PROBABILITY RENORMALIZATION GROUP TREATMENT OF BOND PERCOLATION IN SQUARE, CUBIC AND HYPERCUBIC LATTICES

by

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ABSTRACT

By using the real space Renormalization Group method proposed by Reynolds, Klein and Stanley we treat bond percolation on d-dimensional cubic lattices and obtain (through various extrapolation methods): a) $p_c = 1/2$ (exact), $\nu_p = 1.351 + 0.012\ (-0.020)$ and $\alpha_p = -0.700 + 0.040\ (-0.024)$ for the first-neighbour square lattice; b) $p_c = 0.252 + 0.003\ (-0.007)$ for the first-and second-neighbour square lattice; c) $p_c = 0.2526 \pm 0.0013$, $\nu_p = 0.840 \pm 0.020$ and $\alpha_p = -0.520 \pm 0.060$ for the first-neighbour cubic lattice; d) $p_c = 0.149 \pm 0.010$, $\nu_p = 0.667 \pm 0.030$ and $\alpha_p = -0.67 \pm 0.12$ for the first neighbour 4-dimensional hypercubic lattice.

Whenever comparison is possible these figures agree fairly well with other available results. We also discuss the "magnetic" scaling power y_h for the square lattice. The influence, on p_c and ν_p, of the symmetry of the cluster and of the "direction" of percolation is exhibited through several bidimensional examples.

1. INTRODUCTION

During the last years, the percolation problem (for reviews see Shante and Kirkpatrick (1971) and Essam (1972)) has received a great deal of attention mainly because of its applications to a variety of physical phenomena, its similarity to thermal phase transitions and its relationship (established by Kasteleyn and Fortuin (1969)) with the critical behaviour of the one-component limit of the Ashkin - Teller - Potts model.The Renormalization Group (RG) approaches introduced for cooperative thermodynamic systems (Ma (1973), Wilson and Kogut (1974), Fisher (1974), Niemeyer and Van Leeuwen (1974) and Wallace and Zia (1978)) have been applied to bond and site percolation problems. Harris et al (1975, 1976) and Dasgupta (1976) made a RG ε - expansion ($\varepsilon \equiv 6-d$). Young and Stinchcombe (1975), Stinchcombe and Watson (1976), Kirkpatrick (1977) , Marland and Stinchcombe (1977) have directly renormalized the occupancy probabilities. In particular, Reynolds et al (1977) (hereafter referred to as RKS) have proposed a simple and efficient position space Renormalization Group for the site and bond percolation problems. Some aspects of this treatment have been analysed in the case of site percolation on a square lattice (Tsallis and Schwachheim (1979)). On the other hand, Bernasconi (1978) have formulated an approach for the conductivity of bond-disordered conductance lattices which contains, as a particular case, the RKS bond probability renormalization.

Very recently, Reynolds et al (1978) have also applied their method (RKS) to the site percolation problem on a square lattice using a sequence of increasingly large finite cells and, by convenient extrapolations, have calculated with a rather high degree of accuracy the critical concentration P_c and the "thermal" y_p and "magnetic" y_h scaling powers*. Finally, the influence of the "direction" of percolation through a given finite RG cluster has been investigated by Sarychev (1977) for site percolation on square lattice.

In the present work we treat, through the RKS approach, the bond percolation problem on d-dimensional cubic lattices. Let us summarize this approach. We must first of all make a partition of the lattice into cells or clusters (whose size will be characterized by a length b) which shall be renormal - ized into (usually of the same type) smaller cells(characterized by a length b'). The expansion or rescaling factor is clearly given by b'/b. The macroscopic process shall be simulated, at the finite size cells level, by the (relatively arbitrary) adoption of the "entries" and "exits" (which we will indicate by arrows, see Table 2) of each cluster. This choice clearly defines the "direction" of percolation. Next we associate to the bigger (smaller) cluster a polynomial $R_b(p)$ $(R'_{b'}(p'))$, where by p we denote the independent bond occupancy probability . Finally, the RG is defined by

$$R'_{b'}(p') = R_b(p) \qquad (1)$$

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* We recall that $\nu_p = y_p^{-1}$, $\alpha_p = 2-(d/y_p)$, $\gamma_p = (2y_h-d)/y_p$, $\eta_p = d+2 - 2y_h$,

$$\beta_p = (d - y_h)/y_p \ , \quad \delta_p = y_h/(d - y_h)$$

where p' plays the role of renormalized occupancy probability. The non-trivial fixed point $p^*(b,b')$ gives an approximation for the critical probability p_c we are looking for. Furthermore, the critical exponent ν_p is approximated, at this level, by (see, for example, Niemeyer and Van Leeuwen (1974) and RKS (1977))

$$\nu_p(b,b') = \frac{\ln \frac{b}{b'}}{\ln \lambda_p(b,b')} \qquad (2)$$

where $$\lambda_p(b,b') \equiv \left.\frac{dp'}{dp}\right|_{p^*(b,b')} = \left\{ \frac{dR_b(p)}{dp} \Big/ \frac{dR'_{b'}(p')}{dp} \right\}_{p^*(b,b')}$$

is the eigenvalue of the linearized transformation (1) in the neighbourhood of $p^*(b,b')$. Of course, we expect that

$$p_c = \lim_{b\to\infty} p^*(b,b') \quad \text{and} \quad \nu_p = \lim_{b\to\infty} \nu_p(b,b') \quad \forall\, b'.$$

