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SIMPLE METHOD TO CALCULATE PERCOLATION, ISING AND POTTS CLUSTERS - RENORMALIZATION GROUP APPLICATIONS

by

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ABSTRACT

We introduce a procedure ("break-collapse method") which considerably simplifies the calculation of (two - or multi-rooted) clusters like those commonly appearing in real space renormalization group (RG) 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. The first of them concerns a RG calculation of the critical exponent ν for the isotropic square lattice: we obtain numerical consistence (particularly for $q \to 0$) with den Nijs conjecture. The second application is a compact reformulation of the standard star-triangle and duality transformations which provide the exact critical temperature for the anisotropic triangular and honeycomb lattices.

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 from now on as the break-collapse method (BCM)) which considerably simplifies the performance of such tracing for all conventional d-dimensional uncorrelated-bond-percolation and pure as well as bond-random $\frac{1}{2}$ -spin - Ising and q-state-Potts models (the latter contains, as it 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 (in several senses that will become clear further on) the "deletion-contraction rule" [1-9]; it demands the introduction of convenient variables (transmissivities [10-12]) and graphs which reformulate and extend the "pair connectedness" introduced by Essam in 1971[1,3-9,13]. Though the BCM finds its most immediate applications within the RG framework [9-12, 14-16], 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 and mainly through illus trations) the basic properties associated to the BCM and perform two simple pure Potts ferromagnet applications: isotropic square lattice through RG and anisotropic triangular (and honeycomb) lattice through duality arguments.

Let us consider the i-th q-state Potts bond of a certain array; its Hamiltonian is given by $\mathcal{H}_i = -q J_i \delta_{\sigma,\sigma'}$, 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, the (conditional) probabilities p_i^c and p_i^d for the other site to be respectively in the <u>same</u> configuration (sites"connected") or in a <u>particular different</u> one (sites "disconected") are given by

$$p_i^c = \frac{e^{qJ_i/k_BT}}{e^{qJ_i/k_BT} + (q-1)} \tag{1}$$

and

$$p_i^d = \frac{1}{e^{qJ_i/k_BT} + (q-1)} \tag{2}$$

We define the <u>thermal transmissivity</u> t_i as follows:

$$t_i \equiv p_i^c - p_i^d = \frac{1-e^{-qJ_i/k_BT}}{1+(q-1)e^{-qJ_i/k_BT}} \tag{3}$$

(for q=1 we recover the isomorphism [1] between t and the bond occupancy probability of percolation). If we have two bonds (with transmissivities t_1 and t_2) in series, the equivalent transmissivity t_s is given by (see also Ref. [17]):

$$t_s = t_1 t_2 \tag{4}$$

For a parallel array we obtain

$$t_p = \frac{t_1+t_2+(q-2)t_1 t_2}{1+(q-1)t_1 t_2} \tag{5}$$

which can be rewritten as follows [10-12,18,19]

$$t_p^D = t_1^D \; t_2^D \tag{6}$$

where

$$t_i^D \equiv \frac{1-t_i}{1+(q-1)t_i} \qquad (i=1,2,p) \tag{7}$$

(D stands for "dual"). The generalization of Eqs.(4) and (6) for N bonds is obvious, and enables the calculation of the equivalent transmissivity (noted $G(\{t_i\})$) of any two-terminal array or cluster (connected two-rooted graph) whose topology is reductible in series-parallel sequences. The BCM extends this procedure to <u>any</u> two-terminal cluster (reductible in series-parallel <u>or not</u>). Let us be more specific. If we have a general two-terminal cluster whose bonds have respectively transmissivities $\{t_i\}$ then

$$G(\{t_i\}) = \frac{N(\{t_i\})}{D(\{t_i\})} \tag{8}$$

where both numerator N and denominator D are <u>multilinear</u> func tions 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 noted G_j^b (G_j^c) and given by

$$G_j^b(\{t_i\}') = \frac{N_j^b(\{t_i\}')}{D_j^b(\{t_i\}')} \tag{9}$$

and

$$G_j^c(\{t_i\}') = \frac{N_j^c(\{t_i\}')}{D_j^c(\{t_i\}')} \tag{10}$$

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

$$N(\{t_i\}) = (1-t_j)N_j^b(\{t_i\}')+t_jN_j^c(\{t_i\}') \tag{11}$$

and

$$D(\{t_i\}) = (1-t_j)D_j^b(\{t_i\}')+t_jD_j^c(\{t_i\}') \tag{12}$$

The sequential use of Eqs.(4), (6), (11) and (12) is what we call the "break-collapse method" and enables, with considerable economy of effort, the calculation of <u>any</u> Potts cluster, i.e. the tracing over all the internal degrees of freedom is <u>automatically performed</u> 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 (by using Eqs. (4) and (6))

