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ABSTRACT

Certain types of real-space renormalisation groups (which essentially approximate Bravais lattices through hierarchical ones) do not preserve standard thermodynamic convexity properties. We point out that this serious defect is not intrinsic to any real-space renormalisation. It can be avoided if form-invariance (under uniform translation of the energy scale) of the equation connecting the Bravais lattice (we intend to study) to the hierarchical one (which approximates it) is demanded. In addition to that we analyse expressions for the critical exponents ν and α corresponding to hierarchical lattices; these are consistent with Melrose recent analysis of the fractal intrinsic dimensionality.

Key-words: Real-space renormalisation group; Specific heat; Ising and Potts models; Bravais and hierarchical lattices.

I - INTRODUCTION

During very recent years, extensively used real-space renormalisation-group (RG) methods approximate Bravais lattices (which are translationally invariant) by hierarchical lattices (which are self-similar, i.e. scale-invariant). The point whether these methods are able to satisfy, *for all temperatures* (or analogous intensive parameters, e.g., concentration in diluted systems), thermodynamically correct convexity properties (e.g., *positive* specific heat) is an important one. Some treatments (Niemeijer and van Leeuwen 1976, Kadanoff 1975, Kadanoff et al 1976, Martin and Tsallis 1981 (a); see also Dunfield and Noolandi 1980) do not satisfy (see discussion by Kaufman and Griffiths 1983); others (Martin and Tsallis 1981 (b), 1983) do satisfy. In any case, many of these RG's are commonly said to be *exact* for the hierarchical lattices (Berker and Ostlund 1979, Bleher and Zalys 1979) which intend to approximate d-dimensional Bravais lattices; to be more precise they are said to be exact as long as they concern systems which are *classical*, in the sense that all relevant commutators vanish. Three interesting questions can be raised about the *exactness* of these RG's: (i) do they provide the *exact* critical exponent ν ? ; (ii) assuming a hyperscaling law $2-\alpha = d_f\nu$ ($\alpha \equiv$ specific heat critical exponent), what is the dimensionality d_f to be put therein ? ; (iii) are the standard thermodynamic convexity properties (such as positivity of the specific heat) satisfied ?. The (possible) answers to these questions constitute the central scope of the present paper.

II - CORRELATION LENGTH AND SPECIFIC HEAT

Since critical exponent ν is associated with the correlation length ξ (e.g., $\xi \propto |T-T_c|^{-\nu}$ for thermal phase transitions) question (i) implicitely admits a well defined (fluctuation) correlation function $S(r)$ of the type $\exp(-r/\xi)$, which in turn implies a well defined concept of distance r in hierarchical lattices. Although the general problem of the metric in such lattices is yet unsolved, Melrose 1983 (a, b) has recently given enough insight to make the following reasonable proposal, at least for the two-rooted self-dual Wheatstone-bridge-like hierarchical lattices (the standard $b = 2,3,4$ cases are indicated in Fig. 1; see Tsallis and Levy 1981, Martin and Tsallis 1981 (a) and references therein). The distance between roots (*terminals*) is defined as the length of the shortest path joining them ($r = b^n$ in our example, where n is the number of times we have applied the recurrence which constructs the hierarchical lattice; see Fig. 2) ; $S(r)$ is defined as the correlation function between the two terminals. Within this context, the exact ν for the q-state Potts ferromagnet in the present $b = 2$ example will be given by

$$\nu = \ell n 2 / \ell n \frac{8 + 13\sqrt{q} + 5q}{8 + 7\sqrt{q} + q} \qquad (1)$$

This expression recovers, for $q = 1$ (the bond percolation problem) and $q = 2$ (the spin 1/2 Ising model), the results appearing for instance in Reynolds et al 1977 and Yeomans and Stinchcombe 1979 (a,b) respectively. It might well be that the answer to question (i) is "yes" in general. In particular as we shall see just below, numerical values appearing in Kaufman and Griffiths 1983 are not inconsistent with this point of view (at least for the $b = 2$ case).

