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Möbius Function for the Set of Acyclic Directed Backbone Graphs

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Consider a two-rooted graph G, the edges of which are directed in such a way that there are no cycles and every edge belongs to some self-avoiding walk from root u to root v which follows the direction of the edges. A u–v backbone of G is a subgraph formed by taking the union of any subset of directed self-avoiding walks from u to v. Let $\mathscr{B}_{uv}$ be the set of all such backbones of G partially ordered by set-inclusion. We prove the conjecture of Bhatti and Essam that the Möbius function of this set is given, for acyclic $b, b' \in \mathscr{B}_{uv}$ with $b \leqslant b'$, by $\mu(b, b') = (-1)^{c'-c}$, where c and c' are the respective cycle ranks of b and b'. The significance of this result in percolation theory is reviewed together with previous results for other sets of subgraphs.

KEY WORDS: Möbius function; backbone graphs.

1. INTRODUCTION

Bond percolation was introduced by Broadbent and Hammersley[1] in terms of a model of fluid flowing through a porous medium. They considered a crystal lattice in which each bond had probability p of being open to the flow of fluid independently of all other bonds and noted that there was a threshold p_c above which fluid introduced at a given site had a positive probability of wetting an infinite number of sites. Soon afterwards Domb[2] drew attention to a similar phenomenon in random A–B mixtures, where p is now the probability that a site is of type A. He pointed out that infinite clusters of the A species occur above a threshold probability p_c, and Domb and Sykes[3] showed how p_c could be estimated

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for several different lattices by deriving an expansion of the mean cluster size in powers of p.

More recently, there has been considerable interest in electrical conduction in random resistor networks in which the open bonds of the Broadbent–Hammersley model are replaced by Ohmic resistors. In particular, Fisch and Harris[(4)] obtained power series expansions for an average of the point-to-point resistance in such a medium.

In considering the passage of current between two electrodes, the only resistors which are of interest are those which lie on some conducting walk connecting the electrodes. The union of all such walks has become known as the *backbone* relative to those electrodes.[(5)] In different applications, properties of the backbone other than its resistance are of interest. For example, in a dilute Ising ferromagnet the number of nodal bonds is important in determining the behavior of the low-temperature correlation function near the percolation threshold.[(6)] In electrical terms a nodal bond is one which carries the whole current flowing between the electrodes.

Many other applications are described in a paper by Bhatti and Essam,[(7)] where the use of Möbius functions for deriving power series expansions is described (see also Domb[(8)]). In the original calculation of Domb and Sykes,[(3)] a technique known as the perimeter method was used. Although this method could be applied to the calculation of backbone properties, it requires consideration of all possible clusters connecting the electrodes and it is more efficient to avoid clusters with "dangling bonds" (i.e., bonds which carry no current). The penalty for this is that the probabilities associated with the backbone clusters are less easy to obtain, and hence the need for the Möbius function.

If a directed percolation model is considered in which the resistors are replaced by diodes, then there is a simple formula for the Möbius function. This formula was conjectured by Bhatti and Essam[(7)] and it is the purpose of this paper to supply the missing proof.

In Section 2, several sets of different types of subgraphs of a graph are defined and previous results for their Möbius functions are summarized. The derivation of the Möbius function for the set of acyclic directed backbone subgraphs is given in Section 3, and in Section 4 we place our results in the context of percolation theory.

2. MÖBIUS FUNCTIONS FOR PARTIALLY ORDERED SETS OF SUBGRAPHS

2.1. General Definition of Möbius Function

The use of Möbius functions in combinatorial theory is described in a fundamental paper of Rota,[(9)] where a number of general theorems may be found. Applications to statistical mechanics are given in a review by Domb.[8]

Let $\mathscr{P}$ be a partially ordered set and for p, $p' \in \mathscr{P}$ define the zeta function $\zeta_{\mathscr{P}}$ as

$$\zeta_{\mathscr{P}}(p, p') = \begin{cases} 1, & p \leqslant p' \\ 0, & p \nleqslant p' \end{cases} \tag{2.1}$$

The Möbius function $\mu_{\mathscr{P}}$ of $\mathscr{P}$ is defined to be the inverse of the zeta function, i.e.,

$$\sum_{p'' \in \mathscr{P}} \mu_{\mathscr{P}}(p, p')\, \zeta_{\mathscr{P}}(p'', p') = \delta(p, p') \tag{2.2}$$

where δ is a unit matrix. The elements of μ may be calculated recursively by

$$\mu_{\mathscr{P}}(p, p') = \begin{cases} 1, & p = p' \\ -\displaystyle\sum_{p \leqslant p'' < p'} \mu_{\mathscr{P}}(p, p''), & p < p' \\ 0, & \text{otherwise} \end{cases} \tag{2.3}$$

or alternatively,

$$\mu_{\mathscr{P}}(p, p') = \begin{cases} 1, & p = p' \\ -\displaystyle\sum_{p < p'' \leqslant p'} \mu_{\mathscr{P}}(p'', p'), & p < p' \\ 0, & \text{otherwise} \end{cases} \tag{2.4}$$

The subset of $\mathscr{P}$ whose elements are between p and p' will be known as the segment $[p, p']$, i.e.,

$$[p, p'] = \{p'' \in \mathscr{P} \mid p \leqslant p'' \leqslant p'\} \tag{2.5}$$

Notice that, from the definition of $\mu_{\mathscr{P}}$,

$$\sum_{p'' \in [p, p']} \mu_{\mathscr{P}}(p'', p') = \sum_{p'' \in [p, p']} \mu_{\mathscr{P}}(p, p'') = 0 \tag{2.6}$$

and $\mu_{\mathscr{P}}(p, p')$ depends only on the structure of the segment $[p, p']$.

Let $f(p)$ be a function defined on the elements of $\mathscr{P}$, and let

$$g(p) = \sum_{p' \geqslant p} f(p') = \sum_{p' \in \mathscr{P}} \zeta_{\mathscr{P}}(p, p')\, f(p') \tag{2.7}$$

Then solving for the function f gives

$$f(p) = \sum_{p' \in \mathscr{P}} \mu_{\mathscr{P}}(p, p')\, g(p') \tag{2.8}$$

The segment $[p, p']$ is itself a partially ordered set and its Möbius function is just the restriction of $\mu_{\mathscr{P}}$ to this segment.

2.2. Partially Ordered Sets of Subgraphs

Let $G = (V, E)$ be the graph with vertex set V and edge set E or arc set A when the edges are directed to form arcs. We consider the following sets of subgraphs of G which are considered to be partially ordered by containment, i.e., if g and g' are two subgraphs, then $g \leqslant g'$ if $g \subseteq g'$. If there is no element $\varnothing$ of the set such that $\varnothing < g$ for all g, then such an element is added to the specified set. This element will be known as the null graph. The following definitions are given for undirected graphs, with the additions required for directed graphs in parentheses:

$\mathscr{H} = \{h' = (V', E') \mid V' \subseteq V, E' \subseteq E(V')\}$ [$E(V')$ is the set of edges in G adjacent to V'] is the set of all subgraphs of the graph $G = (V, E)$ including the null graph $\varnothing$.

$\mathscr{H}_{uv}$ is the set of elements of $\mathscr{H}$ for which there is a (directed) walk from u to v, where u and v are two distinct root vertices (such a walk will be called a u–v walk) together with the null graph $\varnothing$.