$$G^b(t) = \frac{N^b(t)}{D^b(t)} = \frac{2t^2+(q-2)t^4}{1+(q-1)t^4} \qquad (13)$$

and

$$G^c(t) = \frac{N^c(t)}{D^c(t)} = \frac{4t^2+4(q-2)t^3+(q-2)^2t^4}{1+2(q-1)t^2+(q-1)^2t^4} \qquad (14)$$

therefore (through Eqs. (11) and (12))

$$G(t) = \frac{2t^2+2t^3+5(q-2)t^4+(q-2)(q-3)t^5}{1+2(q-1)t^3+(q-1)t^4+(q-1)(q-2)t^5} \qquad (15)$$

which coincides with a particular case of the expression reproduced in Ref. [17] and for q=1 (q=2) recovers those appearing in Refs. [9, 14-16 and 20] (Refs. [10-12 and 21]). We can verify on Eqs. (13),(14)and (15) a general property, namely

$$\Sigma(\text{numerator coeffs.}) = \Sigma(\text{denominator coeffs.}) = q^{\kappa} \qquad (16)$$

where κ is the <u>cyclomatic number</u> [22] and is given by

$$\kappa \equiv (\text{number of bonds}) - (\text{number of sites}) + 1 \qquad (17)$$

Furthermore, for q=1 and <u>any</u> graph, D equals unity. An useful corollary of Eqs.(11) and (12) is that

$$\frac{\partial G(\{t_i\})}{\partial t_j} = \frac{N_j^c(\{t_i\}')-N_j^b(\{t_i\}')-G(\{t_i\})\left[D_j^c(\{t_i\}')-D_j^b(\{t_i\}')\right]}{D(\{t_i\})} \qquad (18)$$

Another interesting property concerns planar arrays and duality, and extends Eq.(6). 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 Ref. [23] and references therein; in Figs. 1.b and 1.c as well as in 1.e and 1.f we present two such examples; the clusters of Figs. 1.a and 1.d (b=3 Wheatstone bridge) are both self-dual) and we respectively note G and G^D their equivalent transmissivities, we verify

$$G^D(\{t_i^D\}) = \frac{1-G(\{t_i\})}{1+(q-1)G(\{t_i\})} \tag{19}$$

Let us now perform our first application, namely a RG calculation of the critical point t_c and correlation lengh critical exponent ν of the isotropic homogeneous pure Potts ferromagnet in square lattice. We renormalize Wheatstone bridges of order b (renormalizing linear expansion factor) into a single bond. This choice is particularly well adapted to the square lattice as it recovers its selfduality for any value of b (for q=1,2 see Refs. [9-12,14-16,20,21] and for any q and b=2 see Ref. [17]). The recursive relation is given by

$$t' = t_b(t) \tag{20}$$

where $t_2(t)$ equals G(t) given by Eq.(15) and

$$t_3(t) = [3t^3+8t^4+(8q-6)t^5+(45q-82)t^6+(24q^2-50q+16)t^7 +(2q^3+62q^2-223q+198)t^8+(34q^3-37q^2-270q+422)t^9 +(4q^4+123q^3-952q^2+2287q-1814)t^{10}+(66q^4-593q^3 +2098q^2-3430q+2157)t^{11}+(13q^5-144q^4+671q^3 -1646q^2+2115q-1126)t^{12}+(q^6-13q^5+74q^4-237q^3 +451q^2-482q+224)t^{13}]/[1+(4q-4)t^3+(4q-4)t^4 +(2q^2-2q)t^5+(8q^2-10q+2)t^6+(21q^2-43q+22)t^7 +(10q^3+q^2-62q+51)t^8+(32q^3-107q^2+101q-26)t^9 +(7q^4+51q^3-394q^2+722q-386)t^{10}+(57q^4-445q^3 +1275q^2-1565q+678)t^{11}+(13q^5-135q^4+559q^3 -1143q^2+1138q-432)t^{12}+(q^6-13q^5+71q^4 -207q^3+337q^2-287q+98)t^{13}] \quad (21)$$