It is important to stress that expression (1) is intended to be exact *for all values of q, therefore excluding first-order phase transitions*, in contrast with what occurs for Bravais lattices where non vanishing latent heat exists for $q>q_c(d)$ ($q_c(2)=4$, Baxter 1973 and Straley and Fisher 1973; $q_c(3)\simeq 3$, Jensen and Mouritsen 1979 and Pytte 1980 and references therein). First-order phase transitions are also absent, for all q, in the $b = 3,4$ (Tsallis and Levy 1981) and 5 (unpublished) hierarchical lattices; they are probably absent for *any* finite value of b (incidentally this means that large cell ($b\to\infty$) RG extrapolations might be missleading for approaching, *for arbitrary* q, the Potts model in a Bravais lattice).

With respect to question (ii), we consider the fractal intrinsic dimension $d_f = \ln B/\ln \bar{b}$ (B is the aggregation number, and $\bar{b}$ is the change in linear scale; $B = b^2+(b-1)^2$ and $\bar{b} = b$ for the family of self-dual hierarchical lattices mentioned above) discussed by Melrose 1983 (a,b) (see also references therein) a completely satisfactory proposal. d_f equals $\ln 5/\ln 2$ for Fig.1(a) and therefore the Potts ferromagnet exact α for the associated hierarchical lattice would be given by $\alpha=2-\nu\ln 5/\ln 2$, with ν given by Eq. (1). For $q = 2$ we recover the value $\alpha = - 0.6670$ indicated by Kaufman and Griffiths 1983.

Finally, with respect to question (iii), the fact that some RG treatments (mentioned above) failed in reproducing posi tive specific heats might generate a sceptical view about the capability of real-space renormalisations to present thermodynamically correct behaviours *for all temperatures*. We want to stress that we see no fundamental reason intrinsically preventing such RG's from recovering, for instance, positive specific heats. More than that, we have shown *how* this can be done in Martin and Tsallis 1981 (b) (Ising ferromagnet in d=3,4 like hierarchical lattices; see Figs. 2-4 therein) and Martin and Tsallis 1983 (Potts ferromagnet in planar-like hierarchical lattices; see Fig.2(b) therein). In both cases the specific heat is *positive for all temperatures*. The procedure is very simple (perhaps very general also) indeed, and it is worthy to be quickly recalled.

The dimensionless free energy f per site associated with the Bravais lattice scales, within the RG, according to

$$f(K) = b^{-d} f(K') + g(K) \qquad (2)$$

where K and K' respectively are the original and renormalised dimensionless two-body coupling constants of the model and g(K) is the standard background term (see Niemeijer and van Leeuwen 1976, Martin and Tsallis 1981 (a,b), 1983, and references therein). On the other hand, at the graphs (cells) level, the preservation of the partition function imposes

$$\mathrm{Tr}_{\{\sigma_i\}}\, e^{\mathcal{H}(K;\sigma_1,\sigma_2;\{\sigma_i\})} = e^{\mathcal{H}'(K';\sigma_1,\sigma_2) + K_0'} \qquad (3)$$

where $\mathcal{H}$ and $\mathcal{H}'$ respectively are the dimensionless Hamiltonians corresponding to the original (e.g., Fig. 1 (b)) and renormalized (Fig. 1 (a)) graphs; σ_1 and σ_2 are the random variables associated with the *terminal nodes* of the two-rooted graphs (*open* circles of Fig.1), and $\{\sigma_i\}$ are those associated with the *internal nodes* of the original graph (*full* circles in Fig.1); K'_o is the additive term that has to be included in order to exactly preserve the cell partition function. This equation completely determines $K'=K'(K)$ and $K'_o=K'_o(K)$. We introduce now a *proportionality factor* $D(K)$ (to be determined) through the relation