$\mathscr{C}$ is the set of all elements of $\mathscr{H}$ which are connected, i.e., the subgraph has a walk between every pair of vertices (ignoring orientations) together with the null graph.

$\mathscr{C}_u$ is the subset of graphs in $\mathscr{C}$ which contain the vertex u (and have a directed walk from u to every other vertex of the subgraph) together with the null graph.

$\mathscr{C}_{uv}$ is the subset of $\mathscr{C}_u$ containing the second root vertex v together with the null graph.

$\mathscr{B}_{uv}$ is the set of all u–v backbones (i.e., those $c \in \mathscr{C}_{uv}$ such that every edge of c is on some u–v (directed) walk) together with the null graph. The graph c is said to be coverable.

These sets satisfy:

(P1) Closure under union of their elements.

(P2) $\mathscr{B}_{uv} \subseteq \mathscr{C}_{uv} \subseteq \mathscr{H}_{uv} \subseteq \mathscr{H}$.

(P3) $\mathscr{C}_{uv} \subseteq \mathscr{C}_u \subseteq \mathscr{C} \subseteq \mathscr{H}$ (cf. Fig. 1 for an example of the property $\mathscr{C}_{uv} \subseteq \mathscr{C}_u \subseteq \mathscr{C}$).

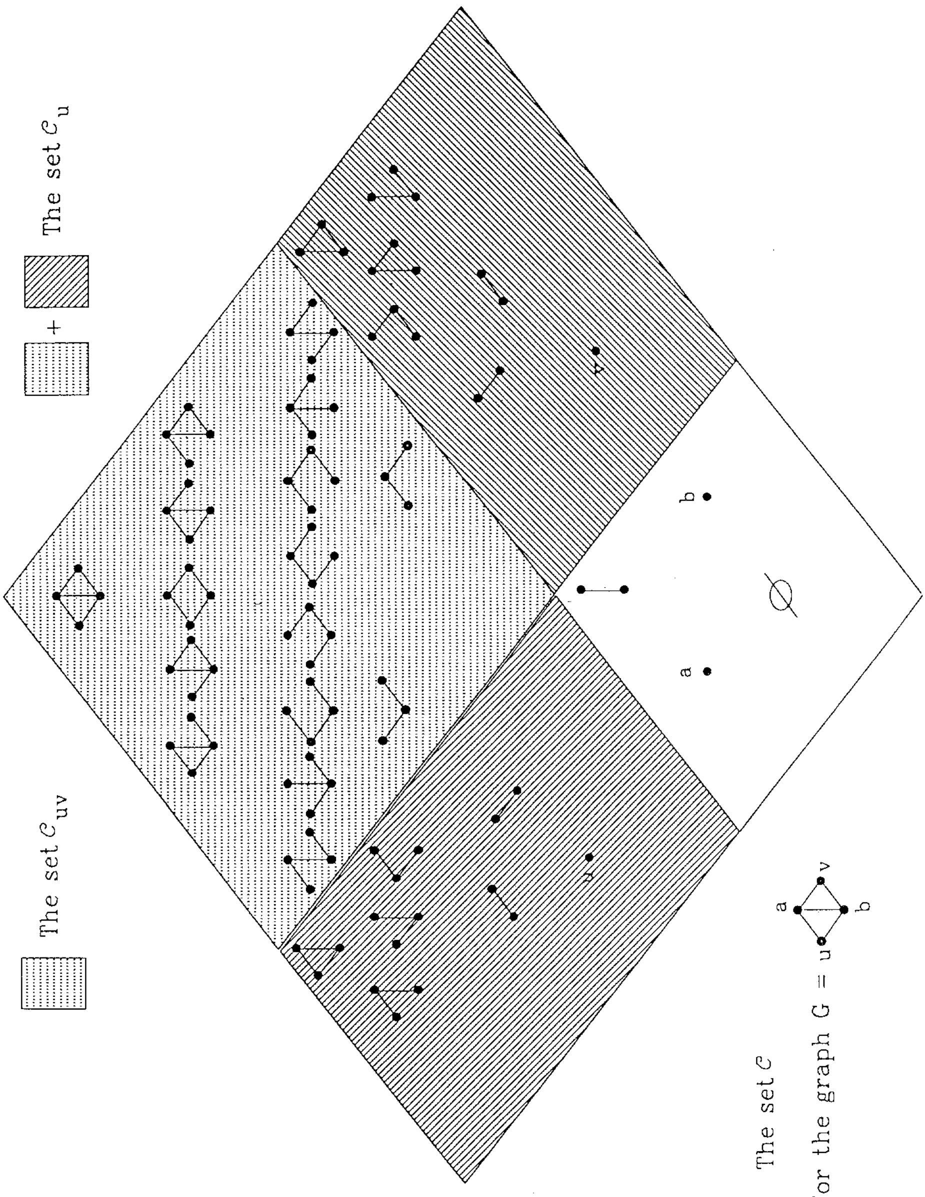

Fig. 1. An example of the subsets $\mathscr{C}_{uv}$ and $\mathscr{C}_u$ of the set of connected graphs $\mathscr{C}$.

(P4) If $\mathscr{G}$ is any of these sets, with Möbius function $\mu_{\mathscr{G}}$, then $\mu_{\mathscr{G}}(g, g')$ depends only on the segment $[g, g']$ of graphs of type $\mathscr{G}$.

(P5) If

$c, c' \in \mathscr{C}_{uv} \backslash \varnothing$, $c \leqslant c'$, the segments $[c, c']$ of $\mathscr{C}_{uv}$, $\mathscr{C}_u$, and $\mathscr{C}$ are equal

$c, c' \in \mathscr{C}_u \backslash \varnothing$, $c \leqslant c'$, the segments $[c, c']$ of $\mathscr{C}_u$ and $\mathscr{C}$ are equal

$h, h' \in \mathscr{H}_{uv} \backslash \varnothing$, $h \leqslant h'$, the segments $[h, h']$ of $\mathscr{H}_{uv}$ and $\mathscr{H}$ are equal

Hence any property derived for segments of $\mathscr{C}$ will be inherited by corresponding segments of $\mathscr{C}_u$ and $\mathscr{C}_{uv}$. The same property holds for $\mathscr{H}$ and $\mathscr{H}_{uv}$. The hereditary property cannot be extended from $\mathscr{H}$ to $\mathscr{C}$, since type $\mathscr{H}$ supergraphs of connected graphs are not necessarily connected.

2.3. The Möbius Functions of $\mathscr{H}$ and $\mathscr{C}$

In this section we recall and extend some previous results.

(a) The simplest Möbius function to derive is that for the segment $[(V, \varnothing), G] \subseteq \mathscr{H}$.

