Simple Method to Calculate Percolation, Ising, and Potts Clusters: Renormalization-Group Applications

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We introduce a procedure which considerably simplifies the calculation of clusters like those commonly appearing in real-space renormalization-group treatments of bond-percolation and pure and random Ising and Potts problems. The method is illustrated through two applications for the q-state Potts ferromagnet.

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Within the framework of various exact or approximate procedures [e.g., real-space renormalization group (RG)] to calculate statistical equilibrium properties, the central operational stage consists in performing traces over all the possible configurations of what we may call the *internal* degrees of freedom of a (usually *finite*) cell or cluster, while what we may call the external or terminal degrees of freedom (of the same cluster) are maintained frozen in convenient particular configurations. The central aim of this paper is to present a new method [referred to from now on as the break-collapse method (BCM) which considerably simplifies the (human or computer) performance of such tracing (no counting of configurations is needed) for all conventional d-dimensional uncorrelated-bond-percolation and pure as well as bond-random spin- $\frac{1}{2}$ Ising and q-state Potts models (the latter contains, as is well known,¹ the other two as particular cases): the cluster might refer to a regular lattice or not, isotropic and homogeneous or not, in the presence or absence of external fields. etc. The BCM reformulates and extends the "deletion-contraction rule" $^{1-3}$; it demands the introduction of convenient variables (transmissivi $ties^4$) and graphs which reformulate and extend the "pair connectedness" introduced by Essam in 1971.^{1-3,5} Though the BCM finds its most immediate applications within the RG framework, ^{3,4,6-8} it has in fact no particular relation with it, and can be used in other contexts (e.g., duality arguments, cluster expansions, etc.). Herein we present (without proof) the BCM basic properties and perform two simple applications.

Let us consider the ith q-state Potts bond of a

certain array; its Hamiltonian is given by $\mathcal{K}_i = -qJ_i\delta_{\sigma,\sigma'}$, where J_i is the coupling constant and σ and σ' are the Potts random variables respectively associated to the two sites of the bond. Once we assume that one site is in a given configuration and denote by $p_i^{\ c}$ and $p_i^{\ d}$ the (conditional) probabilities for the other site to be respectively in the same configuration (sites "connected") or in a particular different one (sites "disconnected"), we may define the thermal transmissivity t_i as

$$t_{i} \equiv p_{i}^{c} - p_{i}^{d} = \frac{1 - \exp(-qJ_{i}/k_{\rm B}T)}{1 + (q - 1)\exp(-qJ_{i}/k_{\rm B}T)}$$
(1)

(for q = 1 we recover the isomorphism¹ between tand the bond occupancy probability of percolation). An alternative way of defining transmissivity is directly through Eq. (1) by disregarding the intermediate definitions of $p_i^{\ c}$ and $p_i^{\ d}$. If we have two bonds (with transmissivities t_1 and t_2) in series, the equivalent transmissivity t_s is given (see also Yeomans and Stinchcombe⁹) by $t_s = t_1 t_2$. For a parallel array we obtain (see also Refs. 4 and 10) $t_p^{\ D} = t_1^{\ D} t_2^{\ D}$, where

$$t_i^{D} \equiv (1 - t_i) / [1 + (q - 1)t_i] \quad (i = 1, 2, p)$$
(2)

(D stands for "dual"). The generalization of these equations for N bonds is obvious. The BCM makes possible the calculation of the equivalent transmissivity [denoted by $G(\{t_i\})$] of any two-terminal cluster (reducible in series-parallel sequences or not). Let us be more specific. If we have a general two-terminal cluster with bond transmissivities $\{t_i\}$ then $G(\{t_i\}) = N(\{t_i\})/$ $D(\{t_i\})$, where both numerator N and denominator D are multilinear functions of the $\{t_i\}$. If we choose the *j*th bond of the set and "break" ("collapse") it, i.e., we impose $t_j=0$ ($t_j=1$), we will have a new equivalent transmissivity denoted $G_j^{\ b}$ ($G_j^{\ c}$) and given by

$$G_{j}^{b}(\{t_{i}\}') = N_{j}^{b}(\{t_{i}\}') / D_{j}^{b}(\{t_{i}\}')$$
$$[G_{j}^{c}(\{t_{i}\}') = N_{j}^{c}(\{t_{i}\}') / D_{j}^{c}(\{t_{i}\}')]$$

where the set $\{t_i\}'$ now excludes t_j . The multilinearity of both N and D leads to