We have calculated $t_4(t)$ as well but is too long to be reproduced here. The recursive relation provides, for all b, the (unstable) fixed point $t=t_c\equiv(1+\sqrt{q})^{-1}$ (besides the trivial ones t=0 and t=1) which is the exact answer [24]. The RG approximation for ν is given by $\nu_b = \ln b/\ln(dt_b(t)/dt)_{t=t_c}$. We have obtained

$$\left.\frac{dt_2}{dt}\right|_{t=t_c} = \frac{8+21q^{1/2}+18q+5q^{3/2}}{8+15q^{1/2}+8q+q^{3/2}} \quad (22)$$

$$\left.\frac{dt_3}{dt}\right|_{t=t_c} = \frac{576+2668q^{1/2}+5143q+5323q^{3/2}+3173q^2+1078q^{5/2}+190q^3+13q^{7/2}}{576+1964q^{1/2}+2711q+1955q^{3/2}+789q^2+176q^{5/2}+20q^3+q^{7/2}} \quad (23)$$

and an expression for $(dt_4/dt)_{t=t_c}$ which is too long to be reproduced here. The associated $\{\nu_b(q)\}$ are represented in Fig.

2 (see also Table 1) and compared with den Nijs conjecture [25] (both branches [26]) and Klein et al conjecture [27]. 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 $\nu(q\to\infty)$ as follows:

$$\nu(q\to\infty) = \lim_{b\to\infty} \lim_{q\to\infty} \nu_b(q) = \lim_{b\to\infty} \frac{\ln b}{\ln\left[b^2+(b-1)^2\right]} = \frac{1}{2}$$

(see Ref. [26] for a possible physical interpretation of this value but for $q\to 0$). We have not been able to discuss the limit $q\to 0$ 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 conjecture [25], namely $\nu = 2/3\left[2+\pi/(\arccos\frac{\sqrt{q}}{2} - \pi)\right] \sim \pi/3\sqrt{q}$ in the limit $q\to 0$. Within 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 re-calculation of the critical surface of the fully anisotropic homogeneous pure Potts ferromagnet in triangular (and honeycomb lattice. We essentially follow along the lines of standard duality and triangle-star transformation [28,29]; 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 equivalent if the point is an <u>articulation</u> one (its deletion separates the graph in two or more pieces;with in 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 (noted G_Δ) and operate on the t_3-bond. The broken and collapsed transmissivities are respectively given by

$$G_3^b(t_1,t_2)= \frac{t_1 t_2}{1} \tag{24}$$

and

$$G_3^c(t_1,t_2)= \frac{t_1+t_2+(q-2)t_1t_2}{1+(q-1)t_1t_2} \tag{25}$$

therefore, through Eqs.(11) and (12),

$$G_\Delta(t_1,t_2,t_3)= \frac{t_1t_2+t_2t_3+t_3t_1+(q-3)t_1t_2t_3}{1+(q-1)t_1t_2t_3} \tag{26}$$

We consider now the graph of Fig.1h (noted G_Y) 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,though Eqs.(11) and (12),

$$G_Y(t_1^D,t_2^D,t_3^D)= t_1^D t_2^D t_3^D/1 \tag{27}$$

where t_i^D is related to t_i (i= 1,2,3) through Eq.(7). The simultaneous performance of duality and star-triangle transformations leads to

$$G_{\Delta}(t_1,t_2,t_3)= G_{Y}(t_1^D,t_2^D,t_3^D) \qquad (28)$$

which, through notation changements, reproduces the exact [28, 29] critical surface we were looking for. Consistently the exact critical surface associated to the honeycomb lattice is given by $G_{\Delta}(t_1^D,t_2^D,t_3^D)= G_{Y}(t_1,t_2,t_3)$.

We have presented herein the basic operational rules of the "break-collapse method", which considerably simplifies human or cumputer effort (no counting of configurations is needed) for the calculation of bond-percolation (q=1), Ising (q=2) and q-state Potts clusters (with two or more terminals exempted from the statistical tracing operations), and have illustrated their use through two simple applications. We are presently working on a certain amount of other properties and extensions of this formalism.

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CAPTION FOR FIGURES AND TABLE

Fig. 1 - Examples of planar clusters. The solid (open) circles denote the internal sites (external sites or roots).

Fig. 2 - The RG correlation length critical exponent ν as a function of q (solid and dashed lines); the exact Ising value (x) and Klein et al [27] (o) and den Nijs [25,26] (dotted and dashed-dotted lines) conjectures are indicated as well.

TABLE 1- RG values of ν; $\nu_b \sim A_b q^{-1/2}$ if $q \to 0$ and $\nu_b \sim B_b(1+C_b q^{-1/2})$ if $q \to \infty$. The values with (*) recover values appearing in Refs. [10-12, 14, 15, 17, 20, 21].

