{N}_4$, suppose that $N-e$ is a nucleus. Then, $(N-e)+e=N\in\mathcal{N}_2$, a contradiction, so $N-e$ cannot be a nucleus. This requires that $N-e$ consist of two components, $V(N)$ containing v and $U(N)$ containing u. Let $v(N)$ be the vertex set of $V(N)$ and denote by $n(u)$ the set of vertices of C_n adjacent to u.

We are now prepared to perform a decomposition of $\mathcal{N}_4$:

$$\mathcal{N}_5=\{N\in\mathcal{N}_4|n(u)\subseteq v(N)\}.$$

It is clear that for $N\in\mathcal{N}_5$, $U(N)=u$ and u is adjacent only to v in N. By deleting both u and e from these nuclei we have the following set:

$$\mathcal{N}_6=\{N-u-e|N\in\mathcal{N}_5\}.$$

It is easily checked that $\mathcal{N}_6\subseteq\mathcal{N}_3$ and $\mathcal{N}_3\subseteq\mathcal{N}_6$ so that $\mathcal{N}_3=\mathcal{N}_6$. This establishes a one–one correspondence between $\mathcal{N}_3$ and $\mathcal{N}_5$; the nuclei of $\mathcal{N}_5$ having one additional edge. The sum over nuclei $N\in\mathcal{N}_3\cup\mathcal{N}_5$ thus vanishes in the manner of (12).

Finally, we consider the remaining nuclei $N\in\mathcal{N}_4-\mathcal{N}_5$. Define:

$$\mathcal{V}=\{V(N)|N\in\mathcal{N}_4-\mathcal{N}_5\}$$
$$\mathcal{N}_V=\{N\in\mathcal{N}_4-\mathcal{N}_5|V(N)=V\}.$$

For a particular $V\in\mathcal{V}$, it is readily verified that C_n-V breaks up into a set of components $\{w_1,\ldots,w_k,C_u(V)\}$ where $w_1,\ldots,w_k$ are isolated vertices and $C_u(V)$ is a *non-trivial* graph containing u. Moreover, it is also easily checked that the possible $U(N)$ for $N\in\mathcal{N}_V$ are precisely the nuclei of $C_u(V)$ that contain u. Since $v\notin C_u(V)$,

$2 \leqslant \nu(C_u(V)) < n$ and we can apply induction:

$$\sum_{N \in \mathcal{N}_4 - \mathcal{N}_5} (-1)^{\varepsilon(N)} = \sum_{V \in \mathcal{V}} \left\{ \sum_{N \in \mathcal{N}_V} (-1)^{\varepsilon(N)} \right\}$$

$$= \sum_{V \in \mathcal{V}} (-1)^{\varepsilon(V)+1} \left\{ \sum_{\substack{\text{nuclei} \\ \{N \subseteq C_u(V) | u \in N\}}} (-1)^{\varepsilon(N)} \right\}$$

$$= 0.$$

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