Lemma 2.1. For $h, h' \in [(V, \varnothing), G]$,

$$\mu_{\mathscr{H}}(h, h') = (-1)^{|E' \backslash E|} \qquad \text{when} \quad h' \geqslant h$$

Proof. The segment is isomorphic with the set of all subsets of the edge set E of the graph G. This is the Boolean case and the Möbius function is given in Rota.[9]

The following alternative proof parallels the proof of our main result in Section 3 (namely, the Möbius function for $\mathscr{B}_{uv}$ when G is directed and acyclic), and the method is presented in this simpler context as an introduction. We note first that the intervals $[h, h']$ and $[\varnothing, h' \backslash h]$, where $h' \backslash h$ is the subgraph of G with edge set $E' \backslash E$ and vertex set V, are related by an order-preserving bijection. Thus,

$$\mu_{\mathscr{H}}(h, h') = \mu_{\mathscr{H}}(\varnothing, h' \backslash h) \tag{2.9}$$

and it is sufficient to prove that

$$\mu_{\mathscr{H}}(\varnothing, h') = (-1)^{|E'|} \tag{2.10}$$

Now $[\varnothing, h']$ consists of all subgraphs of h' and if e is an edge of h', we may partition the defining sum (2.6) for $\mu_{\mathscr{H}}$ according as the edge e does or does not occur in h'; thus,

$$\sum_{h \in [\varnothing, h'] : e \in h} (\mu_{\mathscr{H}}(\varnothing, h) + \mu_{\mathscr{H}}(\varnothing, h_\delta)) = 0 \tag{2.11}$$

where h_δ is the graph h with the edge e deleted. We can now prove by induction on $|E'|$ that

$$\mu_{\mathscr{H}}(\varnothing, h') = -\mu_{\mathscr{H}}(\varnothing, h'_\delta) \tag{2.12}$$

Thus, if $|E'| = 1$, there is only one term in the sum and the result follows. On assuming the result for $|E| < |E'|$, we deduce that terms in (2.11) are zero except for $h = h'$, which is the only term with $|E| = |E'|$, and hence, by induction, (2.12) follows. Equation (2.10) follows from (2.12) again by induction on the order of the set $|E'|$ when we note that h'_δ has one edge less than h'. ∎

By P5, the same result is valid for $\mathscr{H}_{uv} \backslash \varnothing$ and we may use (2.4) to express $\mu_{\mathscr{H}_{uv}}(\varnothing, h')$ as the following sum:

$$\mu_{\mathscr{H}_{uv}}(\varnothing, h') = -\sum_{\varnothing < h \leqslant h'} (-1)^{|E' \backslash E|} \tag{2.13}$$

Lemma 2.1 can be extended to the whole of $\mathscr{H}$.

Lemma 2.2. For $h \in \mathscr{H}$, define the edge set $E^+ = E(V(h))$ and the subgraph $h^+ = (E^+, V) \subseteq G$. Then

$$\mu_{\mathscr{H}}(h, h') = \begin{cases} (-1)^{|E' \backslash E(h)|} (-1)^{|V \backslash V(h)|}, & h' \in [h, h^+] \\ 0, & \text{otherwise} \end{cases} \tag{2.14}$$

We are also able to show that $\mu_{\mathscr{H}_{uv}}(\varnothing, h') = 0$ unless $h' \in \mathscr{B}_{uv}$.

Lemma 2.3. Given $h' \in \mathscr{H}_{uv} \backslash \varnothing$,

$$\mu_{\mathscr{H}_{uv}}(\varnothing, h') = 0 \tag{2.15}$$

when $h' \in \mathscr{H}_{uv} \backslash \mathscr{B}_{uv}$, and

$$\mu_{\mathscr{H}_{uv}}(\varnothing, h') = \mu_{\mathscr{B}_{uv}}(\varnothing, h') \tag{2.16}$$

which is given by (2.15), for $h' \in \mathscr{B}_{uv}$.

Proof. For $h' \in \mathscr{H}_{uv} \backslash \mathscr{B}_{uv}$, define b_0 to be the maximal backbone subgraph of h' (b_0 is precisely the backbone formed from the union of all

u–v self-avoiding walks in h'). Define $S(h') = \{h: h < h' \text{ and } h \nleq b_0\}$. Then $S(h') \subset \mathscr{H}_{uv} \setminus \mathscr{B}_{uv}$ and using (2.6),

$$\begin{aligned} \mu_{\mathscr{H}_{uv}}(\varnothing, h') &= - \sum_{\varnothing \leqslant h < h'} \mu_{\mathscr{H}_{uv}}(\varnothing, h) \\ &= - \sum_{\varnothing \leqslant h \leqslant b_0} \mu_{\mathscr{H}_{uv}}(\varnothing, h) - \sum_{h \in S(h')} \mu_{\mathscr{H}_{uv}}(\varnothing, h) \\ &= 0 - \sum_{h \in S(h')} \mu_{\mathscr{H}_{uv}}(\varnothing, h) \end{aligned} \tag{2.17}$$

Assume that for all u–v connected and nonbackbone $h < h'$, $\mu_{\mathscr{H}_{uv}}(\varnothing, h) = 0$; then from (2.18) we deduce $\mu_{\mathscr{H}_{uv}}(\varnothing, h') = 0$. Hence Eq. (2.15) follows from (2.17) by induction, the minimal case of a nonbackbone, u–v connected graph is given by an arc set consisting of a single walk and an extra arc. The various possibilities are illustrated in Fig. 2 and all satisfy the hypothesis of $\mu_{\mathscr{H}_{uv}}(\varnothing, h') = 0$.

Equation (2.16) can be obtained inductively by using the recursive property (2.3) of Möbius functions together with Eq. (2.15). ▮

(b) We now turn to the sets of connected subgraphs $\mathscr{C}$, $\mathscr{C}_u$, and $\mathscr{C}_{uv}$. Denote by c a typical connected graph. The edge perimeter $\pi_G(c)$ is the set

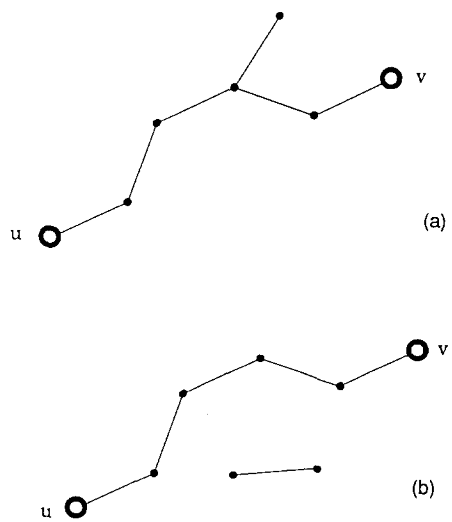

Fig. 2. The two cases of minimal nonbackbone u–v connected graphs considered in Lemma 2.1. In the directed case (a) the dangling bond is oriented into or away from the u–v walk.

of edges of G which do not belong to c, but which have at least one (initial) vertex in c.

Let c^+ be the connected graph having edge set $E(c) \cup \pi_G(c)$ together with all incident vertices. By construction, c^+ belongs to the same set as c. In the case of $\mathscr{C}$ it was shown by Essam *et al.*[10] that for $c \neq \varnothing$,

$$\mu_{\mathscr{C}}(c, c') = \begin{cases} (-1)^{|E' \setminus E(c)|} & \text{for} \quad c' \in [c, c^+] \\ 0 & \text{otherwise} \end{cases} \tag{2.18}$$

and for $c = \varnothing$, from the general formula (2.3)

$$\begin{aligned} \mu_{\mathscr{C}}(\varnothing, c') &= - \sum_{\varnothing < c \leqslant c'} \mu_{\mathscr{C}}(c, c') \\ &= - \sum_{c \in \mathscr{C};\, c' \in [c, c^+]} (-1)^{|E' \setminus E(c)|} \end{aligned} \tag{2.19}$$

If $c' \in [c, c^+]$, then c is said to be a nucleus of c', i.e., $c \in N(c')$. With this notation

$$\mu_{\mathscr{C}}(\varnothing, c') = - \sum_{c \in N(c')} (-1)^{|E' \setminus E(c)|} \tag{2.20}$$

