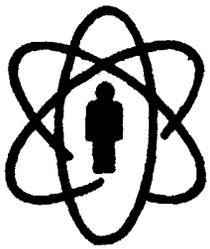

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RENORMALISATION-GROUP SPECIFIC HEAT OF THE SQUARE LATTICE POTTS FERROMAGNET

by

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RENORMALISATION-GROUP SPECIFIC HEAT OF THE SQUARE LATTICE POTTS FERROMAGNET

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ABSTRACT

The free and internal energies and specific heat of the q-state Potts ferromagnet are discussed. A real space renormalisation group approach is presented which recovers a considerable amount of exact particular results for all dimensionalities (hypercubic lattices). The square lattice case is calculated in detail by using self-dual clusters (which provide the exact critical point for all q). Comparison with Onsager results (q=2) is satisfactory; the general tendencies for $q \neq 2$ ($1 \leq q \leq 4$) are exhibited, and the bond percolation limit ($q \to 1$) is worked out with some detail.

During recent years an increasing amount of efforts is being dedicated to the study of the q-state Potts model; this is fully justified if we consider its intrinsic theoretical interest on one hand, and its experimental applications on the other (for a recent and excellent tutorial review see Wu 1982). Because of their relative simplicity, the planar lattices ferromagnets are the most intensively studied and conjectural (exact) proposals for both the thermal and magnetic critical exponents (respectively y_T and y_H) are already available. In what concerns the critical frontiers, those with the anisotropic square, triangular and honeycomb lattices are well established (see Wu 1982 and references therein); futhermore a conjectural (exact) critical frontier has recently been proposed (Tsallis 1982) for the anisotropic 3-12 lattice (which contains the Kagomé lattice as particular case) and its dual; finally, approximate values for the critical points of a great variety of planar and non planar lattices are available as well (see Tsallis and de Magalhães 1981, de Magalhães and Tsallis 1981 and references therein). However quite little is known about the thermal variation, <u>for all temperatures</u>, of relevant quantities (excepting of course the q=2 case which corresponds to the spin - $\frac{1}{2}$ Ising model). The present work is dedicated to a real space renormalisation group (RG) calculation of the square specific heat for all temperatures, and follows along the lines of Mártin and Tsallis 1981a,b. Let us anticipate that the present treatment does not exhibit clear indications of the

q=4 crossover to first-order phase thansitions (Baxter 1973) and is therefore restricted to $0 \leq q \leq 4$.

We consider the following ferromagnetic dimensionless Hamiltonian

$$\mathcal{H}_\gamma(\{\sigma_i\}) = K \sum_{<i,j>} (q\,\delta_{\sigma_i,\sigma_j} + \gamma) \quad (\sigma_i = 1,2,\ldots,q, \forall i) \tag{1}$$

where $K \geq 0$, γ is an arbitrary additive constant, and $<i,j>$ runs over all pairs of first-neighbouring sites of a given d-dimensional lattice; we note $\mathcal{H}'_\gamma(\{\sigma_i'\})$ the renormalized lattice Hamiltonian (associated with a linear expansion factor $b>1$). The partition function invariance implies

$$\sum_{\{\sigma_i'\}} \exp[G_\gamma + \mathcal{H}'_\gamma(\{\sigma_i'\})] = \sum_{\{\sigma_i\}} \exp[\mathcal{H}_\gamma(\{\sigma_i\})] \tag{2}$$

where both sums run over all spin configurations, and G_γ is the usual additive constant (see for example Neimeijer and van Leeuwen 1976). From Eq.(2) immediately follows, in the thermodynamical limit, the relation

$$f_\gamma(K) = g_\gamma(K) + b^{-d} f_\gamma(K') \tag{3}$$

where f_γ is the dimensionless free energy per site and $g_\gamma \equiv G_\gamma/N$, N being the number of sites of the original lattice.

From now on we shall be concerned with the hypercubic lattices (d=1, d=2 and d=3 respectively refer to the linear chain, square and simple cubic lattices). Generalising along the lines of previous works (Reynolds et al 1977, 1980 Yeomans and Stinchcombe 1979,1980, Chaves et al 1979, 1980,Tsallis

and Levy 1980, 1981, Levy et al 1980, de Magalhães et al 1980, Curado et al 1981, Chao et al 1981, Mártin and Tsallis 1981a, b) on bond percolation, Ising and Potts problems, we shall choose, in order to construct our RG recursive relations, the family of two terminal clusters (or more precisely two-rooted graphs) which is illustrated in Fig. 1 (note that the d=2 elements are <u>self-dual</u>, a fact which makes them very suitable for the square lattice, self dual itself). To be more explicit we shall renormalise a b-sized d-dimensional two-terminal cluster into a single bond, whose terminal spins will be noted μ_A and μ_B ($\mu_A, \mu_B = 1,2,\ldots,q$). At the clusters level, the analogous of Eq.(2) is given by

$$\exp\left[L'_\gamma + K'(q\delta_{\mu_A,\mu_B}+\gamma)\right] = \sum_{\{\sigma_i\}} \exp\left[K(q\Pi_{\mu_A\mu_B}+\gamma n_b\right] \qquad (4)$$

where $n_b = b^d+(b-1)^2(d-1)b^{d-2}$ is the total number of bonds of the cluster, the sum runs over all the <u>internal</u> spins configurations, and $\Pi_{\mu_A\mu_B}$ equals the sum of <u>all</u> two-spin interactions of the cluster. For example, for the cluster of Fig. 1a, we have $\Pi_{\mu_A\mu_B} = \delta_{\mu_A,\sigma_1} + \delta_{\mu_A,\sigma_2} + \delta_{\sigma_1,\sigma_2} + \delta_{\sigma_1,\mu_B} + \delta_{\sigma_2,\mu_B}$ and, from Eq.(4), we obtain

$$K' = \frac{1}{q}\, \ell n\, \frac{w_1}{w_2} \qquad (5)$$

$$w_1 \equiv e^{5qK}+2(q-1)e^{2qK}+(q-1)e^{qK}+(q-1)(q-2)$$

$$w_2 \equiv 2e^{3qK}+2e^{2qK}+5(q-2)e^{qK}+(q-2)(q-3)$$

$$L'_\gamma = 5\gamma K + \frac{\gamma}{q}\, \ell n\, \frac{w_2}{w_1} + \ell n\, w_2 \qquad (6)$$