	ν				A_b	B_b	C_b
q / b	1	2	3	4	$q \to 0$	$q \to \infty$	
2	1.4277*	1.1486*	1.0236*	0.9484*	$\frac{4 \ln 2}{3} \simeq 0.924$	$\frac{\ln 2}{\ln 5} \simeq 0.431$	$\frac{22}{5 \ln 5} \simeq 2.73$
3	1.3797*	1.1094*	0.9883	0.9156	$\frac{9 \ln 3}{11} \simeq 0.899$	$\frac{\ln 3}{\ln 13} \simeq 0.428$	$\frac{70}{13 \ln 13} \simeq 2.10$
4	1.3627*	1.0950*	0.9752	0.9033	$\frac{56 \ln 4}{87} \simeq 0.892$	$\frac{\ln 4}{\ln 25} \simeq 0.431$	$\frac{154}{25 \ln 25} \simeq 1.91$
exact(a) or $b \to \infty$ (b) or conjectures(c)	4/3 (c) [15] 1.3547 (c) [17]	1 (a)	5/6 (c) [15]	2/3 (c) [15]	$\frac{\pi}{3} \simeq 1.047$ (c) [15]	$\frac{1}{2}$ (b)	?

TABLE 1

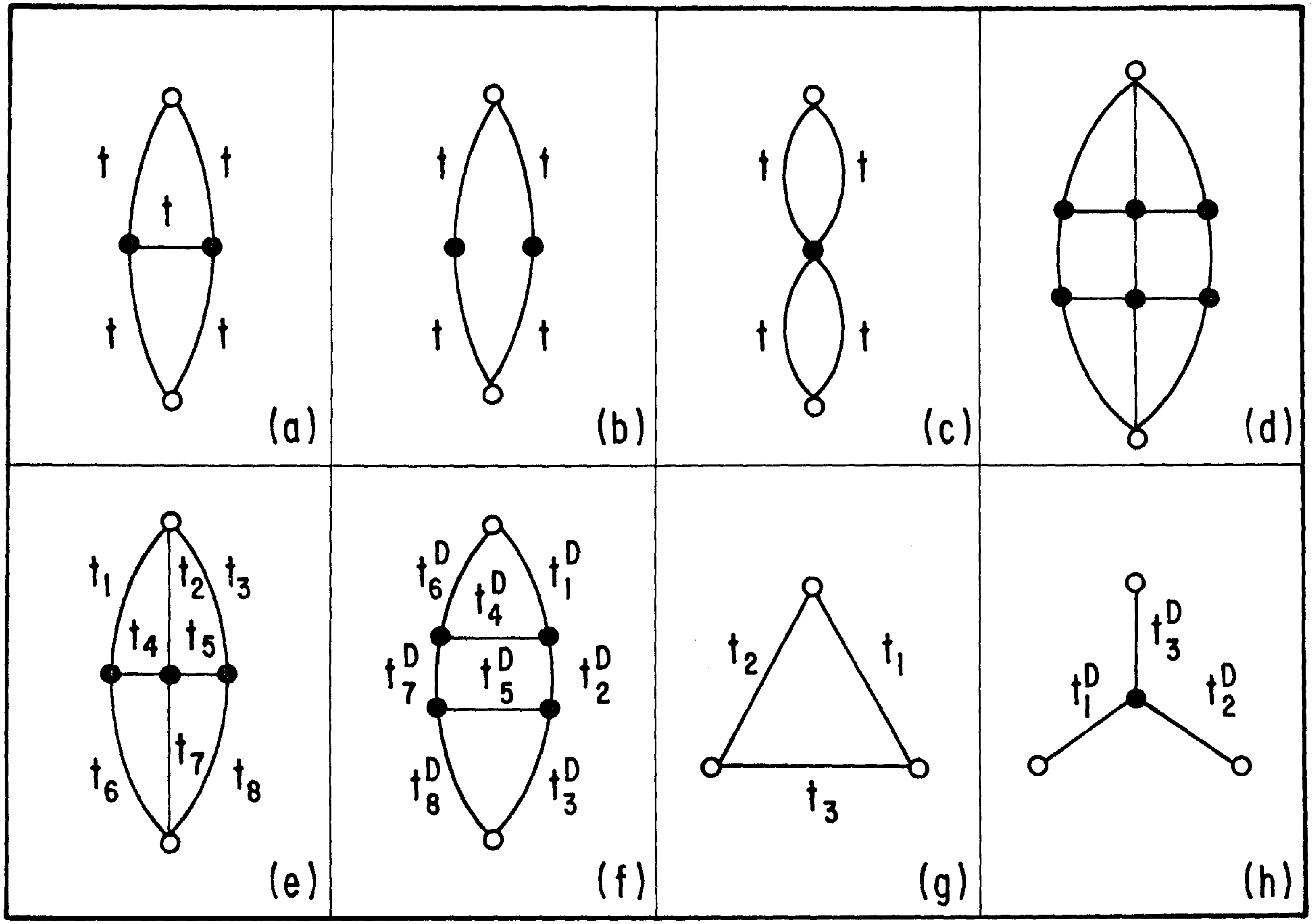
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FIG. 1