Equations (2.18) and (2.20) hold for $\mathscr{C}_u$ and $\mathscr{C}_{uv}$ by property P5. Finally, we note that Lemma 2.3 is also true when $\mathscr{H}_{uv}$ is replaced by $\mathscr{C}_{uv}$. The argument follows in exactly the same way and hence (2.20) implies

$$\mu_{\mathscr{B}_{uv}}(\varnothing, b') = - \sum_{b \in N(b')} (-1)^{|E' \setminus E(b)|} \quad \blacksquare \tag{2.21}$$

3. THE MÖBIUS FUNCTION FOR ACYCLIC DIRECTED BACKBONE GRAPHS

In this section $\mathscr{B}_{uv}$ refers to acyclic directed backbone subgraphs for the 2-rooted acyclic directed graph G. First we show how the segment $[b_0, b] \subseteq \mathscr{B}_{uv}$ is associated with the complete partially ordered set of backbones $\mathscr{P}$ of a 2-rooted graph derived from the difference of the arc sets $A(b) \setminus A(b_0)$. The discussion then reduces to considering the Möbius function $\mu_{\mathscr{B}}$ for $[\varnothing, b]$, $b \in \mathscr{B}_{uv}$. This result is derived directly and also as a consequence of a deletion-contraction rule obtained by an application of a theorem of Rota.[9] Undirected backbones are also considered.

3.1. Derivation of the Möbius Function

The first step in deriving the value of $\mu_{\mathscr{B}_{uv}}(b_0, b)$ on $\mathscr{B}_{uv}$ is to show that the segment $[b_0, b]$ of $\mathscr{B}_{uv}$ corresponds to the partially ordered set of backbones of some associated "rooted difference" graph.

Define the difference graph $b^D = b \backslash b_0$ to consist of the arc set $A(b) \backslash A(b_0)$ together with its adjacent vertices in b. We now describe a unique construction which obtains a coverable 2-rooted graph $(b \backslash b_0)_R$, with roots u and v, from the graph b^D. Boundary vertices are the vertices of b^D, other than u and v, which also belong to b_0 (see, for example, $w_1,..., w_5$ in Fig. 3). The graph b is then modified at the boundary vertex w as follows:

(a) If the vertex w has an inset of arcs I in b^D, then disconnect the inset I from w and introduce a new vertex w_I for the set I together with a new arc oriented from w_I to the root v (see Fig. 3).

(b) If the vertex w has an outset of arcs O in b^D, then disconnect the outset O from w and introduce another new vertex w_O for the set O together with a new arc oriented from u to w_O (see Fig. 3).

If this procedure is carried out at each of the boundary vertices, we obtain a graph of the same cycle rank as b which consists of two parallel graphs relative to the root points u and v, one of which is the subgraph b_0 and the other is defined to be the *rooted difference graph* $(b \backslash b_0)_R$ (see Fig. 3).

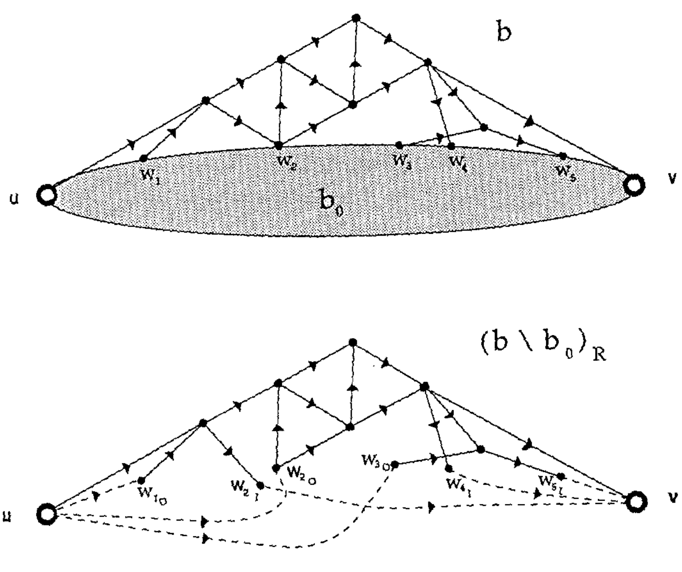

Fig. 3. An example of the construction of the derived 2-rooted graph $(b \backslash b_0)_R$ from a backbone b containing the graph b_0. The arcs of b_0 are removed and the boundary vertices $w_1 \cdots w_5$ are split, if necessary, and connected to the roots u and v.

Lemma 3.1. The cycle rank of the graph $(b\backslash b_0)_R$ is given by $c(b)-c(b_0)-1$.

Proof. In both of the cases (a) and (b) described above, the surgery for each boundary vertex has involved the addition of precisely one arc and one vertex and hence the cycle rank $c(b)=A(b)-V(b)+1$ of the graph b is not changed in either case. A simple cycle count for a parallel graph b formed from the subgraphs b', b'' satisfies $c(b)=c(b')+c(b'')+1$. Therefore the graph obtained from the above construction satisfies

$$c((b\backslash b_0)_R)=c(b)-c(b_0)-1 \quad \blacksquare \tag{3.1}$$

Lemma 3.2. There is an order-preserving bijection between the segment $[b_0, b]$ of $\mathscr{B}_{uv}$ and the partially ordered set $\mathscr{P}$ of the backbones of the graph $(b\backslash b_0)_R$.

Proof. Consider two subgraphs $b', b'' \in [b_0, b]$ such that $b_0 < b' < b''$. The mapping between $[b_0, b]$ and $\mathscr{P}$ which we consider is given by $b' \to (b'\backslash b_0)_R$ for $b' \neq b_0$ and $b_0 \to \varnothing$. Then the arc sets satisfy $A(b')\backslash A(b_0) \subset A(b'')\backslash A(b_0)$ and the boundary vertices for b' are a subset of those of b'' relative to the same graph b_0. Thus, the set of arcs between the root and boundary vertices in $(b'\backslash b_0)_R$ is a subset of those in $(b''\backslash b_0)_R$ and so $(b'\backslash b_0)_R < (b''\backslash b_0)_R$ and the mapping is order preserving.

Now consider $b'_R, b''_R \in \mathscr{P}$ with $\varnothing < b'_R < b''_R$. Then both b'_R and b''_R are formed from arc sets of u–v self-avoiding walks. For each such walk in b'_R which contains arcs not in $A(b)\backslash A(b_0)$, replace these arcs (which connect root and boundary vertices) by corresponding walks in b_0. The acyclic property of b ensures that the resulting u–v walks are self-avoiding. This process produces a backbone in b. We take its arc union with b_0 to obtain a supergraph backbone b' of b_0 such that $(b'\backslash b_0)_R = b'_R$. Clearly, the same procedure applied to b''_R will give a supergraph backbone b'' of b' such that $(b''\backslash b_0)_R = b''_R$. Thus, we have an order-preserving bijection between $\mathscr{P}$ and $[b_0, b]$. $\blacksquare$

Lemma 3.2 can be interpreted as showing that the zeta functions for the two partially ordered sets are conjugate by the order-preserving bijection given and hence their inverses, the corresponding Möbius functions, are also equal. This means that if the Möbius functions is $\mu_{\mathscr{P}}$ on $\mathscr{P}$, then the restriction of $\mu_{\mathscr{B}_{uv}}$ to the segment $[b_0, b]$ is given by $\mu_{\mathscr{P}}$; in particular,

$$\mu_{\mathscr{B}_{uv}}(b_0, b) = \mu_{\mathscr{P}}(\varnothing, (b\backslash b_0)_R) \tag{3.2}$$

[cf. (2.9)]. We have now reduced the problem to that of calculating the Möbius function of an appropriately defined backbone relative to the empty set. This calculation is done by induction on the number of arcs in the graph. The Möbius function of an acyclic $b \in \mathscr{B}_{uv}$ is related to the contracted and deleted graphs b_γ and b_δ, respectively, of the graph b obtained by contracting or deleting a specified arc of b. We define an admissable arc to be an arc $a = (\overrightarrow{u, w})$, $w \neq v$, of the u–v rooted graph b.