These equations recover, for $q = 2$ and $\gamma = -1$, those appearing, in Mártin and Tsallis 1981a (page 5647); Eq.(4) recovers, for $q = 2$, $\gamma = -1$ and $d = 3$, the vanishing magnetic field Eq.(6) of Mártin and Tsallis 1981b (note, in both cases, the nomenclature identification $L'_\gamma \equiv K'_o$). Eq.(4) provides, for any $d > 1$, a function $K'(K)$ which presents two trivial (stable) fixed points, namely $K = 0$ and $K = \infty$, as well as a non trivial one (noted K_c and unstable), which, for $d \neq 1, 2, \infty$, depends on b; in the limit $d \to 1 (d \to \infty)$, K_c diverges (vanishes) thus yielding the exact result for all values of b and q; for $d = 2$, $K_c = \frac{1}{q} \ell n(1+\sqrt{q})$ thus yielding the exact result for all values of b and q (this is a consequence of the already mentioned self-duality); finally for $1 < d < 2$ ($d > 2$ but finite), the present approach presumably underestimates (overestimates), for any finite value of b, the real critical temperature, and hopefully tends, for all values of q, to the exact result in the limit $b \to \infty$ (numerical support to this speculation can be found in de Magalhães et al 1980 for $q = 1$, and in Mártin and Tsallis 1981 b for $q = 2$).

Let us now relate $g_\gamma(K)$ and $L'_\gamma(K)$ by introducing a new function $D(K)$ (which has to be found) through the following equation

$$g_\gamma(K) = D(K) L'_\gamma(K) \tag{7}$$

By substituting this into Eq.(3) we obtain

$$f_\gamma(K) = D(K) L'_\gamma(K) + b^{-d} f_\gamma(K') \tag{8}$$

If we perform now the transformation $\gamma \to \gamma+\lambda$, λ being an arbi-

trary real number (i.e. if we translate the zero energy), the hypercubic lattice free energy transforms as $f_\gamma(K) \to f_{\gamma+\lambda}(K) = f_\gamma(K) + d\lambda K$ (see Eq.(1)). Consequently g_γ transforms as $g_\gamma(K) \to g_{\gamma+\lambda}(K) = g_\gamma(K) + d\lambda \left[K - b^{-d}K'(K)\right]$ in order to preserve Eq.(3). Analogously the preservation of Eq.(4) implies that L'_γ transforms as $L'_\gamma(K) \to L'_{\gamma+\lambda}(K) = L_\gamma(K) + \lambda\left[n_b K - K'(K)\right]$. Finally, following along the lines of Mărtin and Tsallis 1981b, we impose that Eq.(7) is preserved in form (i.e. D(K) does not depend on λ), and immediately obtain that

$$D(K) = \frac{d}{n_b} \frac{K - b^{-d}K'(K)}{K - n_b^{-1}K'(K)} \tag{9}$$

which univoquely determines the function D(K). It can be shown that, in the limit $K \to 0$ ($K \to \infty$), $K' \propto K^b$ ($K' \sim b^{d-1}K$). Consequently, while K grows from zero to infinity, D(K) decreases (monotonically) from d/n_b to $d(b-1)/(bn_b - b^d)$. Furthermore, in the limit $b \to \infty$, $n_b \sim db^d$, therefore D becomes a pure topological number ($D \sim b^{-d}$) for all temperatures.

We have now all the elements for establishing, through succesive derivations of Eq.(8), the complete set of operational recursive relations which numerically provide, as functions of the inverse temperature K, the free energy, the internal energy ($\propto df_\gamma/dK$) and the specific heat per site $C = k_B K^2 (d^2 f_\gamma / dK^2)$ (C independs on γ); these relations are (besides Eq.(8))

$$\frac{df_\gamma}{dK} = \frac{dD}{dK} L'_\gamma + D \frac{dL'_\gamma}{dK} + b^{-d} \frac{df_\gamma}{dK'} \frac{dK'}{dK} \tag{10}$$

$$\frac{d^2 f_\gamma}{dK^2} = \frac{d^2 D}{dK^2} L'^{}_\gamma + 2 \frac{dD}{dK} \frac{dL'_\gamma}{dK} + D \frac{d^2 L'_\gamma}{dK^2} + b^{-d} \left[\frac{d^2 f_\gamma}{dK'^2} \left(\frac{dK'}{dK} \right)^2 + \frac{df_\gamma}{dK'} \frac{d^2 K'}{dK^2} \right] \quad (11)$$

