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GAUSSIAN-CLUSTER MODELS OF PERCOLATION AND SELF-AVOIDING WALKS

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October 1983

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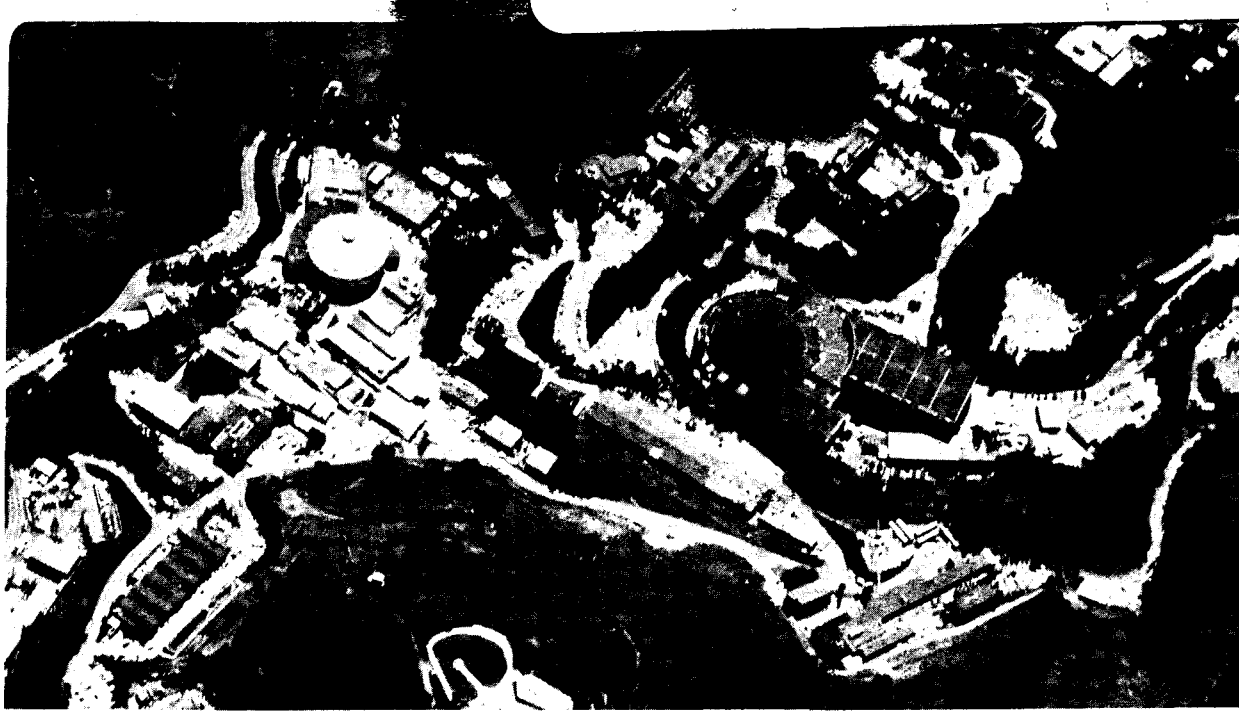

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# GAUSSIAN-CLUSTER MODELS OF PERCOLATION AND SELF-AVOIDING WALKS*

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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.

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## 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[1] and the series expansions for models defined on a $D$-dimensional hypercubic lattice where $D$ also appears explicitly[2]. 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[3]. 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 labeled $1, 2, \ldots, n$. If we associate each edge of $C$ with the pair of vertices it connects, then

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

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 Ford and Uhlenbeck[4] in their study of a gas of particles having the pairwise interaction $-\beta V(r) = \log(1 - \exp(-ar^2))$.

## 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 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 $\rho$ reproduces the site-type problem.

Our approach to analyzing this model will be to obtain the so-called "cluster numbers"[5]. 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 $\overline{n}_k(x_1, \ldots, x_N)$. Averaging this quantity over all ensembles of points gives the cluster numbers appropriate to a uniform, random distribution of points:

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

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 $k$ (labeled) vertices, $\mathcal{C}_k$. For a particular graph $C \in \mathcal{C}_k$ with vertices labeled



$1, \ldots, k$, one associates the following probability factor with each pair of vertices $1 \le i < j \le k$:

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

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 $\rho$ 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 utilizing expressions involving only gaussian integrals, we will be interested in expanding in powers of the density:

$$\frac{1}{V^{N-k}} \int d^D z_1 \cdots \int d^D z_{N-k} \prod_{i=1}^{N-k} (1 + f(z_i)) \to \exp\left(\rho \int d^D z \, f(z)\right)$$

$$= 1 + \rho \int d^D z_1 \, f(z_1) + \frac{\rho^2}{2!} \int d^D z_1 \int d^D z_2 \, f(z_1) f(z_2) + \cdots \tag{4}$$

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 $C \in \mathcal{C}_k$ and taking into account the relationship between $n_k$ and $p_k$ we arrive at

the expansion

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

where,

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

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

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

organized in the form

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

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

(*i*) $B$ is connected;