By introducing a "ghost" site (Kasteleyn and Fortuin (1969)), the scaling power y_h can be calculated in a similar way (see Reynolds et al (1978)).

In section 2 we discuss the bond percolation on square lattices (p_c, ν_p, y_h for the first-neighbour case and, as universality is expected to hold, only p_c for the first-and second-neighbour case). In section 3 we present the results (p_c and ν_p) for cubic and hypercubic first-neighbour bond percolation. In section 4 we analyze, through some examples, the influence of the symmetry of the cluster and of the "direction" of percolation.

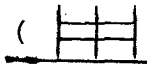
2. SQUARE LATTICE

In this section we apply the above procedure to the square lattice. Let us first of all consider only first-neighbour bonds. We shall adopt the family of (self-dual) clusters obtained by straightforward generalization of the H-shaped ("Wheatstone bridge", see also Bernasconi (1978)) cluster introduced by RKS. The associated polynomials may be written as follows

$$R_b(p) = \sum_{i=0}^{n_b} A_b^{(i)} p^i (1-p)^{n_b - i} \qquad (3)$$

where

$$A_b^{(i)} + A_b^{(n_b - i)} = \frac{n_b !}{i!\,(n_b - i)!} \qquad \forall i, \forall b \qquad (4)$$

The degree n_b of the polynomial is equal to the number of (relevant*) bonds of the cluster and the coefficient $A_b^{(i)}$ is the number of percolating configurations with i unblocked bonds (for a given b). Relation (4) holds because of the self-duality of the chosen family of clusters, and implies that all the $R_b(p)$ are centro-symmetric with respect to the point (1/2,1/2). Hence they are particularly suitable for the first-neighbour square lattice, as the fixed point p*(b,b') is equal to the exact value $p_c = 1/2$ for <u>any</u> choice of b and b'. For instance, we may verify the above properties on the following example ( - shaped cluster):

* For example, the cluster in Fig. 2 has 16 bonds, but only 14 "relevant" ones.

$$R_3(p) = p^{13} + 13\,p^{12}(1-p) + 78\,p^{11}(1-p)^2 + 283\,p^{10}(1-p)^3 +$$

$$+ 677\,p^9(1-p)^4 + 1078\,p^8(1-p)^5 + 1089\,p^7(1-p)^6 +$$

$$+ 627\,p^6(1-p)^7 + 209\,p^5(1-p)^8 + 38\,p^4(1-p)^9 + 3\,p^3(1-p)^{10} =$$

$$= 18\,p^{13} - 117\,p^{12} + 298\,p^{11} - 352\,p^{10} + 149\,p^9 + 39\,p^8 -$$

$$- 10\,p^7 - 37\,p^6 + 2\,p^5 + 8\,p^4 + 3\,p^3 \qquad (5)$$

We were able to establish this kind of closed forms only for $b \leqslant 4$ (see Table 1); bigger values ($5 \leqslant b \leqslant 15$) were treated by a Monte Carlo method, which essentially consists in presenting every coefficient of the polynomial (3) in the following form

$$A_b^{(i)} = r_b^{(i)} \frac{n_b!}{i!\,(n_b - i)!} \qquad (6)$$

Where $r_b^{(i)}$ can be interpreted as the probability that a cluster (of size b) with i randomly distributed unblocked bonds (hence $(n_b - i)$ blocked bonds) percolates. The Monte Carlo approximation is introduced at the level where $r_b^{(i)}$ is replaced by the frequency of percolating configurations satisfying the conditions we have just described. We have worked, for all values of b (and not only for the first-neighbour square lattice we are discussing here, but also for the first-and second-neigh - bour square and simple cubic lattices we shall present later) around $N_b\, n_b \gtrsim 10^6$, where by N_b we denote the total number of Monte Carlo runs. Whenever comparison between Monte Carlo and closed form results was possible the agreement was very good.