Note. $[\varnothing, b_\delta]$ is a segment of $[\varnothing, b]$, whereas $[\varnothing, b_\gamma]$ is a different partially ordered set.

Let b be an acyclic backbone containing the admissible arc $a = (\overrightarrow{uw})$. If b_γ and b_δ are the contracted and deleted graphs of b relative to the arc a, we can deduce the following result.

Lemma 3.3. Suppose the vertex w of the acyclic backbone b is such that:

(i) $A(b)\backslash a$ has only outward arcs at w; then b_γ is a backbone and

$$\mu_{\mathscr{B}_{uv}}(\varnothing, b) = \mu_{\mathscr{B}_{uv}}(\varnothing, b_\gamma) \tag{3.3}$$

(ii) $A(b)\backslash a$ has both inward- and outward-directed arcs at w; then b_δ is a backbone and [cf. (2.12)]

$$\mu_{\mathscr{B}_{uv}}(\varnothing, b) = -\mu_{\mathscr{B}_{uv}}(\varnothing, b_\delta) \tag{3.4}$$

Proof. In case (i), $b' \leqslant b''$ if and only if $b'_\gamma \leqslant b''_\gamma$. Moreover, if b' is a backbone, then so is b'_γ. Therefore, the partially ordered sets of backbones $[\varnothing, b]$ and $[\varnothing, b_\gamma]$ are related by an order-preserving bijection. Hence (3.3) follows.

For case (ii), consider the set of self-avoiding walks on b which either contain the arc a or do not pass through the vertex w. Let b_0 be the backbone graph formed from the union of the arc sets of these walks. This graph has the property that there are no walks passing through w which do not contain the arc a. Consider the segment $[\varnothing, b_0]$. We have, by (2.6),

$$\sum_{\varnothing \leqslant b' \leqslant b_0} \mu_{\mathscr{B}_{uv}}(\varnothing, b') = 0 \tag{3.5}$$

Now consider the partially ordered set $\mathscr{D} = \{b' \leqslant b \mid b' \not\leqslant b_0\}$. From (3.5) together with (2.6) applied to $[\varnothing, b]$

$$\sum_{b' \in \mathscr{D}} \mu_{\mathscr{B}_{uv}}(\varnothing, b') = 0 \tag{3.6}$$

The elements of $\mathscr{D}$ can be paired as illustrated in Fig. 4. Every $b' \in \mathscr{D}$ contains an arc other than a with end vertex w. If $b' \in \mathscr{D}$, where $a \in A(b')$,

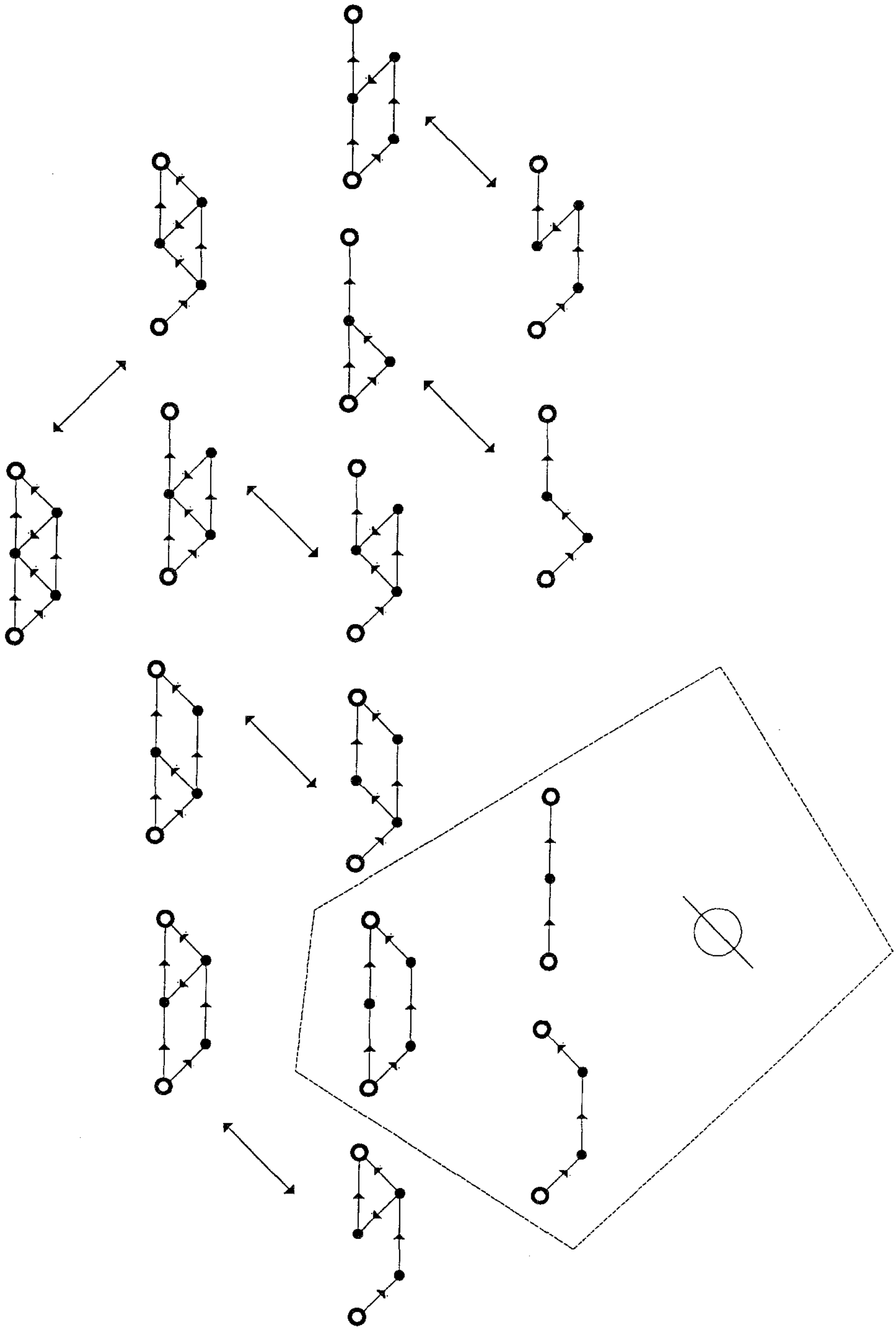

Fig. 4. An example of the segment $[\varnothing, b_0] \subseteq [\varnothing, b]$ and the complementary set $\mathscr{D}$ together with its pairings described in Lemma 3.3.

then b'' with arc set $A(b')\backslash a$ is also a backbone and clearly not a subgraph of b_0 and thus $b'' \in \mathscr{D}$. Similarly, if $b' \in \mathscr{D}$ with $a \notin A(b')$, then b'' with arc set $A(b') \cup a$ is an element of $\mathscr{D}$. Thus we can pair graphs in $\mathscr{D}$ whose arc sets differ by the arc a. Now suppose that for all backbone graphs $b' \in \mathscr{D}$ containing arc a with less than $|A(b)|$ arcs,

$$\mu_{\mathscr{B}_{uv}}(\varnothing, b') + \mu_{\mathscr{B}_{uv}}(\varnothing, b'_\delta) = 0 \tag{3.7}$$

It then follows by induction from (3.6) that

$$\mu_{\mathscr{B}_{uv}}(\varnothing, b) + \mu_{\mathscr{B}_{uv}}(\varnothing, b_\delta) = 0 \tag{3.8}$$

once the trivial case is checked of a pair of graphs obtained from a walk together with the arc a (cf. Fig. 2).