The analysis of relation (4) and the use of Eqs.(8)-(11) yields (through tedious and quite complex graph considerations) the following general results for $K = 0$:

$$f_\gamma(0) = \frac{db^d (1-b^{-1})}{n_b (1-b^{-d})} \ell nq \xrightarrow{(b\to\infty)} \ell nq \quad (\underline{\text{exact}}); \quad (12)$$

$$\left. \frac{df_\gamma}{dK} \right|_{K=0} = \begin{cases} d(1+\gamma) - \dfrac{d(d-1)}{(d+3)^2} \ell nq & \text{if } b=2 \\ d(1+\gamma) \quad (\underline{\text{exact}}) & \text{if } b \geq 3 \ ; \end{cases} \quad (13)$$

$$\left. \frac{d^2 f_\gamma}{dK^2} \right|_{K=0} = \begin{cases} d(q-1) - \dfrac{d(d-1)}{(d+3)^3} \left[(2d^2+5d+1) + 2(d+3)(q-2) \right] \ell nq & \text{if } b=2 \\ d(q-1) - \dfrac{16d(d-1)}{(4d+5)^2} \ell nq & \text{if } b=3 \\ d(q-1) \quad (\underline{\text{exact}}) & \text{if } b \geq 4 \ ; \end{cases} \quad (14)$$

and, for $b \geq 5$ (because of their complexity and relative irrelevance, we have not looked for the analytic expressions corresponding to $b < 5$),

$$\left. \frac{d^3 f_\gamma}{dK^3} \right|_{K=0} = d(q+1) \left[(q-2) + \frac{12(b-1)(d-1)}{b^2 + (b-1)^2 (d-1)} \right] \quad (15)$$

$$\xrightarrow{(b\to\infty)} d(q-1)(q-2) \quad (\underline{\text{exact}})$$

and finally

$$\left.\frac{d^j f_\gamma}{dK^j}\right|_{K=0} = \left.\frac{d^j f_\gamma^{exact}}{dK^j}\right|_{K=0} + o(jd/b) \qquad (16)$$

therefore, in the limit $b \to \infty$, <u>all</u> derivatives are exact at K=0. Analogously we obtain, in the limit $K \to \infty$,

$$f_\gamma \sim d(q+\gamma)K \qquad (\underline{\text{exact}}) \qquad (17)$$

The trivial case q=1 (to be not confused with the non trivial limit $q \to 1$ which will be discussed later on and which is isomorphic to bond percolation; Kasteleyn and Fortuin 1969) deserves a special mention: the present RG yields, for <u>all</u> values of b and K, $f_\gamma = d(1+\gamma)K$ hwich is the <u>exact</u> result for all dimensionalities. Finally, in the case d=1 we obtain, for <u>all</u> values of b, K and q, $f_\gamma = \ell n\{e^{\gamma K}[e^{qK} + (q-1)]\}$, which is the <u>exact</u> result.

For the case d = 2 (square lattice) we have numerically worked out equations (10) and (11) (together with Eqs.(4) and (9)) for b = 2,3,4,5 and q = 2,3,4 as well as $q \to 1$; the results are presented in Figs. 2-4 and Table 1 (we recall that the present RG yields, for all values of b and q, the <u>exact</u> critical point K_c). In Fig.2 we compare the q = 2 RG results with Onsager's exact result; in particular, in Fig.2.b we exhibit how the present procedure (based on Eq.(9)), which is the natural extension of the one we introduced in Martin and Tsallis 1981b for the d > 2 Ising model, is superior to the one we had used in Martin and Tsallis 1981a for the d = 2 Ising model (note the

disappearance of the slightly negative values for the specific heat in the high-K region).

The present results (particularly Eqs.(12)-(17), Figs. 2 and 3 and Table 1) strongly suggest that the RG approach here introduced converges, in the limit $b \to \infty$, towards the (still unknown for $q \neq 2$) exact free and internal energies and specific heat, for all values of K. However it might occur that this is true only for the low-K region (see Eq.(16)); indeed the apparent absence (up to b=5) of RG indications for the expected $q > 4$ first-order phase transitions could be related to convergence anomalies in the neighbourhood of the critical point (or to a need for a larger RG parameter-space).

In Fig.4 we have presented, as a function of the bond independent occupancy probability $p \equiv 1-e^{-K} \in [0,1]$ (see Kasteleyn and Fortuin 1969), the non trivial percolation quantity $C_p \equiv k_B^{-1}(\partial C/\partial q)_{q=1} = \lim_{q\to 1} C/k_B(q-1)$. Let us give some details on the bond percolation limit ($q \to 1$); we recall that two sites of the lattice are said to belong to the same cluster (do not confuse with the same word used in the sense of Fig.1) if and only if they are connected by occupied bonds (each isolated site is considered as a cluster as well). It is well known (Kasteleyn and Fortuin 1969, Fortuin and Kasteleyn 1972, Stephen 1976 and Wu 1977) that the average number of clusters per site is given by $n_p(p) \equiv \left[\frac{\partial \tilde{f}(\tilde{K})}{\partial q}\right]_{q=1}$ with $p \equiv 1-e^{-\tilde{K}}$ and $\tilde{f}(\tilde{K}) \equiv f_{\gamma=0}(K)$ where $\tilde{K} \equiv qK$. Consequently Eq. (8) implies

$$n_p(p) = \left[\tilde{L}'(\tilde{K}(p))\,\frac{\partial \tilde{D}(\tilde{K}(p))}{\partial q} + \tilde{D}(\tilde{K}(p))\,\frac{\partial \tilde{L}'(\tilde{K}(p))}{\partial p}\right]_{q=1} + b^{-d}\{n_p(p') + \left[\frac{\partial \tilde{f}(\tilde{K}')}{\partial K'}\,\frac{\partial \tilde{K}'}{\partial q}\right]_{q=1}^{\tilde{K}'=\tilde{K}(p')}\}$$

where $\tilde{D}(\tilde{K}) \equiv D(\tilde{K})$ and $\tilde{L}'(\tilde{K}) \equiv L_{\gamma=0}(K)$.