In Fig. 1 we have plotted $\nu_p(b,1)$ against b^{-1}. We observe that for $b \geqslant 4$ the numbers oscillate randomly around their mean value 1.351 (2/3 of the points belong to the interval [1.347; 1.365]). Our best proposal is given by $1.351 \begin{smallmatrix} + 0.012 \\ - 0.020 \end{smallmatrix}$, which leads to

$$\alpha_p = -0.700 \begin{smallmatrix} + 0.040 \\ - 0.024 \end{smallmatrix}$$

In what concerns the "magnetic" scaling power y_h we have performed the calculations only for $b,b' \leqslant 4$ ($y_h(3,2)=2.060$; $y_h(4,2) = 2.058$; $y_h(4,3) = 2.056$; see Table 1 for $y_h(b,1)$). By different kinds of extrapolation we arrive to the result 2.0 ± 0.1, which compares to other available results (around 1.9; see Table 1). However we must recognize that the central value 2.0 is probably wrong (for instance, it leads to $\beta_p = \eta_p = \delta_p^{-1} = 0$, which are certainly very hard to believe from the physical analysis of this particular case).

Let us turn our attention to the first-and second-neighbour square lattice within the assumption that there is an unique occupancy probability p. We have used a family of clusters which generalizes the previous one (see, for example, in Fig. 2 the case $b = 2$). We have obtained closed forms for $b \leqslant 3$ and Monte Carlo forms for $b = 4,5$. For illustration, let us present two examples:

$$R_1(p) = p^3 + 3\,p^2(1-p) + 3p(1-p)^2 = p^3 - 3p^2 + 3p \qquad (7)$$

$$R_2(p) = p^{14} + 14\,p^{13}(1-p) + 91\,p^{12}(1-p)^2 + 364\,p^{11}(1-p)^3 + 1001\,p^{10}(1-p)^4 +$$

$$+2002\,p^9(1-p)^5 + 3001\,p^8(1-p)^6 + 3412\,p^7(1-p)^7 + 2919\,p^6(1-p)^8 +$$

$$+ 1810\, p^5(1-p)^9 + 743\, p^4(1-p)^{10} + 164\, p^3(1-p)^{11} + 14\, p^2(1-p)^{12} =$$

$$= 4\, p^{14} - 48\, p^{13} + 259\, p^{12} - 824\, p^{11} + 1696\, p^{10} - 2312\, p^9 + 2007\, p^8 -$$

$$- 908\, p^7 - 66\, p^6 + 320\, p^5 - 137\, p^4 - 4\, p^3 + 14\, p^2 \qquad (8)$$

See Table 1 for the closed form values of $p^*(b,1)$. We also obtained $p^*(4,1) \simeq 0.2734$, $p^*(5,1) \simeq 0.2696$, $p^*(3,2) \simeq 0.2688$, $p^*(4,2) \simeq 0.2652$, $p^*(4,3) \simeq 0.2614$, $p^*(5,2) \simeq 0.2624$, $p^*(5,3) \simeq 0.2589$ and $p^*(5,4) \simeq 0.2563$. Through two different extrapolation methods (one of them consists in plotting $p^*(b,1)$ against b^{-1/ν_p} (see, for example, Reynolds et al (1978) and also Section 3); and the second is a variant adapted to $b' \geq 2$) we arrive to our best proposal $p_c = 0.252\ ^{+\ 0.003}_{-\ 0.007}$. As universality is expected to hold, we have calculated neither ν_p nor y_h. For comparison, we recall that the estimates for the corresponding value for the <u>site</u> problem are 0.410 ± 0.010 and 0.387 ± 0.014 (see Essam, 1972), which are greater than our bond result, as required by theory.

3. CUBIC AND HYPERCUBIC LATTICES

Let us first examine the bond percolation on first-neighbour simple cubic lattice. The family of clusters we have chosen are the straightforward generalization for d=3 of the corresponding family we used in the previous section (for example, b=2 corresponds to ). We have established a closed form of $R_b(p)$ only for b=2 (which is exactly the same as that presented in equation (16) of Bernasconi (1978)).

We treated $3 \leqslant b \leqslant 7$ with a Monte Carlo method. The plot of $\nu_p(b,1)$ versus b^{-1} shown in Fig. 1 did not allow us to obtain a reliable estimate of ν_p. In Fig. 3 we plot $p^*(b,1)$ against b^{-1/ν_p} as suggested by the finite-size relation (Fisher (1971), Sur et al (1976)):

$$p_c - p^*(b,1) \sim b^{-1/\nu_p}$$

The best fit of our data (corresponding to a linear correlation close to 0.9994) was obtained with the following values: $p_c = 0.2526 \pm 0.0013$ and $\nu_p = 0.840 \pm 0.020$ which compare well with other available results (see Table 1). Let us add that, in the fitting process, p_c remains almost unchanged for a rather wide range of ν_p ($0.79 \leqslant \nu_p \leqslant 0.89$). For the case $b=2$ we have also established the scaling factor y_h (see Table 1).