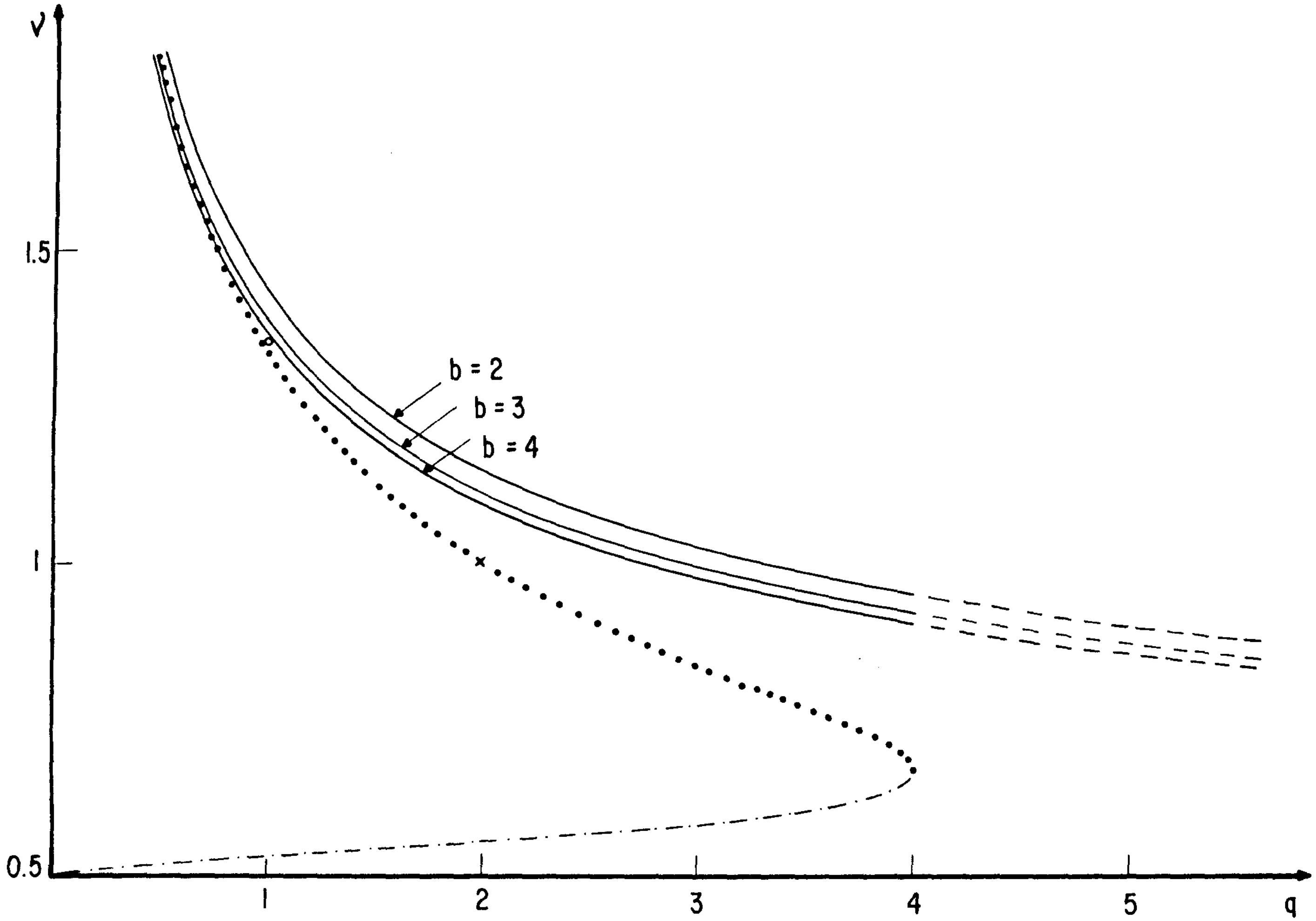

FIG.2