Furthermore by using Eqs. (12)-(15) we obtain

$$n_p(0) = \frac{db^d(1-b^{-1})}{n_b(1-b^{-d})} \xrightarrow{(b\to\infty)} 1 \quad (\underline{\text{exact}}); \tag{19}$$

$$\left.\frac{dn_p}{dp}\right|_{p=0} = \begin{cases} -d\left[1+\dfrac{d-1}{(d+3)^2}\right] & \text{if } b=2 \\ \\ -d \quad (\underline{\text{exact}}) & \text{if } b \geq 3; \end{cases} \tag{20}$$

$$\left.\frac{d^2n_p}{dp^2}\right|_{p=0} = \begin{cases} -\dfrac{2d(d-1)(d^2+2d-1)}{(d+3)^3} & \text{if } b=2 \\ \\ -\dfrac{16d(d-1)}{(4d+5)^2} & \text{if } b=3 \\ \\ 0 \quad (\text{exact}) & \text{if } b\geq 4; \end{cases} \tag{21}$$

$$\left.\frac{d^3n_p(p)}{dp^3}\right|_{p=0} = \frac{12d(d-1)(b-1)}{b^2+(d-1)(b-1)^2} \xrightarrow{(b\to\infty)} 0 \quad (\underline{\text{exact}}) \text{ if } b\geq 5 \tag{22}$$

The use of Eq. (16) leads to the fact that, in the limit $b \to \infty$, the exact derivatives $(d^j n_p/dp^j)_{p=0}$ are recovered for all values of j and d. For d=1, the trivial exact result $n_p(p) = 1 - p$ is obtained for all values of b. In Fig. 5 we present $n_p(p)$ for the case $d = b = 2$.

Let us conclude by recalling that we have treated, within a real space renormalisation group framework, the specific heat (and related quantities) associated with the square-lattice q-state Potts ferromagnet. Although we cannot prove that the present approach tends (at least for the high-temperature region), in the limit of increasingly large cells, towards the (unknown for $q \neq 2$) exact result, several positive tests (some d=1 results as well as Fig.2 and Eqs.(12)-(17) and consequently Eqs.(19)-(23)) are encouraging in that sense (at least as long as the first-order phase transitions, existing for sufficiently high q, are not involved). Therefore results like those exhibited in Figs.3-5 can possibly be considered as reasonable approximations of reality.

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CAPTION FOR FIGURES AND TABLE

Fig. 1 - Examples of two-terminal clusters (or two-rooted graphs); o(•) denotes terminal (internal) sites or nodes. (a) d=b=2; (b) d=b=3; (c) d=4 and b=2

Fig. 2 - Specific heat as a function of the inverse reduced temperature for the d=2 Ising ferromagnet (q=2); the arrows indicate the critical point (exact). Onsager:... present RG:——; Mártin and Tsallis 1981a RG: ——.——.——. (a) influence of the RG cluster size b; (b) beneficial effect of the present RG procedure (Eq.(9))

Fig. 3 - RG specific heat as a function of the inverse reduced temperature for the d=2 q-state Potts ferromagnet (... for b=2, ∀q; ——for b=5, 4 and 3 if q=2, 3 and 4 respectively); the arrows indicate the critical points (exact); the downwards arrow indicates the critical point associated with the limit $q \to 1$ (C vanishes for all K, in this limit).

Fig. 4 - The d=b=2 RG percolation "specific heat" $C_p \equiv k_B^{-1}(\partial C/\partial q)_{q=1}$ as a function of the bond occupancy probability $p \equiv 1-e^{-K}$; the arrow indicates the critical point (exact).

Fig. 5 - The d=b=2 RG percolation "free energy" (i.e. average number of clusters per site) $n_p \equiv (\partial f_o/\partial q)_{q=1}$ as a function of the bond occupancy probability $p \equiv 1-e^{-K}$; the arrow indicates the critical point (exact).

Table 1 - Present d=2 RG critical values (and comparison with exact results whenever available) for the average number of clusters per site n_p, reduced internal energy $df_{-q/2}/dK$, bond percolation "specific heat" C_p, specific heat C and α exponent ($C \propto |K-K_c|^{-\alpha}$ and $C_p \propto |p-p_c|^{-\alpha}$ in the neighbourhood of the critical point); α is calculated from $2-\alpha=d\nu$ where $\nu = \ell n b / \ell n (dK'/dK)_{K=K_c}$. The $q = 2$ exact results are from Onsager 1944; the $q \neq 2$ exact results for α are from den Nijs 1979 conjecture (for $q=4$ a logarithmic factor in the specific heat appears as well; Nauenberg and Scalapino 1980 and Cardy et al 1980), and those for $(df_{-q/2}/dK)_{Kc}$ are from Baxter et al. 1978 ($(df_{-q/2}/dK)_{Kc} = \sqrt{q}$). We recover previous results from one and/or the other of the following references: (a) Reynolds et al 1977, Chaves et al 1979, 1980, de Magalhães et al 1980; (b) Yeomans and Stinchcombe 1980; (c) Tsallis and Levy 1981; (d) Yeomans and Stinchcombe 1979, Tsallis and Levy 1980, Levy et al 1980; (e) Mártin and Tsallis 1981a, Curado et al 1981.