$$g(K) = D(K)\, K'_o\,(K) \tag{4}$$

Let us now analyse what happens if we shift the zero-energy point by adding an *arbitrary constant* λ to the energy associated with each single bond: f transforms according to $f(K) \to f(K) + \lambda dK$, and consequently Eq. (2) implies

$$g(K) \to g(K) + \lambda d\left[K-b^{-d}K'(K)\right] \tag{5}$$

At the cell level, Eq. (3) implies

$$K'_o(K) \to K'_o(K) + \lambda\left[b^{d_f}\, K-K'(K)\right] \tag{6}$$

If we *impose* now that Eq. (4) remains *form-invariant under uniform translation of the energy scale* (i.e., $D(K)$ does not change with λ), in a similar way the Maxwell equations are form-invariant under the Lorentz transformation, it immediately follows that

$$D(K) = \frac{d[b^d K - K'(K)]}{b^d[b^{d_f} K - K'(K)]} \qquad (7)$$

This equation closes the operational procedure as (together with Eq. (4)) it provides g(K), which (together with the recursive relation (2)) enables the calculation of quantities such as the specific heat.

If we are studying the hierarchical lattice itself, then d is replaced by d_f (see comment further on), therefore $D = d_f/b^{d_f}$ is a purely topological number, thus yielding (by using Eqs. (2) and (4)).

$$f(K) = b^{-d_f}[f(K') + d_f K_o'(K)] \qquad (8)$$

Note that d_f plays in this expression precisely the same role that d (number of bonds per site) plays in the standard recursive relation associated with a d-dimensional Bravais lattice.

If we are instead interested in a hopefully closer approximation to the d-dimensional Bravais lattice, then D(K) contains both topological *and* thermal informations; typically D(K) smoothly and monotonously varies from $D(0) = d\,b^{-d_f}$ to $D(\infty) = d\,b^{-d_f}(1-b^{-1})/(1-b^{-1+d-d_f})$ when K increases from zero to infinity. If the family of hierarchical lattices is appropriately chosen, one should expect $\lim_{b\to\infty} d_f = d$, hence $D(K) \sim d\,b^{-d}$ *for all values of K*. Although the above facts go in the right sense, it is obvious that they do not yet constitute a *proof* that the $b \to \infty$ limit of the specific heat associated with hierarchical lattices coincides, for all temperatures, with the specific heat associated with the corresponding Bravais lattice (the situation is even less clear for other quantities such as order parameter, susceptibility, etc.).

Before going on let us comment on the fact that, for the treatment of the hierarchical lattice itself, we have replaced (see above Eq. (8)) d by d_f. Consider the total number of bonds $N_{bonds}^{(n)}$ ($N_{bonds}^{(1)} \equiv B$) and the total number of sites $N_{sites}^{(n)}$ associated with the degree of iteration n (see Fig. 2). For the self-dual lattices appearing in Fig. 1, it is easy to verify that

$$N_{bonds}^{(n)} = \left[b^2 + (b-1)^2\right]^n \qquad (b = 1,2,\ldots;\ n = 0,1,2,\ldots) \tag{9}$$

On the other hand, the following recursive relation is satisfied:

$$\begin{aligned} N_{sites}^{(n)} &= b(b-1)\ N_{bonds}^{(n-1)} + N_{sites}^{(n-1)} \\ &= b(b-1)\ \left[b^2 + (b-1)^2\right]^{n-1} + N_{sites}^{(n-1)} \end{aligned} \tag{10}$$

$$(b = 1,2,\ldots,\ n = 1,2\ldots)$$

hence

$$N_{sites}^{(n)} = b(b-1) \sum_{i=0}^{n-1} \left[b^2 + (b-1)^2\right]^i + 2$$

and finally

$$N_{sites}^{(n)} = \frac{\left[b^2 + (b-1)^2\right]^n + 3}{2} \qquad (b = 1,2,\ldots;\ n=0,1,2,\ldots) \tag{11}$$

This equation yields, in the $n \to \infty$ limit,

$$\frac{N_{sites}^{(n-1)}}{N_{sites}^{(n)}} = \frac{\left[b^2 + (b-1)^2\right]^{n-1} + 3}{\left[b^2 + (b-1)^2\right]^n + 3} \to \frac{1}{b^2 + (b-1)^2} = b^{-d_f} \tag{12}$$

which provides the geometrical interpretation of the b^{-d_f} factor appearing in Eq. (8).