Let us now turn our attention onto the four-dimensional first-neighbour simple hypercubic lattice. Once more the chosen family of clusters is of the same type of those used for $d=2,3$. The unique closed form we established is for $b=2$:

$$\begin{aligned} R_2(p) = & -1862\,p^{28} + 38416\,p^{27} + 374204\,p^{26} + 2285136\,p^{25} - 9794464\,p^{24} + \\ & + 31250840\,p^{23} - 76787640\,p^{22} + 148188216\,p^{21} - 226831310\,p^{20} + \\ & + 275829488\,p^{19} - 264550124\,p^{18} + 196352600\,p^{17} - 108377337\,p^{16} + \\ & + 40698288\,p^{15} - 7838992\,p^{14} - 631312\,p^{13} + 525580\,p^{12} + 93736\,p^{11} - \\ & - 77264\,p^{10} - 3144\,p^{9} + 3694\,p^{8} + 2296\,p^{7} - 376\,p^{6} - 264\,p^{5} - 28\,p^{4} + \\ & + 24\,p^{3} + 8\,p^{2} \end{aligned} \qquad (9)$$

The fixed point $p^*(2,1)$ and $\nu_p(2,1)$ are indicated in Table 1. In spite of the fact we have not studied bigger values of b, it is possible to estimate p_c in the following way. Let us first define the ratio $f_d \equiv p_c/p^*(2,1)$ for different dimensionalities. Hence $f_2 = 0.5/0.5=1$ and $f_3 \simeq 0.2526/0.2085 \simeq 1.2115$. A linear extrapolation leads to $f_4 \simeq 1.4230$, and as we know $p^*(2,1)$ for d=4 we can immediately obtain our first estimate $p_c \simeq 0.1443$. Furthermore, we have used another type of extrapolation, namely: let us define the ratio $g_d \equiv p_c$ (site)$/p_c$ (bond), hence $g_2 \simeq 0.5935/0.5 \simeq 1.187$ (the value 0.5935 has been taken from Reynolds et al (1978)) and $g_3 \simeq 0.312/0.2526 \simeq 1.2352$ (the value 0.312 has been taken from Kirkpatrick (1976)). A linear extrapolation leads to $g_4 \simeq 1.2833$, hence (by using p_c (site; d=4) $\simeq 0.198$ from Kirkpatrick (1976)) p_c(bond)$\simeq$0.1543, which is quite close to our first estimate. Finally, our proposal will be the mean value $p_c = 0.149 \pm 0.010$. The simple procedure we have adopted here is not, of course, expected to be trustful for more than, let us say, one "step" in dimension (from d=3 to d=4 in our case); it can not take into account , for instance, that $d \to \infty$ implies $g_d \to 1$, as expected from general theory. The value of ν_p has been determined by the same kind of procedure. By defining $h_d = \nu_p(2,1)/\nu_p$ ($h_2 \simeq 1.428/1.351 \simeq 1.0570$, $h_3 \simeq 1.031/0.840 \simeq 1.2274$, hence $h_4 \simeq 1.3978$) we have obtained $\nu_p = 0.667 \pm 0.030$, which compares fairly well with Kirkpatrick's result (see Table 1) for site percolation.

4. SYMMETRY OF THE CLUSTER AND DIRECTION OF PERCOLATION

In order to investigate how the symmetry of the basic cell influences the results, we have calculated, for the square lattice, p_c and ν_p using the "assymmetric" clusters shown in Table 2 (the first four examples). We observe that the graphs associated to the first and third cells are dual one of the other (as well as the second and fourth ones among them) and, consequently, their renormalized probabilities satisfy the relation

$$R_b(p) + R_{b_D}(1-p) = 1 \tag{10}$$

from which follows that

$$p^*(b,1) + p^*_D(b_D,1) = 1 \tag{11}$$

and

$$\frac{\nu_p(b,1)}{\nu_p^D(b_D,1)} = \frac{\ln b}{\ln b_D} \tag{12}$$

where the indice D refers to "dual".

Note that a "vertical" percolation in the third cell (giving a renormalized probability bond p'_v) corresponds to an "horizontal" one in the first cell (with a renormalized probability bond p'_H and vice-versa (the same happens for the fourth and second cells).

All the first four clusters violate the full $\pi/2$ rotational symmetry of the square lattice. Comparing the results for the first and second (or the third and fourth) clusters, we verify that $p^*(b,1)$ and $\nu_p(b,1)$ approach to the expected values as b increases. This, of course, happens because the lack of symmetry becomes more "diluted" in larger cells.

Let us conclude this point by saying that a comparison of Tables 1 and 2 shows that the results get sensibly worse when we use clusters which do not preserve the total symmetry of the lattice.