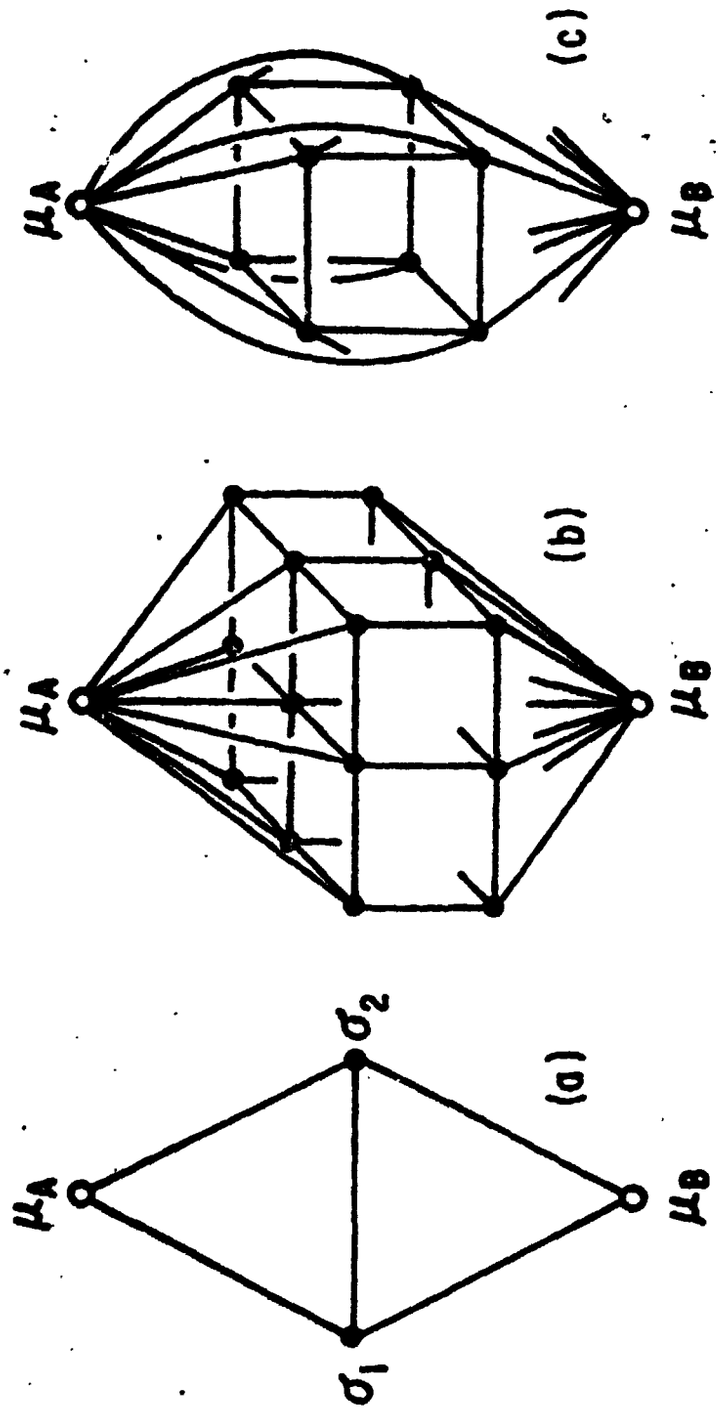
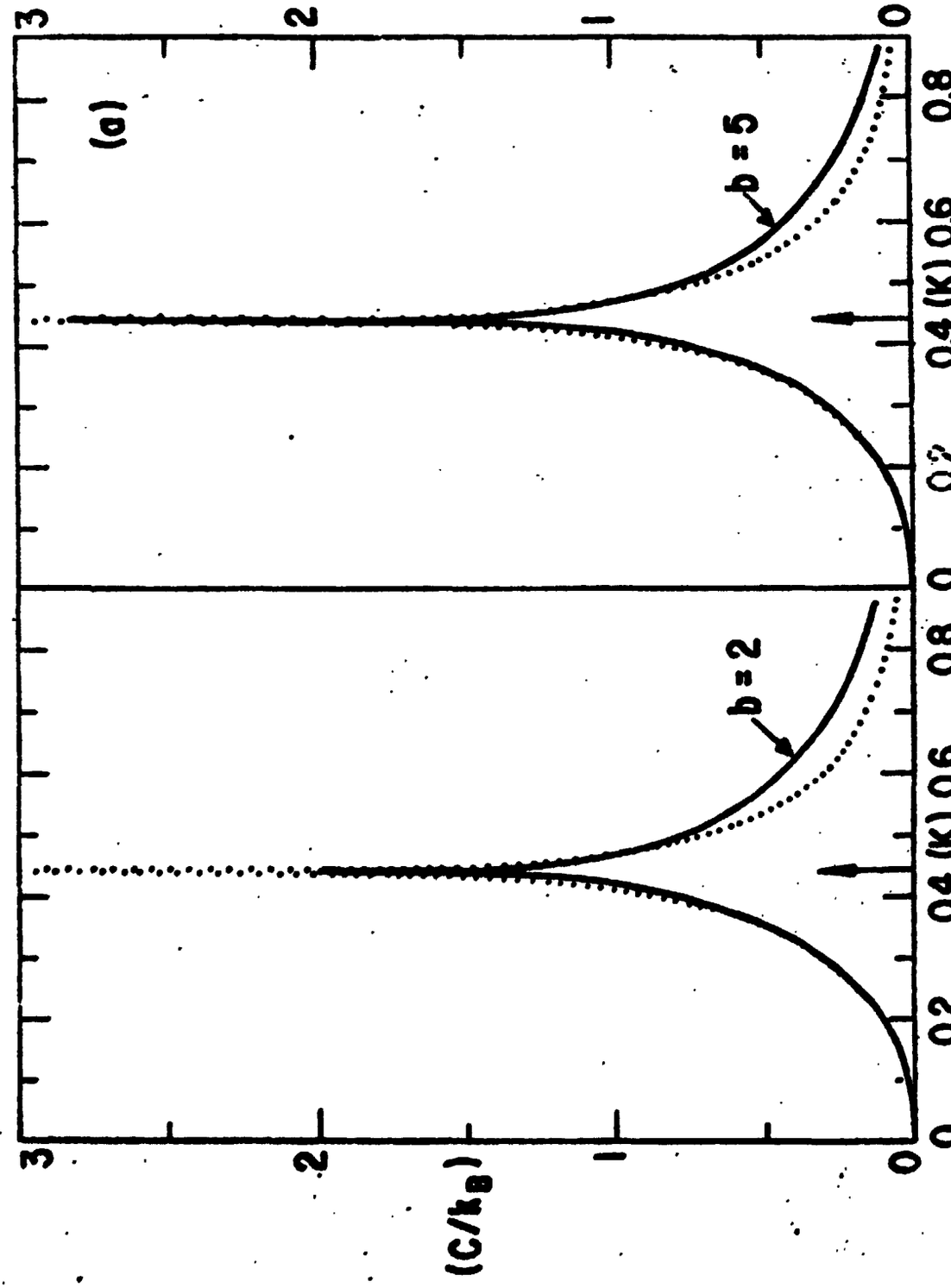