$$N(\{t_i\}) = (1 - t_j) N_j^{b}(\{t_i\}') + t_j N_j^{c}(\{t_i\}')$$

and

$$D(\{t_i\}) = (1 - t_j) D_j^{b}(\{t_i\}') + t_j D_j^{c}(\{t_i\}').$$

The sequential use of these equations is what we call the "break-collapse method" and makes possible, with considerable economy of effort, the calculation of *any* Potts cluster; i.e., the tracing over all the internal degrees of freedom is *automatically performed* through the simple algorithms and topological operations just mentioned. Let us illustrate the procedure on the example of Fig. 1(a) (b=2 Wheatstone bridge), whose broken and collapsed clusters are respectively indicated in Figs. 1(b) and 1(c), where we have operated on the central bond of Fig. 1(a); we obtain

$$G^{b}(t) = \frac{N^{b}(t)}{D^{b}(t)} = \frac{2t^{2} + (q-2)t^{4}}{1 + (q-1)t^{4}}$$
(3)

and

$$G^{c}(t) = \frac{N^{c}(t)}{D^{c}(t)} = \frac{4t^{2} + 4(q-2)t^{3} + (q-2)^{2}t^{4}}{1 + 2(q-1)t^{2} + (q-1)^{2}t^{4}} .$$
(4)

Therefore G(t)

$$=\frac{2t^2+2t^3+5(q-2)t^4+(q-2)(q-3)t^5}{1+2(q-1)t^3+(q-1)t^4+(q-1)(q-2)t^5},$$
 (5)

which coincides with a particular case of the expression reproduced in Ref. 9 and for q = 1 (q = 2) recovers those appearing in Refs. 3, 6-8, and 11 (Refs. 4 and 12). We can verify on the above examples a general property, namely

 \sum (numerator coeffs.)

=
$$\sum$$
(denominator coeffs.) = q^{κ} , (6)

where κ is the cyclomatic number ¹³ [$\kappa \equiv$ (number of bonds) – (number of sites) +1]. Furthermore, for q = 1 and any graph, D equals unity. The BCM provides a quick way for calculating $\partial G(\{t_i\})/\partial t_j$.

Another interesting property concerns planar arrays and duality. If we consider any pair of dual clusters (i.e., superimposable in such a way that each bond of one cluster crosses one and only one bond of the other; see Essam and Fish er^{14} and references therein; see Fig. 1) and denote by G and G^{D} , respectively, their equivalent transmissivities, we verify that

$$G^{D}(\{t_{i}^{D}\}) = [1 - G(\{t_{i}\})] / [1 + (q - 1)G(\{t_{i}\})].$$



FIG. 1. Planar clusters. The solid (open) circles denote the internal sites (external sites or roots). (b), (c), and (e), (f) are dual pairs; (a) and (d) are self-dual.



FIG. 2. The RG critical exponent ν as a function of q (solid and dashed lines); the exact Ising values (cross) and the conjectures of Klein *et al.* (Ref. 17) (open circle), den Nijs [dotted line (Ref. 15)], and Nienhuis *et al.* [dash-dotted line (Ref. 16)] are indicated as well.

Let us now perform our first application, namely a RG calculation of the critical point t_c and correlation-length critical exponent ν of the isotropic, homogeneous, pure, Potts ferromagnet in the square lattice. We renormalize Wheatstone bridges of order b (whose self-duality recovers that of the square lattice; for q = 1, 2 see Refs. 3, 4, 6-8, 11, and 12 and for any q and b = 2 see Ref. 9) into a single bond. The recursive relation is given by $t' = t_b(t)$; $t_2(t)$ equals G(t) given by Eq. (5); $t_3(t)$ and $t_4(t)$ are too long to be reproduced herein. The recursive relation provides, for all b, the (unstable) nontrivial fixed point $t = t_c \equiv (1 + \sqrt{q})^{-1}$ (exact answer). The

RG approximation for ν is given by $\nu_b = \ln b / \ln[dt_b(t)/dt]_{t=t_c}$: See Fig. 2 and Table I. Although ν is defined only for $q \leq 4$ (the transition is known to be a first-order one for q > 4) we may formally calculate $\nu(q \rightarrow \infty)$ and obtain $\frac{1}{2}$: See Ref. 16 for a possible physical interpretation of this value but for $q \rightarrow 0$. We have not been able to discuss the limit $q \rightarrow 0$ for b > 4, but for $b \leq 4$ we have obtained $\nu_b \propto 1/\sqrt{q}$ (this is probably true for all b): this result coincides with den Nijs's conjecture, ¹⁵ namely

$$\nu = \frac{2}{3} \left\{ 2 + \pi / \left[\arccos(\frac{1}{2} \sqrt{q}) - \pi \right] \right\} \sim \pi / 3 \sqrt{q}$$

in the limit $q \rightarrow 0$ (see also Blöte, Nightingale, and Derrida¹⁸). In this respect let us remark that numerical analysis of $\nu_b(q)$ for b = 2, 3, 4 and q = 1, 2 suggests that the present RG approximation converges (towards the exact result) faster for small values of q.