In the last three examples of Table 2, we have constructed a renormalization group by use of a "biased" percolation. The values of $p^*(b,1)$ and $\nu_p(b,1)$ for $b = 2,3$ indicated in Table 2 are considerably worse than the previous ones (see Table 1 for $d = 2$) and they exhibit a slower convergence to the known results.

5. CONCLUSION

Let us conclude by saying that the RKS proposal for RG proved to be very efficient for bond percolation. In particular, the generalized H-shaped clusters are, because of their self-duality, extremely well adapted to the first-neighbour square lattice, as they lead to the exact result $p_c = 1/2$ for any order, and they present a fast convergence in what concerns ν_p.

All our numerical results (d = 2 with or without inclusion of second neighbours, d = 3 and d = 4) for p_c and ν_p (hence α_p) compare fairly well with other available results, with the unique exception of y_h for d = 2 (we obtained $y_h \simeq 2$ instead of $y_h \simeq 1.9$ which is the most commonly accepted value). This discrepancy is not surprising as we did not try to increase the number of points of the series in order to see what happens.

To the best of our knowledge our proposals $p_c = 0.252 \begin{smallmatrix} + 0.003 \\ - 0.007 \end{smallmatrix}$ for the first-and second-neighbour square lattice and $p_c = 0.149 \pm 0.010$ for the simple d = 4 hypercubic lattice are the first ones available in literature (this is not the case for site percolation; see, for example, Essam (1972) and Kirkpatrick (1976)). Also let us add that the former value is strangely close to our proposal for simple cubic lattice $p_c = 0.2526 \pm 0.0013$.

Finally we exhibited, through several examples, that clusters which do not entirely respect the symmetry of the lattice or inconvenient "directions" of percolation on them may

seriously deteriorate the numerical values as well as the quickness of the convergence process, though they present the correct tendencies in all the cases.

CAPTION FOR FIGURES AND TABLES:

Fig. 1 - The approximative critical exponent $\nu_p(b,1)$ as a function of the inverse renormalization expansion parameter for simple square and cubic lattices. ("E" means that the particular point has been obtained from a closed form expression; the others were obtained through a Monte Carlo method).

Fig. 2 - An example (b=2) of the renormalization clusters we used to discuss the bond percolation in the first-and second-neighbour square lattice.

Fig. 3 - The approximative critical probability $p^*(b,1)$ for the simple cubic lattice as a function of b^{-1/ν_p} with $\nu_p = 0.840$. ("E" means that the particular point has been obtained from a closed form expression; the others were obtained through a Monte Carlo method).

Table 1 - Results obtained for the bond percolation on the first-and-second neighbour square, simple cubic and simple hypercubic lattices ($z \equiv$ coordination number). The values we obtained by Monte Carlo method are not quoted here. (*) These values coincide with those obtained by Bernasconi (1978). (†) These values were derived by us through use of scaling laws and values established (for other critical exponents) by the quoted authors.

(a) Dunn et al (1975)

(b) Reynolds et al (1978)

(c) Klein et al (preprint)

(d) Sykes and Essam (1964)

(e) Vyssotsky et al (1961)

(f) Kirkpatrick (1976)

Table 2 - Results obtained, through closed forms, for the bond percolation on the first-neighbour square lattice; the first four clusters do not completely preserve the symmetry of the lattice, and the last three ones refer to a biased "direction" of percolation.