FIG.1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b=2
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0.8
1
2
3

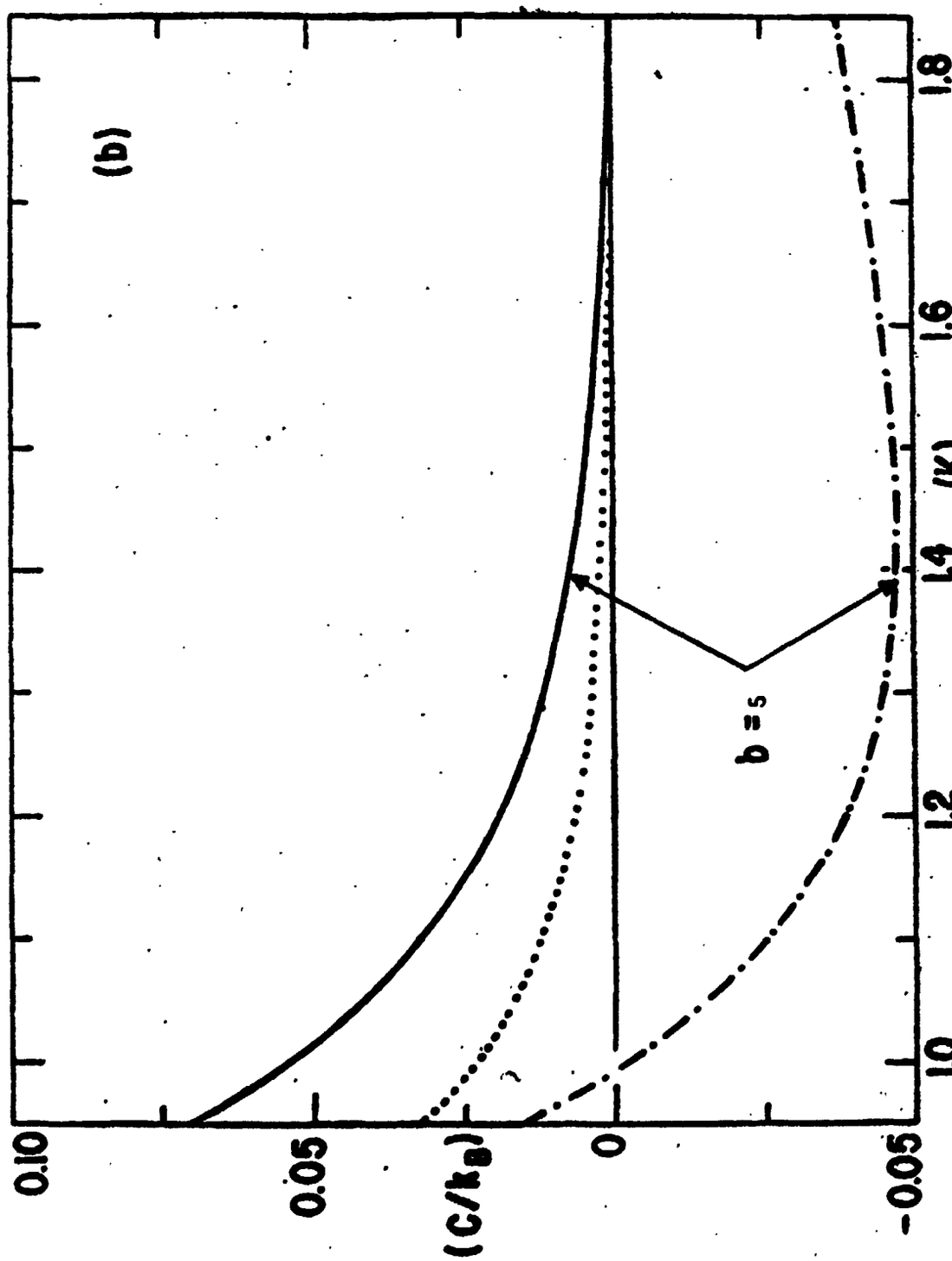

Fig. 2

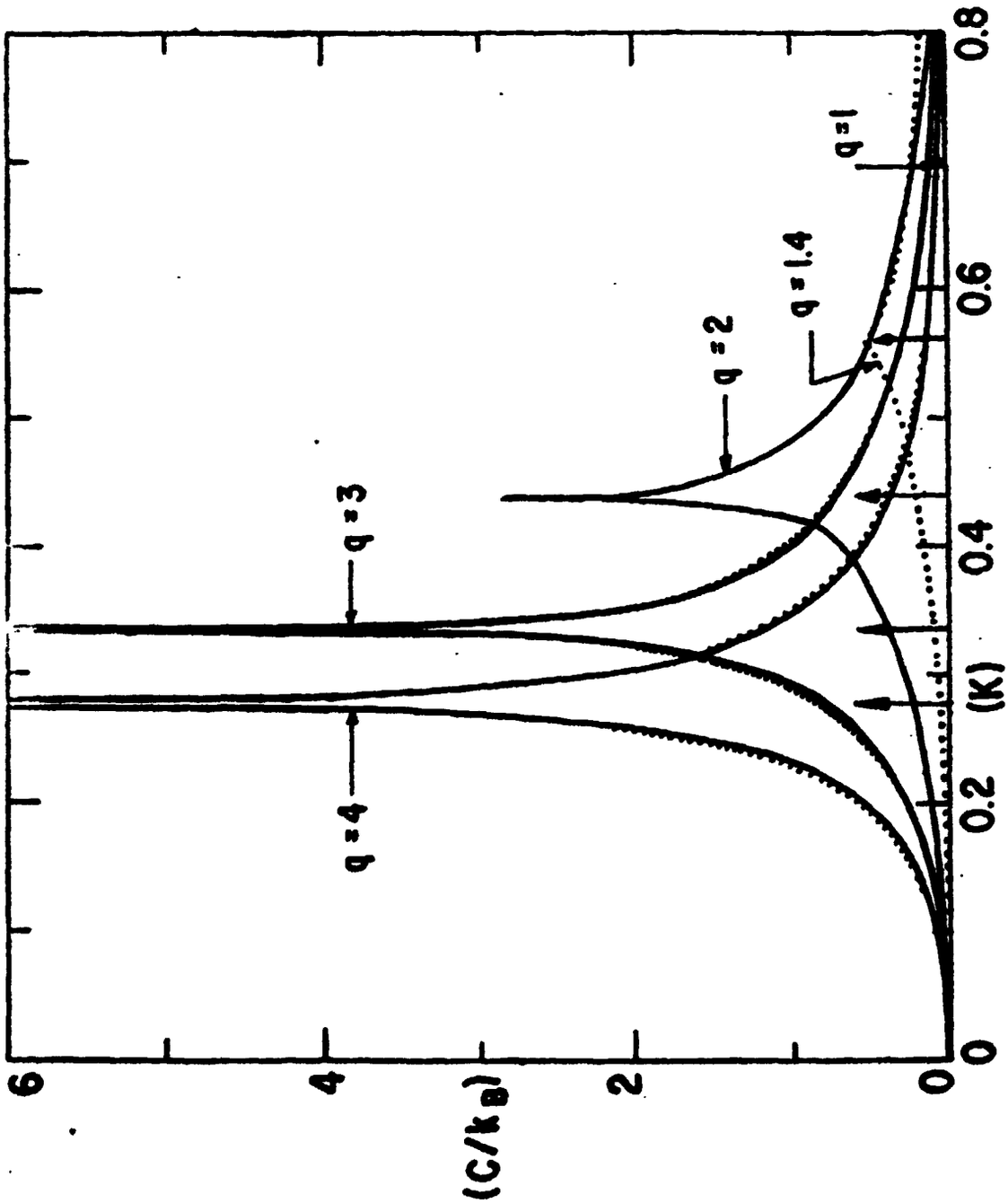

FIG.3

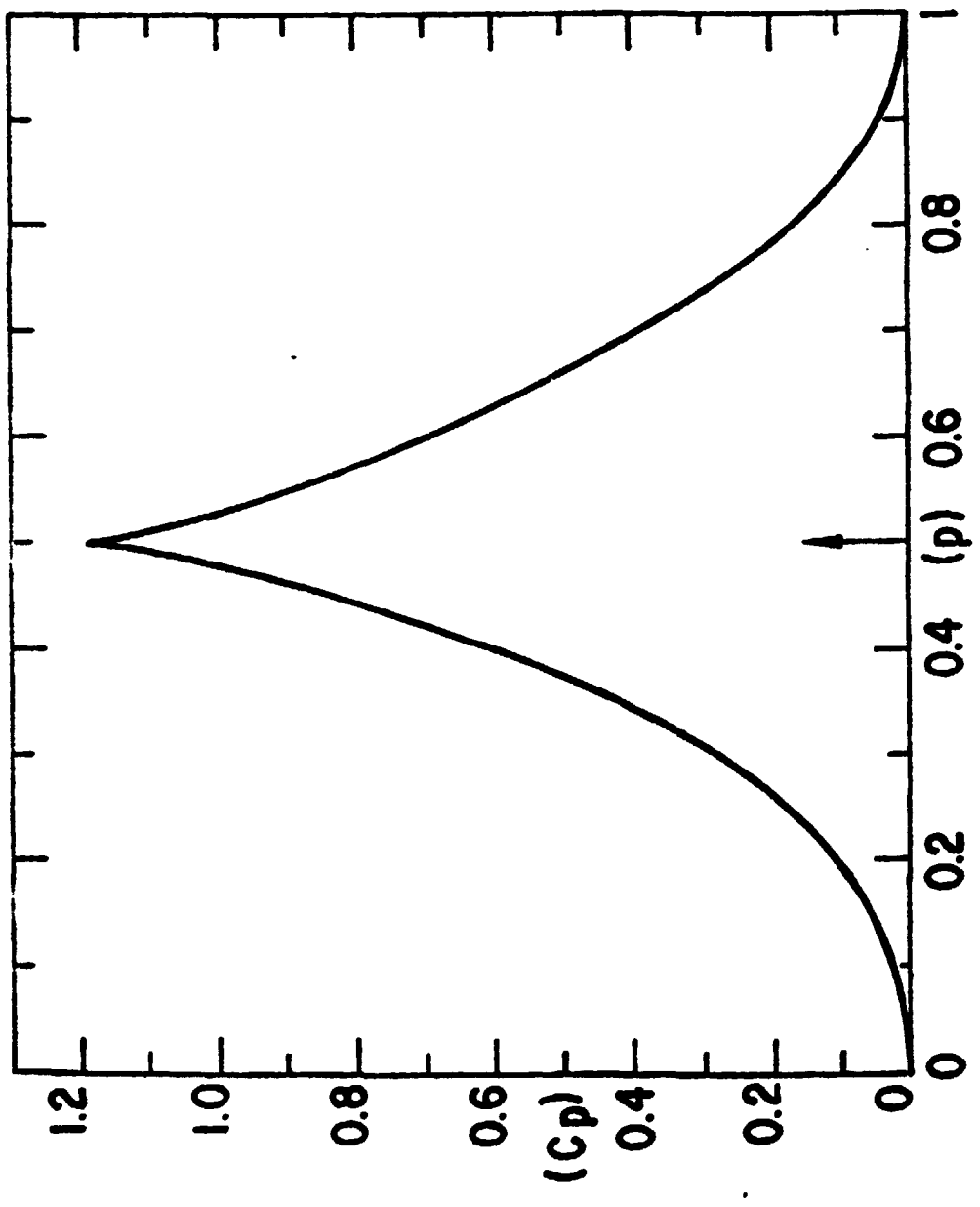

FIG. 4

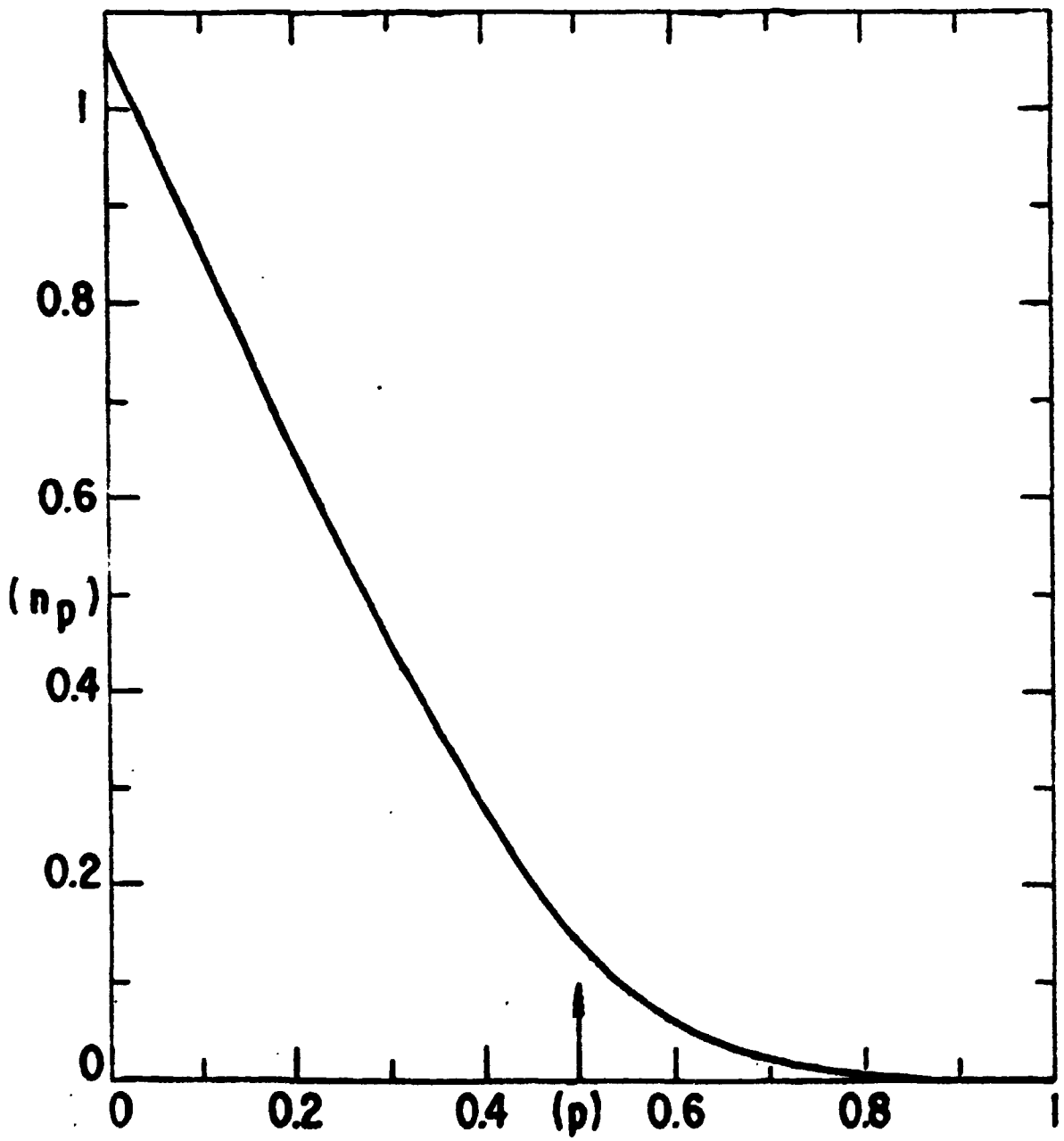

FIG. 5

		b = 2	b = 3	b = 4	b = 5	exact