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

The vertices not in the backbone 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 backbone 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 backbone $B \subseteq C$, there are three types of edges $e$ of $C$. First, if $e \in B$ then $e$ contributes a gaussian factor with a plus sign according to (3a). Second, if the endpoints of $e$ belong to $B$ but $e \notin B$ then (3b) applies and the gaussian factor comes with a minus sign. Third, if one of the endpoints of $e$ belongs to $C - B$ then the origin of the relevant gaussian was (4) and also carries a minus sign. The parity of the contribution due to a particular backbone $B \subseteq C$ is thus

$$(-1)^{\epsilon(C) - \epsilon(B)} ,$$

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

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

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

$$= \cdots + \frac{x^{k+n-1}}{(k+n)!} \left(\frac{1}{\tau(C)}\right)^{D/2} (-1)^{\epsilon(C)-\epsilon(B)} y^k + \cdots$$

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

$$W(C;y) = \sum_{\substack{backbones \\ B \subseteq C}} (-1)^{\epsilon(C)-\epsilon(B)} y^{\nu(B)}\,, \tag{7}$$

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

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

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

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 nontrivial, simple, connected graph and let $v$ be any vertex of $C$. Then,

$$\sum_{\substack{backbones \\ \{B \subseteq C \mid v \in B\}}} (-1)^{\epsilon(B)} = 0\,, \tag{8}$$



where the summation is over all backbones 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 $B \subseteq C$ be a backbone of $C$. Suppose $v \notin B$. Then, since $B$ is a backbone $v$ is adjacent only to vertices of $B$. Now $B$ is connected so we conclude that $C - v$ is connected contrary to the statement that $v$ is a cut vertex. Thus $v \in B$ and the statement of the theorem follows immediately from (7) and Lemma 1. ∎

*Theorem 2.* Let $C$ be a nontrivial, simple, connected graph. Then

$$\frac{d}{dy} W(C;1) = 0\,.$$

*Proof.*

$$(-1)^{\epsilon(C)} \frac{d}{dy} W(C;1) = \sum_{\substack{backbones \\ B \subseteq C}} (-1)^{\epsilon(B)}\, \nu(B)$$

$$= \sum_{v \in C} \left\{ \sum_{\substack{backbones \\ \{B \subseteq C \mid v \in B\}}} (-1)^{\epsilon(B)} \right\}$$

$$= 0$$

∎

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

$$P_{finite}(x) = \sum_{k=1}^{\infty} k n_k(x)$$
$$= \frac{d}{dy}\mathsf{F}(x,1)$$
$$= 1\,,$$

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

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

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

Here the weight $W(S;1)$ is nonzero only for graphs without cut vertices ("stars") by Theorem 1. Below are the first few terms:

$$\mathsf{S}(x)^{-1} = 1 - \frac{1}{2}x + \frac{1}{6}\left(\frac{1}{3}\right)^{D/2} x^2 + \left[\frac{1}{8}\left(\frac{1}{4}\right)^{D/2} - \frac{1}{4}\left(\frac{1}{8}\right)^{D/2} + \frac{1}{12}\left(\frac{1}{16}\right)^{D/2}\right] x^3 + \cdots$$

The formal $D = 0$ limit of $\mathsf{S}(x)$ is readily evaluated since now the gaussian integrations do not involve $\tau(S)$ but are simply $\pm 1$. A



convenient starting point is (5) where we first argue that the summation over connected graphs $C \in \mathcal{C}_k$ collapses to the single term involving the *complete* graph $K_k$. Any graph with two nonadjacent 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,

$$n_k = \frac{x^{k-1}}{k!} \sum_{n=0}^{\infty} \frac{x^n}{n!} \left\{ \sum_{i=1}^{k} (-1)^i \binom{k}{i} \right\}^n$$
$$= \frac{x^{k-1}}{k!} e^{-x} \qquad (D = 0)$$
$$\mathsf{S}(x)^{-1} = \frac{1 - e^{-x}}{x}\,.$$

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

**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 ($n \ge 2$):

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

The first product above realizes the chain constraint and by itself reproduces the behavior of the unrestricted walk if one identifies $Z_n$ with the num-

ber of walks of length $n-1$. The second product, over all nonconsecutive pairs of points, enforces the excluded volume constraint and renders the problem nontrivial.