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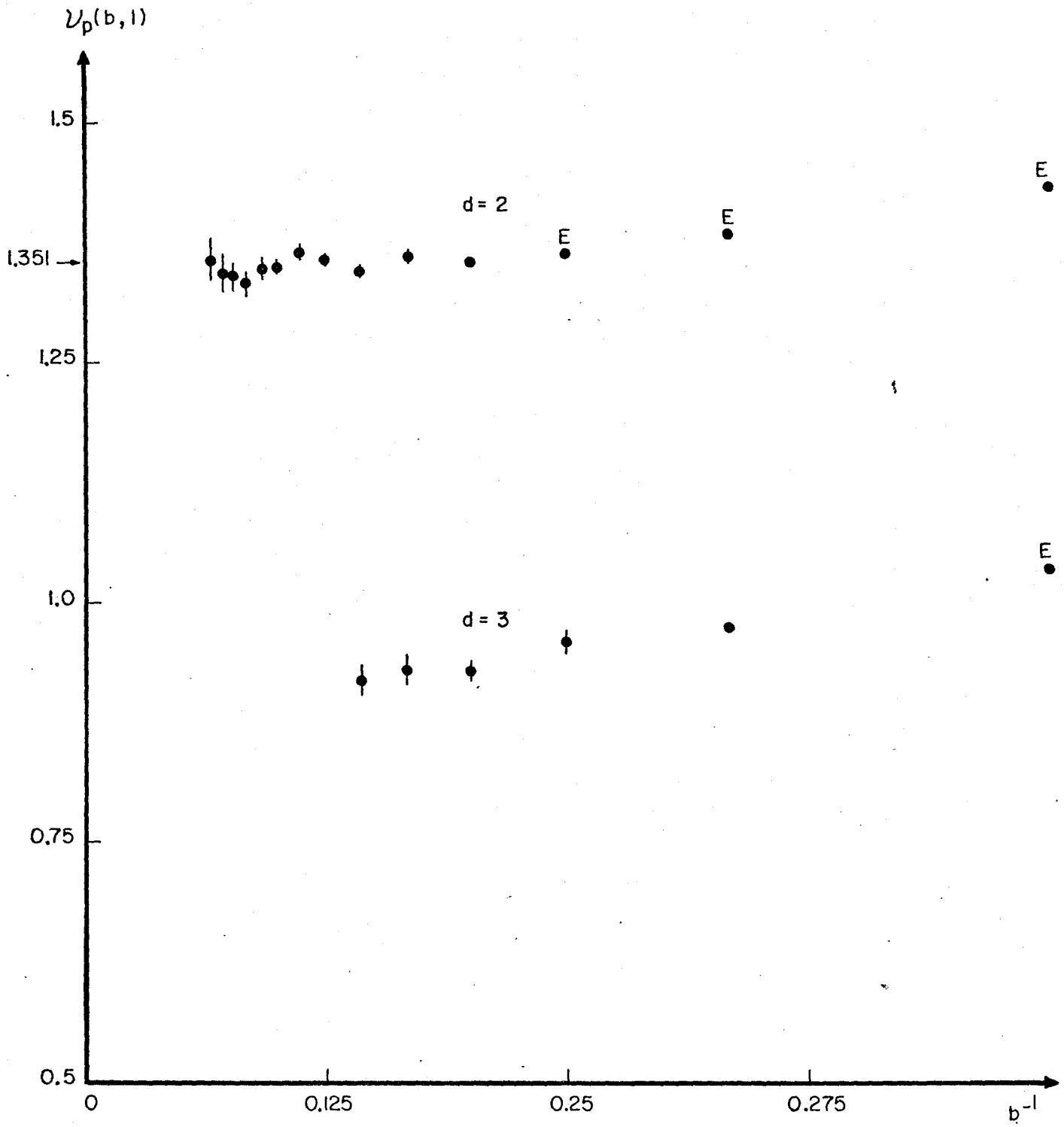