Let us now perform our second application, namely a compact recalculation of the critical surface of the fully anisotropic, homogeneous, pure. Potts ferromagnet in the triangular (and honeycomb) lattice. We essentially follow along the lines of standard duality and triangle-star transformation¹⁹; they are, however, reformulated within the present framework. We must now use three-rooted graphs but this does not increase the operational complexity as the BCM holds as stated before for any *n*-rooted graph with the convention that the collapse of two terminals or of one terminal and one internal site provides a terminal, whereas the collapse of two internal sites provides an internal site; furthermore, internal and terminal sites are strictly

TABLE 1. RG values of ν ; $\nu_b \sim A_b q^{-1/2}$ if $q \rightarrow 0$ and $\nu_b \sim B_b (1 + C_b q^{-1/2})$ if $q \rightarrow \infty$. The values with asterisks recover values appearing in Refs. 4, 6, 7, 9, 11, and 12.

	ν				A _b	B _b	С _b
b	1	2	3	4	$q \rightarrow 0$	$q ightarrow \infty$	
2	1.4277*	1.1486*	1.0236*	0.9484*	$\frac{4\ln 2}{3}\simeq 0.924$	$rac{\ln 2}{\ln 5}\simeq 0.431$	$\frac{22}{5\ln 5} \simeq 2.73$
3	1.3797*	1.1094*	0.9883	0.9156	$\frac{9\ln\!3}{11}\simeq 0.899$	$rac{\mathrm{ln3}}{\mathrm{ln13}}\simeq0.428$	$\frac{70}{13\ln 13} \simeq 2.10$
4	1.3627*	1.0950*	0.9752	0.9033	$\frac{56\ln 4}{87} \simeq 0.892$	$rac{\mathrm{ln}4}{\mathrm{ln}25} \simeq 0.431$	$\frac{154}{25\ln 25} \simeq 1.91$
exact (a) or							
$b \rightarrow \infty$ (b) or	4/3 (c) ^a	1 (a)	5/6 (c) ^a	2/3 (c) ^a	$\frac{\pi}{3} \simeq 1.04$ (c) ^a	$\frac{1}{2}$ (b)	?
conjectures (c)	1.3547 (c) ^b					-	

^aSee Ref. 15.

^bSee Ref. 17.

equivalent if the point is an *articulation* point (its deletion separates the graph into two or more pieces; within the present context each piece must contain at least one terminal site) and the transmissivity of a graph with one or more isolated roots vanishes. Let us first consider the graph of Fig. 1(g) (denoted by G_{Δ}); we obtain $G_3^{\ b}(t_1, t_2) = t_1 t_2/1$ and

$$G_3^{\ c}(t_1, t_2) = \frac{t_1 + t_2 + (q - 2)t_1t_2}{1 + (q - 1)t_1t_2} , \qquad (7)$$

and hence

$$G_{\Delta}(t_1, t_2, t_3) = \frac{t_1 t_2 + t_2 t_3 + t_3 t_1 + (q-3) t_1 t_2 t_3}{1 + (q-1) t_1 t_2 t_3}.$$
 (8)

We consider now the graph of Fig. 1(h) (denoted by G_{γ}) and operate on the t_3^{D} bond. The transmissivity of the broken graph vanishes and that of the collapsed one equals $t_1^{D}t_2^{D}/1$; therefore

$$G_{\gamma}(t_1^{\ D}, t_2^{\ D}, t_3^{\ D}) = t_1^{\ D} t_2^{\ D} t_3^{\ D} / 1, \qquad (9)$$

where t_i^{D} is related to t_i (i=1, 2, 3) through Eq. (2). The simultaneous performance of duality and star-triangle transformations leads to $G_{\Delta}(t_1, t_2, t_3) = G_{\gamma}(t_1^{D}, t_2^{D}, t_3^{D})$ which, through notation changes, reproduces the *exact* result.¹⁹ For the honeycomb lattice we obtain $G_{\Delta}(t_1^{D}, t_2^{D}, t_3^{D})$ $= G_{\gamma}(t_1, t_2, t_3)$. We are presently working on a certain amount of other properties and extensions of this formalism.

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