We might generalize the above results for the d-dimensional-like hierarchical lattices illustrated in Fig. 3, and which intend to simulate d-dimensional simple hypercubic lattices. It is straightforward to obtain

$$N^{(n)}_{bonds} = \left[(d-1)b^{d-2}(b-1)^2 + b^d\right]^n \tag{13}$$

$$(b = 1,2,...;\ n = 0,1,2,...)$$

$$N^{(n)}_{sites} = b^{d-1}(b-1)\ N^{(n-1)}_{bonds} + N^{(n-1)}_{sites} \tag{14}$$

$$(b=1,2,...;n=1,2,...)$$

and

$$N^{(n)}_{sites} = \frac{b^{d-1}\left\{\left[(d-1)b^{d-2}(b-1)^2 + b^d\right]^n - 1\right\}}{(d-1)b^{d-2}\ (b-1) + (1+b+b^2+...+b^{d-1})} + 2 \tag{15}$$

$$(b=1,2,...;n=0,1,2...)$$

which respectively recover, for $d = 2$, Eqs.(9), (10) and (11). Eq. (15) yields, in the $n \to \infty$ limit,

$$\frac{N^{(n-1)}_{sites}}{N^{(n)}_{sites}} \to \frac{1}{(d-1)b^{d-2}(b-1)^2 + b^d} = b^{-d_f} \tag{16}$$

where we have used the definition

$$d_f \equiv \frac{\ell n\ B}{\ell n\ \bar{b}} = \frac{\ell n\left[(d-1)b^{d-2}(b-1)^2 + b^d\right]}{\ell n\ b} \tag{17}$$

which extends the $d = 2$ case considered before.

Another interesting remark is the fact that Eqs. (13) and (14) lead, in the $n \to \infty$ limit, to

$$\frac{N^{(n)}_{bonds}}{N^{(n)}_{sites}} = \frac{(d-1)b^{d-2}(b-1)^2 + b^d - 1}{b^{d-1}(b-1)} \tag{18}$$

which, for $d = 2$, yields $2 (\forall b)$ but in general differs from both d and d_f, and which, in the $b \to \infty$ limit, yields d (as desirable).

Although less analysed than herein, the whole procedure is illustrated in detail in Martin and Tsallis 1981 (a), 1983. The consequences of the apparently inocuous form-invariance hypothesis concerning Eq. (4) are quite instructive indeed: specific heats presenting (within similar frameworks *but* which do not allow for appropriate K-dependence of D) strongly negative values for large regions of K, *automatically* (without introducing any adjustable parameter) become positive for *all* finite temperatures. It is not obvious whether the form-invariance hypothesis suffices to provide positive specific heat for *any* (classical) model. But it might well be so; in that case a proof would be extremely welcome. In addition to that, the procedure provides (at least for the cases we are aware of) a specific heat high-temperature expansion which contains an enlarging set of *exact* (for the d-dimensional Bravais lattice) terms if both $\bar{b}$ and B (associated with the corresponding hierarchical lattices) increase in such a way that $d_f = \ln B/\ln \bar{b} \to d$.