Fig. 1

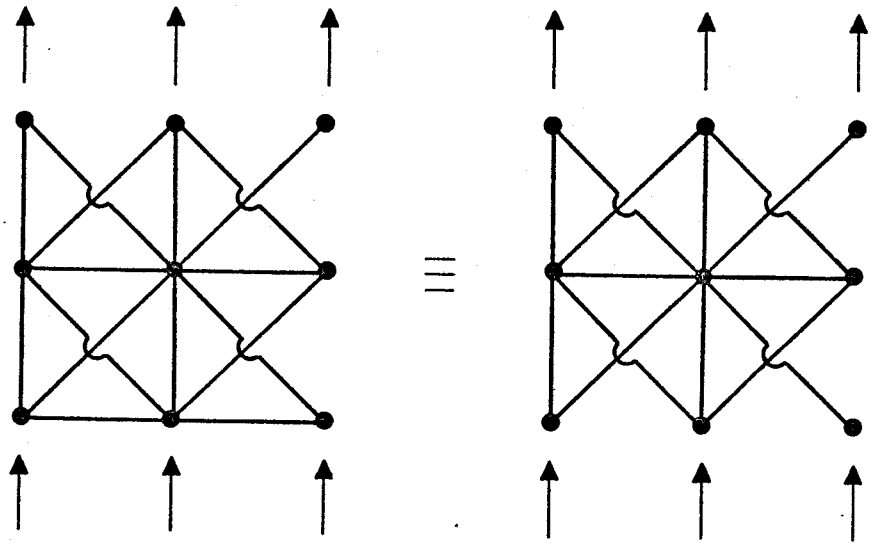


Fig. 2

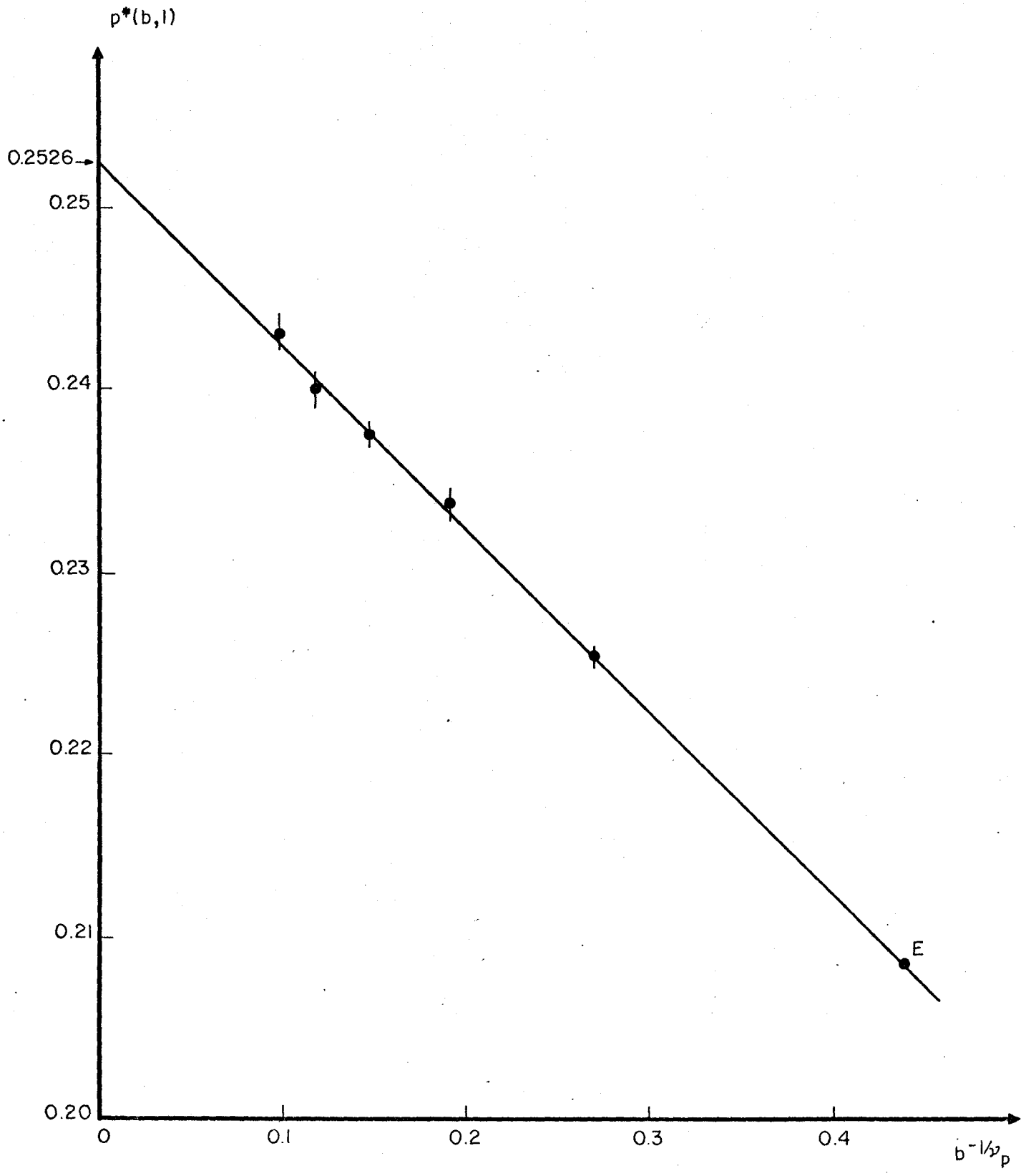
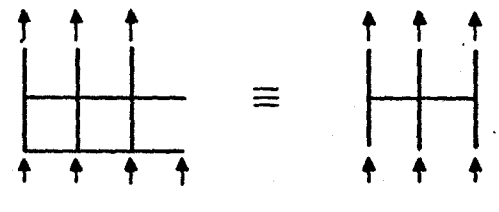
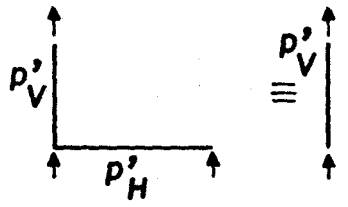
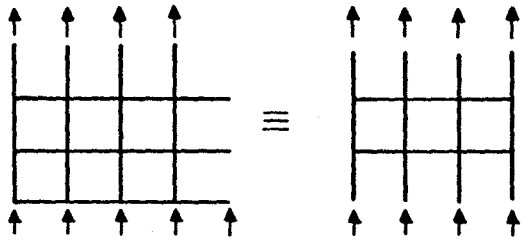
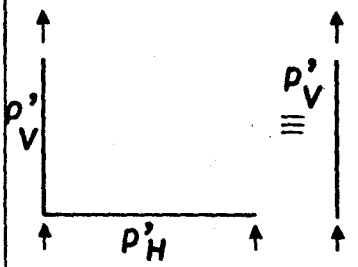
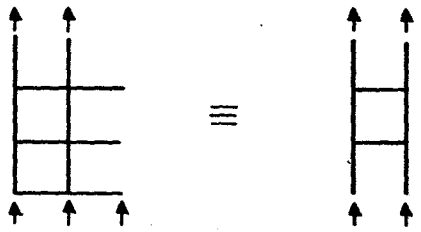
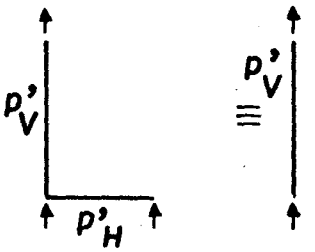
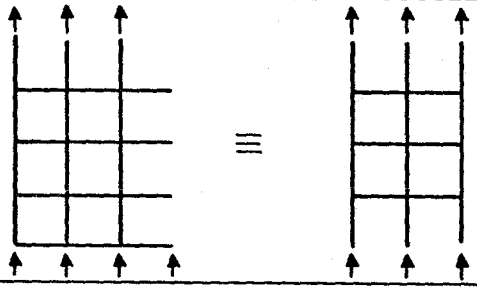
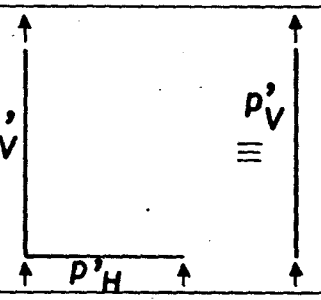
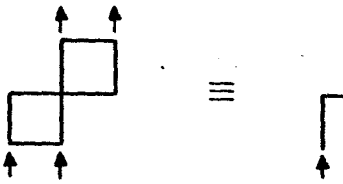
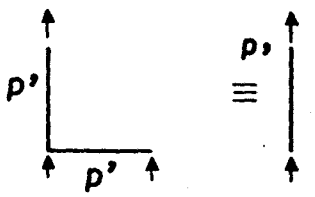
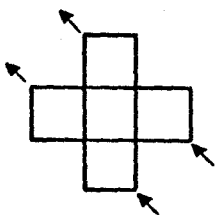
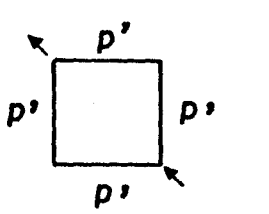
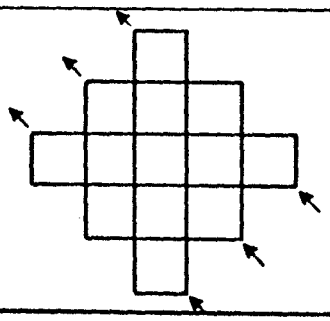
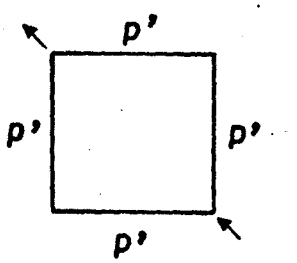