q → 1	$n_p(p_c)$	0.1406	-	-	-	-
	$1/C_p(p_c)$	0.8410	-	-	-	-
	α	[a,b,c] -0.8553	[a,c] -0.7594	[a,c] -0.7254	[a] -0.7106	-2/3
q = 2	$df_{-q/2}/dK\|_{K_c}$	1.3412	1.3465	1.3566	1.3652	$\sqrt{2} = 1.4142$
	$k_B/C(K_c)$	0.5024	0.4059	0.3712	0.3536	0
	α	[b,c,d,c] -0.2973	[c,e] -0.2187	[c,e] -0.1900	[e] -0.1758	$0(\ell n)$
q = 3	$df_{-q/2}/dK\|_{K_c}$	1.5420	1.5520	1.5764	-	$\sqrt{3} = 1.7321$
	$k_B/C(K_c)$	0.0558	0	0	0	0
	α	[b,c] -0.0471	[c] 0.0234	[c] 0.0495	0.0633	1/3
q = 4	$df_{-q/2}/dK\|_{K_c}$	1.6563	1.6691	-	-	$\sqrt{4} = 2$
	$k_B/C(K_c)$	0	0	0	0	0
	α	[b,c] 0.1033	[c] 0.1688	[c] 0.1934	0.2068	2/3

TABLE 1

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