Lemma 3.4. The Möbius function of the partially ordered set $\mathscr{B}_{uv}$, where b is an acyclic backbone, satisfies

$$\mu_{\mathscr{B}_{uv}}(\varnothing, b) = (-1)^{c(b)+1} \tag{3.9}$$

Proof. This follows from Lemma 3.3 by induction on the number of arcs in the graph b. Assume that the Möbius function of any acyclic backbone subgraph b' of b with less than n arcs satisfies

$$\mu_{\mathscr{B}_{uv}}(\varnothing, b') = (-1)^{c(b')+1}$$

Now consider a backbone b with n arcs. From Lemma 3.3, we have two cases; either

$$\mu_{\mathscr{B}_{uv}}(\varnothing, b) = \mu_{\mathscr{B}_{uv}}(\varnothing, b_\gamma) \tag{3.10}$$

where b_γ is an acyclic backbone graph, or

$$\mu_{\mathscr{B}_{uv}}(\varnothing, b) = -\mu_{\mathscr{B}_{uv}}(\varnothing, b_\delta) \tag{3.11}$$

where b_δ is an acyclic backbone graph.

The cycle ranks of b and b_γ are the same and differ by one from that of b_δ. The result follows by induction once the trivial case of a backbone graph consisting of one edge is checked. ▮

Theorem 3.1. The Möbius function of the partially ordered set $\mathscr{B}_{uv}$ of acyclic directed backbones is given by

$$\mu_{\mathscr{B}_{uv}}(b', b'') = (-1)^{c(b'')-c(b')} \tag{3.12}$$

when $b' \leqslant b''$.

Proof. The cycle rank of the graph $(b \backslash b_0)_R$ is given by Eq. (3.1), and (3.2) with (3.9) gives (3.12) as required. ▮

3.2. Deletion-Contraction Rule

The properties described in Lemma 3.3 can also be obtained from a deletion-contraction rule. However, the contracted and deleted graphs of a backbone cannot both be backbones, and may not even be connected, and so we need to consider the partially ordered set $\mathscr{H}_{uv}$. To obtain the rule, we use a simple modification of a result given in ref. 9, p. 348:

Theorem 3.2. Let $\mathscr{P}$, $\mathscr{Q}$ be finite, partially ordered sets with their minimum and maximum elements denoted by 0 and 1, respectively. Let $p: \mathscr{Q} \to \mathscr{P}$ and $q: \mathscr{P} \to \mathscr{Q}$ be order-preserving functions between $\mathscr{P}$ and $\mathscr{Q}$ such that:

(a) $p(x) = 0$ if and only if $x = 0$.

(b) $q(0) = 0$.

(c) $pq(x) \geqslant x$ and $qp(x) \leqslant x$.

Then the Möbius functions of $\mathscr{P}$ and $\mathscr{Q}$ satisfy

$$\mu_{\mathscr{Q}}(0, 1) = \sum_{\{a:\, q(a) = 1\}} \mu_{\mathscr{P}}(0, a) \quad ▮ \tag{3.13}$$

Lemma 3.5. Let a be an admissable arc of the u–v rooted acyclic backbone graph $b \in \mathscr{B}_{uv}$. Then the Möbius functions for the deleted and contracted graphs b_δ and b_γ, respectively, satisfy

$$\mu_{\mathscr{H}_{uv}}(\varnothing, b_\gamma) = \mu_{\mathscr{H}_{uv}}(\varnothing, b) + \mu_{\mathscr{H}_{uv}}(\varnothing, b_\delta) \tag{3.14}$$

if b_δ is u–v connected, and

$$\mu_{\mathscr{H}_{uv}}(\varnothing, b_\gamma) = \mu_{\mathscr{H}_{uv}}(\varnothing, b) \tag{3.15}$$

if b_δ is not u–v connected.

Proof. Let $\mathscr{P}$ and $\mathscr{Q}$ be the partially ordered sets of u–v connected subgraphs of b and its contraction b_γ by some admissible arc a, together with the empty sets. Define the map q of Theorem 3.2 by $q(b') = h'$, where h' is the contraction of the graph with arc set $A(b') \cup \{a\}$. The admissibility of a ensures that every contracted subgraph of b is u–v connected. The map p is defined to be the injection $h' \mapsto h''$, where h'' has the arc set $A(h') \cup \{a\}$. It is now easy to check that the hypotheses of Theorem 3.2 are valid. Observe that the set $S = \{a \in \mathscr{P}: q(a) = b_\gamma\}$ is either

$\{b\}$ or $\{b_\delta, b\}$, depending on whether or not $b_\delta \in \mathscr{P}$, i.e., on whether or not b_δ is u–v connected. Equations (3.14) and (3.15) now follow from Eq. (3.13). ∎

Lemma 3.3 follows from Lemma 2.3 together with the following.

Lemma 3.6. The Möbius function $\mu_{\mathscr{H}_{uv}}$ for the partially ordered set $\mathscr{H}_{uv}$ satisfies, for backbone b, either

$$\mu_{\mathscr{H}_{uv}}(\varnothing, b) = \mu_{\mathscr{H}_{uv}}(\varnothing, b_\gamma) \tag{3.16}$$

where b_γ is a backbone, when either b_δ is not u–v connected or the vertex w is a source in b_δ; or

$$\mu_{\mathscr{H}_{uv}}(\varnothing, b) = -\mu_{\mathscr{H}_{uv}}(\varnothing, b_\delta) \tag{3.17}$$

when b_δ is u–v connected and w is not a source in b_δ.

In each case the contracted and deleted graphs are themselves backbones.

Proof. We consider the various cases:

(i) The graph b_δ is u–v connected.

(a) The vertex w is a source in b_δ, then b_δ is not coverable and so by Lemma 2.3 we have $\mu_{\mathscr{H}_{uv}}(\varnothing, b_\delta) = 0$ and (3.14) simplifies to (3.16).

(b) The vertex w is not a source of the graph b_δ; then b_δ is acyclic and a backbone. Note that the walks from u to w when joined with those from w to v form self-avoiding walks which cover all arcs of b_δ covered by walks containing the deleted arc a. In this case, b_γ is not coverable (the vertex v is not a source), although it is u–v connected, and so $\mu_{\mathscr{H}_{uv}}(\varnothing, b_\gamma) = 0$. In this case, (3.14) simplifies to Eq. (3.17).