Fig. 3

TABLE 1

Lattice	Subject	b	p_c	ν_p	y_h
d = 2 z = 4	b' = 1	2	1/2*	1.428	1.907
		3	1/2*	1.380*	1.963
		4	1/2	1.363	1.982
	Our best proposal	∞	1/2 (exact)	$1.351 \begin{smallmatrix} + 0.012 \\ - 0.020 \end{smallmatrix}$	2.0 ± 0.1
	Other proposals	-	1/2 (exact)	1.34 ± 0.02 [a] 1.356 ± 0.015 [b] $\frac{\ln\sqrt{3}}{\ln(3/2)} \simeq 1.3547$ [b] [c]	1.89 ± 0.02 [a] (†) 1.898 ± 0.003 [b]
d = 2 z = 8	b' = 1	2	0.2874	-	-
		3	0.2786	-	-
	Our best proposal	∞	$0.252 \begin{smallmatrix} + 0.003 \\ - 0.007 \end{smallmatrix}$	-	-
d = 3 z = 6	b' = 1	2	0.2085*	1.031*	2.739
	Our best proposal	∞	0.2526 ± 0.0013	0.840 ± 0.020	-
	Other proposals	-	0.247 ± 0.005 [d] 0.254 ± 0.013 [e]	0.82 ± 0.05 [a] 0.86 ± 0.03 [f]	2.54 ± 0.13 [a] (†) 2.55 ± 0.17 [f] (†)
d = 4 z = 8	b' = 1	2	0.1014	0.932	-
	Our best proposal	∞	0.149 ± 0.010	0.667 ± 0.030	-
	Other proposals	-	-	0.66 ± 0.04 [f] (†)	-

TABLE 2

ORIGINAL CLUSTER	RENORMALIZED/CLUSTER	b	$p^*(b,1)$	$\nu_p(b,1)$
		2	0.304	1.155
		3	0.410	1.231
		3	0.696	1.829
		4	0.590	1.553
		2	0.671	1.429
		2	0.449	1.593
		3	0.466	1.555