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:

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

Here $h(C)$ counts the number of *hamiltonian paths* in $C$, *i.e.* the number of permutations of the vertices $v(1)v(2)\cdots v(n)$ such that $v(i)$ and $v(i+1)$ are adjacent in $C$ for $1 \leq i < n$. We can improve upon (10) by using the fact that a general connected graph can be decomposed into a tree of nontrivial 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

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

$$\mathsf{z}(x) = \sum_{\substack{nontrivial \\ stars \\ S}} \frac{(-1)^{\epsilon(S)-\nu(S)+1}}{\nu(S)!} h(S) \left(\frac{1}{\tau(S)}\right)^{D/2} x^{\nu(S)-1}$$

then,

$$\begin{aligned} \mathsf{G}(x) &= \sum_{k=1}^{\infty} \mathsf{z}^k \\ &= \frac{\mathsf{z}(x)}{1-\mathsf{z}(x)} . \end{aligned} \tag{11}$$



To understand (11), consider a particular sequence of nontrivial 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 $C = S_1 S_2 \cdots S_k$ 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 $\tau(C) = \tau(S_1)\tau(S_2)\cdots\tau(S_k)$ 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 $\mathsf{z}(x)$ begins:

$$\mathsf{z}(x) = x - \left(\frac{1}{3}\right)^{D/2} x^2 + \left[-\left(\frac{1}{4}\right)^{D/2} + 3\left(\frac{1}{8}\right)^{D/2} - \left(\frac{1}{16}\right)^{D/2}\right] x^3 + \cdots$$

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 $n \geq 2$. Thus,

$$\begin{aligned} \mathsf{G}(x) &= x \\ \mathsf{z}(x) &= \frac{x}{1+x} . \end{aligned} \qquad (D = 0)$$

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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 backbones 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 $\mathcal{B}_v$, the set of backbones $B\subseteq C_n$ that contain $v$. We begin by defining the sets

$$\mathcal{B}_1=\{B\in\mathcal{B}_v \mid e\notin B \text{ and } u\in B\}$$
$$\mathcal{B}_2=\{B+e \mid B\in\mathcal{B}_1\}\,.$$

Clearly, $\mathcal{B}_2\subseteq\mathcal{B}_v$ and moreover, $\mathcal{B}_1\bigcap\mathcal{B}_2=\emptyset$. Thus,

$$\sum_{B\in\mathcal{B}_1\bigcup\mathcal{B}_2}(-1)^{\epsilon(B)}=\sum_{B\in\mathcal{B}_1}(-1)^{\epsilon(B)}+\sum_{B\in\mathcal{B}_1}(-1)^{\epsilon(B)+1} \tag{12}$$
$$=0\,.$$

The set of backbones in the complement, $\mathcal{B}_v-(\mathcal{B}_1\bigcup\mathcal{B}_2)$, is decomposed further:

$$\mathcal{B}_3=\{B\in\mathcal{B}_v \mid u\notin B\}$$
$$\mathcal{B}_4=\{B\in\mathcal{B}_v-\mathcal{B}_2 \mid e\in B\}$$



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

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

$$\mathcal{B}_5=\{B\in\mathcal{B}_4 \mid n(u)\subseteq v(B)\}$$

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

$$\mathcal{B}_6=\{B-u-e \mid B\in\mathcal{B}_5\}$$

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

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

$$\mathcal{V}=\{V(B) \mid B\in\mathcal{B}_4-\mathcal{B}_5\}$$
$$\mathcal{B}_V=\{B\in\mathcal{B}_4-\mathcal{B}_5 \mid V(B)=V\}$$

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 *nontrivial* graph containing $u$. Moreover, it is also easily checked that the possible $U(B)$ for $B\in\mathcal{B}_V$ are precisely the backbones of $C_u(V)$ that contain $u$. Since $v\notin C_u(V)$, $2\leq\nu(C_u(V))<n$

and we can apply induction:

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

$$= \sum_{V \in \mathcal{V}} (-1)^{\epsilon(V)+1} \left\{ \sum_{\substack{backbones \\ \{B \subseteq C_u(V) \mid u \in B\}}} (-1)^{\epsilon(B)} \right\}$$

$$= 0$$

∎



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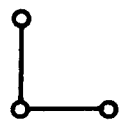
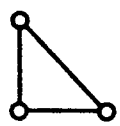
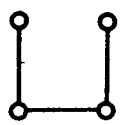
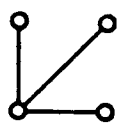
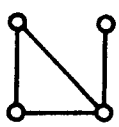
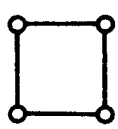
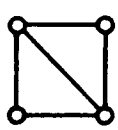
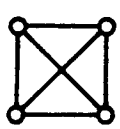
| $C$ | $\sigma(C)$ | $\tau(C)$ | $W(C;y)$ | $h(C)$ |
|---|---|---|---|---|
| | 1 | 1 | $y$ | 1 |
| | 2 | 1 | $y^2 - 2y$ | 2 |
|  | 2 | 1 | $y^3 - 2y^2 + y$ | 2 |
|  | 6 | 3 | $-2y^3 + 3y^2$ | 6 |
|  | 2 | 1 | $y^4 - 2y^3 + y^2$ | 2 |
|  | 6 | 1 | $y^4 - 3y^3 + 3y^2 - y$ | 0 |
|  | 2 | 3 | $-2y^4 + 4y^3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

Table 1

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