(ii) The graph b_δ is not u–v connected. Here we have the case given by Eq. (3.15), which is rewritten as (3.16). ∎

3.3. Undirected Backbones

We now obtain a relationship between the Möbius functions $\mu_{\mathscr{B}_{uv}}$ and $\mu_{\mathscr{B}_{\vec{uv}}}$ of the undirected and directed backbone graphs, respectively. Let $b, b' \in \mathscr{B}_{uv}$ be such that $b \leqslant b'$. Let $D(b') \in \mathscr{C}_{uv}$ be the directed graph obtained by replacing each edge of b' by an antiparallel pair of directed arcs. Define $\vec{b}' \in \mathscr{B}_{\vec{uv}}$ to be the maximal directed backbone in $D(b')$ and define $D(b)$ similarly. Then there is a natural map q: $[\vec{b}, \vec{b}'] \to [b, b']$ such that $q(\vec{b}'')$, $\vec{b}'' \in [\vec{b}, \vec{b}']$, is the undirected graph obtained from $\vec{b}''$ by removing directings or identifying a pair of antiparallel edges to a single undirected edge. We define $p: [b, b'] \to [\vec{b}, \vec{b}']$ now by taking $p(b'')$, $b'' \in [b, b']$, to be the maximal backbone $\vec{b}'' \in \mathscr{B}_{\vec{uv}}$ such that $q(\vec{b}'') = b''$. It then follows that $pq(\vec{b}'') \geqslant \vec{b}''$ and $qp(\vec{b}'') = b''$.

We use Theorem 3.2 to prove:

Lemma 3.7. Let b, $b' \in \mathscr{B}_{uv}$ with $b \leqslant b'$. Then with the map q defined as above

$$\mu_{\mathscr{B}_{uv}}(b, b') = \sum_{\{\vec{b}'' : q(\vec{b}'') = b'\}} \mu_{\mathscr{B}_{\vec{uv}}}(\vec{b}, \vec{b}'') \tag{3.18}$$

where $\vec{b} = p(b)$.

Proof. Define $\mathscr{P} = [\vec{b}, \vec{b}']$ and $\mathscr{Q} = [b, b']$, where $\vec{b}' = p(b')$ and $\vec{b} = p(b)$. Note that $\vec{b}$ is the only directed backbone in $\mathscr{P}$ related to b by either p or q and so conditions (a) and (b) of Theorem 3.2 are satisfied. The inequalities required in condition (c) are satisfied by the properties of p and q given above. ∎

4. APPLICATION TO PERCOLATION THEORY

4.1. Percolation Models

An important application of Möbius functions is to percolation theory. We now define a percolation model and discuss the role of Möbius functions in the associated probability theory.

Suppose that the element e (vertex or edge) of a graph G occurs with probability p_e independently of all other elements, and is otherwise absent. For any given realization the subgraph $g \in G$ is said to occur if all of its elements occur. The probability that g occurs is

$$\mathrm{pr}(g) = \prod_{e \in g} p_e \tag{4.1}$$

If $p_e = 1$ for all $e \in V$, then we have a bond percolation model, and if $p_e = 1$ for all $e \in E$, we have a site percolation model on G. The general case is a mixed or site-bond percolation model on G. Let $\mathscr{G}$ be one of the partially ordered sets of subgraphs defined above in Section 2.2 and let μ be its Möbius function. Using property P1, in any realization there is a unique maximal element $g \in \mathscr{G}$ which occurs, i.e., g occurs, but no other subgraph $g' \in \mathscr{G}$ occurs which contains g. The probability that the maximal element of $\mathscr{G}$ which occurs is g is denoted by $P(p, g)$, where $p = \{p_e, e \in G\}$. Now, for g, $g' \in \mathscr{G}$,

$$\sum_{g' \geqslant g} P(p, g') = \mathrm{pr}(g) \tag{4.2}$$

and hence from (2.8)

$$P(p, g) = \sum_{g' \geq g} \mu(g, g') \operatorname{pr}(g') \tag{4.3}$$

The element $g \in \mathscr{G}$ occurs iff the maximal element g' realized in $\mathscr{G}$ satisfies $g' \geq g$. Note that $P(p, \varnothing)$ is the probability that no element of $\mathscr{G}$ other than $\varnothing$ occurs. Therefore

$$P(p, \varnothing) = \sum_{g' \geq \varnothing} \mu(\varnothing, g') \operatorname{pr}(g') \tag{4.4}$$

For bond and site percolation, except when $\mathscr{G} = \mathscr{B}_{uv}$, it is possible to simplify (4.3) using the explicit formula for μ.

(i) If $\mathscr{G} = \mathscr{H}$ or $\mathscr{H}_{uv}$, then for $h \in \mathscr{G}$ and $h \neq \varnothing$, using the results of Section 2.3(a),

$$P(p, h) = \sum_{h' \in [h, h^+]} \mu_{\mathscr{H}}(h, h') \operatorname{pr}(h') \tag{4.5}$$

$$= \operatorname{pr}(h) \sum_{h' \in [h, h^+]} (-1)^{|E' \setminus E(h)|} (-1)^{|V' \setminus V(h)|} \prod_{e \in h'} p_e \tag{4.6}$$

where E' is the edge set of h' and $E(h)$ is that of h.

For bond percolation, recalling that $G = (V, E)$, we consider only subgraphs h for which $h \in [(V, \varnothing), G]$ and hence $h^+ = G$. We then obtain from (4.6)

$$P(p, h) = \operatorname{pr}(h) \sum_{h' \geq h} \prod_{e \in E' \setminus E(h)} (-p_e)$$

$$= \prod_{e \in E(h)} p_e \prod_{e \in E \setminus E(h)} (1 - p_e) \tag{4.7}$$

as expected, since $1 - p_e$ is the probability that the edge e does not occur and h is maximal if no edge of $E \setminus E(h)$ occurs.

For mixed percolation models (4.6) must be used directly.

For site percolation, it is sometimes convenient to use a special subset $\mathscr{S} \subseteq \mathscr{H}$ known as the *section* subgraph of G, where $\mathscr{S} = \{h \in \mathscr{H} \mid E(V(h)) = E(h)\}$. This partially ordered set is isomorphic to the set of all subsets of V and hence has Möbius function

$$\mu_{\mathscr{S}}(s, s') = (-1)^{|V' \setminus V(s)|} \tag{4.8}$$

$(s' \geq s)$, which leads to

$$P(p, s) = \prod_{v \in V(h)} p_v \prod_{v \in V \setminus V(h)} (1 - p_v) \tag{4.9}$$

corresponding to (4.7).

(ii) If $\mathscr{G} = \mathscr{C}$, $\mathscr{C}_u$, or $\mathscr{C}_{uv}$, then for $c \neq \varnothing$,

$$P(p, c) = \sum_{c' \geqslant c} \mu_{\mathscr{G}}(c, c') \operatorname{pr}(c') = \sum_{c' \in [c, c^+]} (-1)^{|E' \setminus E(c)|} \operatorname{pr}(c') \quad (4.10)$$

For bond percolation

$$P(p, c) = \sum_{E(c) \subseteq E' \subseteq \pi_G(c) \cup E(c)} (-1)^{|E' \setminus E(c)|} \prod_{e \in E'} p_e \quad (4.11)$$

$$= \prod_{e \in E(c)} p_e \prod_{e \in \pi_G(c)} (1 - p_e) \quad (4.12)$$

which may be expressed by saying that c is the maximal element of $\mathscr{G}$ which occurs provided that no perimeter edge of c also occurs (such an occurrence would mean that a connected supergraph of c occurs). This form was used in deriving the power series expansions in ref. 3 by what has become known as the perimeter method.

A result analogous to (4.12) holds for site percolation with $c \in \mathscr{S}$, $E(c)$ replaced by $V(c)$, and $\pi_G(c)$ the set of vertices not in c but adjacent to c in G. For mixed percolation (4.10) must be used.

4.2. Pair Connectedness

The probability that at least one (directed) walk from u to v occurs is known as the pair connectedness $C_{uv}(p, G)$ of vertices u and v. Let $\mathscr{G}$ be $\mathscr{H}_{uv}$, $\mathscr{C}_{uv}$, or $\mathscr{B}_{uv}$; then in any realization, at least one u–v walk occurs if and only if one of the elements of $\mathscr{G} \setminus \varnothing$ occurs and hence from (4.4)

$$\begin{aligned} C(p, G) &= 1 - P(p, \varnothing) \\ &= 1 - \sum_{g' \geqslant \varnothing} \mu(\varnothing, g') \operatorname{pr}(g') \\ &= -\sum_{g' > \varnothing} \mu(\varnothing, g') \operatorname{pr}(g') \end{aligned} \quad (4.13)$$

The weight attached to the graph g' in the polynomial expression of $C(p, G)$ in the p variables is known as the d weight, $d(g')$, of g'. Hence, for $g' \neq \varnothing$,

$$d(g') = -\mu(\varnothing, g') \quad (4.14)$$

where now μ can be taken as the Möbius function for $\mathscr{H}_{uv}$, $\mathscr{C}_{uv}$, or $\mathscr{B}_{uv}$. This is consistent with Lemma 2.2, where we deduce that $\mu(\varnothing, g')$ is the same for all three partially ordered sets when g' is backbone and zero otherwise.

4.3. Expectation Values

Suppose that Z is a random variable, the value of which is determined by that element of $\mathscr{G}$ which is maximal in G'. Denote this value by $Z(g)$; then

$$\mathscr{E}(Z) = \sum_{g \in \mathscr{G}} Z(g)\, P(p, g) \tag{4.15}$$

Substituting (4.3) in (4.15) gives

$$\begin{aligned}\mathscr{E}(Z) &= \sum_{g \in \mathscr{G}} Z(g) \sum_{g' \geqslant g} \mu(g, g')\, \mathrm{pr}(g') \\ &= \sum_{g' \in \mathscr{G}} W(g')\, \mathrm{pr}(g')\end{aligned} \tag{4.16}$$

where the weight

$$W(g') = \sum_{g \leqslant g'} Z(g)\, \mu(g, g') \tag{4.17}$$

Using (2.2), we may invert (4.17) to give

$$\sum_{g \leqslant g'} W(g) = Z(g') \tag{4.18}$$

which may be used to calculate the weights recursively and is useful when an explicit form of the Möbius function is not available. This is known (in a wider context) as the finite cluster method (see ref. 12, pp. 322–330, and ref. 8, Section IV).

If $Z(g) = \gamma(g)$, the connectedness indicator, i.e.,

$$\gamma(g) = \begin{cases} 1 & \text{if there is a } u\text{–}v \text{ walk in } g \\ 0 & \text{if not} \end{cases} \tag{4.19}$$

then $\mathscr{E}(\gamma) = C(p, g)$, the pair-connectedness, and $W(g') = d(g')$. Thus, if μ is the Möbius function of $\mathscr{G}$,

$$d(g') = \sum_{g \leqslant g'} \gamma(g)\, \mu(g, g') \tag{4.20}$$

If $\mathscr{G} = \mathscr{H}_{uv}$, $\mathscr{C}_{uv}$, or $\mathscr{B}_{uv}$, and $g \in \mathscr{G}$, then $\gamma(g) = 1$ unless $g = \varnothing$, so, using (2.4),

$$d(g') = \sum_{\varnothing < g < g'} \mu(g, g') = -\mu(\varnothing, g') \tag{4.21}$$

in agreement with (4.14).

4.4. Backbone Variables

If the value of the random variable Z is determined by the maximal u–v backbone which occurs, it is known as a backbone variable. The connectedness indicator γ of Section 4.3 is such a variable, as is the resistance between u and v. Many others are given in ref. 13.

If Z is a backbone variable, then Eq. (4.16) applies with $\mathscr{G} = \mathscr{H}_{uv}$, $\mathscr{C}_{uv}$, or $\mathscr{B}_{uv}$ and equating coefficients of $\mathrm{pr}(g')$ in the resulting formulas leads to the following extension of Lemma 2.3.

Lemma 4.1. Suppose that $Z(\varnothing)=0$ and that Z is a backbone variable; then, given $h' \in \mathscr{H}_{uv} \backslash \mathscr{B}_{uv}$, the weight defined in (4.17) satisfies $W(h')=0$.

Proof. The result may be derived directly from the definition (4.7) following the proof and notation of Lemma 2.3. First note that $Z(\varnothing)=0$ together with (4.17) gives $W(\varnothing)=0$. From (4.18), using the fact that Z is a backbone variable,

$$\begin{aligned} W(h') &= Z(h') - \sum_{h<h'} W(h) \\ &= Z(b_0) - \sum_{\varnothing \leqslant h \leqslant b_0} W(h) - \sum_{h \in S(h')} W(h) \\ &= -\sum_{h \in S(h')} W(h) \end{aligned} \tag{4.22}$$

The result follows by induction since $W(\varnothing)=0$ and $W(h)=0$ for the minimal nonbackbone graph which consists of a walk together with an extra edge (cf. Fig. 2). ∎

5. DISCUSSION

Möbius functions for partially ordered sets of subgraphs of a graph and their applications to percolation theory have been reviewed. Depending on the nature of the percolation function to be calculated, one or more of the partially ordered sets defined in Section 2.2 will be appropriate. In early work on percolation theory,[3] connected unrooted subgraphs which we denoted by $\mathscr{C}$ were used. In calculating the pair-connectedness or point-to-point resistance in a percolation model, graphs with roots u and v containing a walk from u to v are more appropriate. Of the three classes of this type considered ($\mathscr{H}_{uv}$, $\mathscr{C}_{uv}$, $\mathscr{B}_{uv}$), the backbone graphs are least numerous and, where appropriate, should be used for computational efficiency. The restriction to $\mathscr{B}_{uv}$ is possible whenever the random variable Z, whose expected value we wish to calculate, is a backbone variable, i.e., one whose value for any configuration depends only on the maximal u–v backbone which occurs. The only major new result of this paper is the proof of the conjecture of Bhatti and Essam[7] which gives an explicit formula for the Möbius function of the set of acyclic directed backbones.

A special case of the backbone Möbius function is $\mu_{\mathscr{B}_{uv}}(\emptyset, b) = -d(b)$, which is the *d-weight* arising in a power series expansion for pair-connectedness. It has been shown in ref. 11 that the *d-weight* for an undirected backbone graph is the sum of the directed *d-weights* over all possible acyclic directed backbones which may be obtained by directing the edges of b. In the case of the general Möbius function for undirected backbones we have shown in Section 3.3 that a similar expression may be obtained, but now a wider sum must be considered involving graphs with antiparallel arc pairs. When no such pairs are present, the weight of the graph is the directed Möbius function, but the general rule which determines the weights has yet to be discovered. This is an important topic for further research, since most applications involve undirected graphs.

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