The framework discussed here simultaneously takes into account (in Eq. (7)) *both* the Bravais lattice and the family of hierarchical lattices which approximates it; in this sense, it could be a better approximation to the Bravais lattice than to *only* consider the set of hierarchical lattices (see for example Kaufman and Griffiths 1983 and references therein). Although it could of course be fortuitous, it is worthy to remark that, for b=q=2, the framework analysed here provides, *as it should if intended to approximate the d=2 Bravais lattice* ($\alpha^{exact} = 0(\ell n)$), a stronger specific heat singularity ($\alpha = -0.2973$) than that provided by the simple consideration of the corresponding hierarchical lattice, which yields (Kaufman and Griffiths 1983) $\alpha = -0.6670$.

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CAPTION FOR FIGURE

Fig. 1 - Family of two-terminal self-dual Wheatstone-bridge-like graphs (each of them, together with the graph (a), determines, through the standard recurrence procedure, an hierarchical lattice). The open (full) circles indicate the terminal (internal) nodes of the graph.

Fig. 2 - Recursive construction of the $b = 2$ Wheatstone-bridge hierarchical lattice (corresponding to Fig. 1(b)); n is the degree of iteration (the hierarchical lattice itself corresponds to the $n \to \infty$ limit).

Fig. 3 - d- dimensional-like hierarchical lattices ($n=1$ degree of iteration). (a) and (b) correspond to $d = 3$; (c) corresponds to $d = 4$.

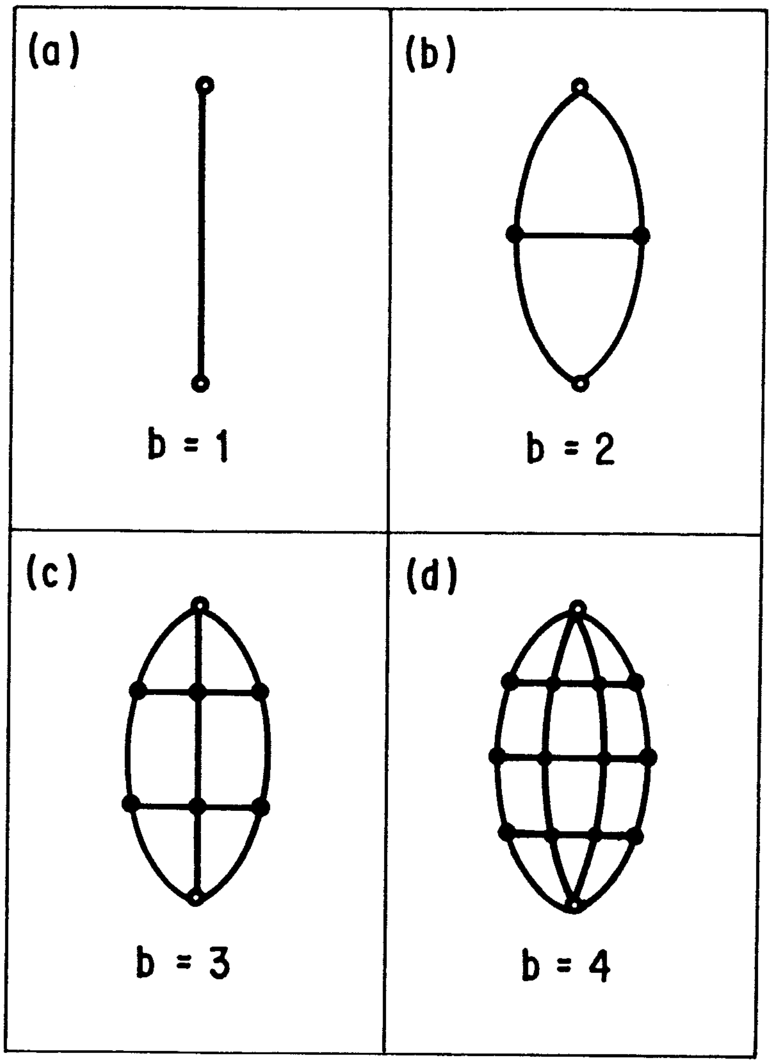

FIG.1

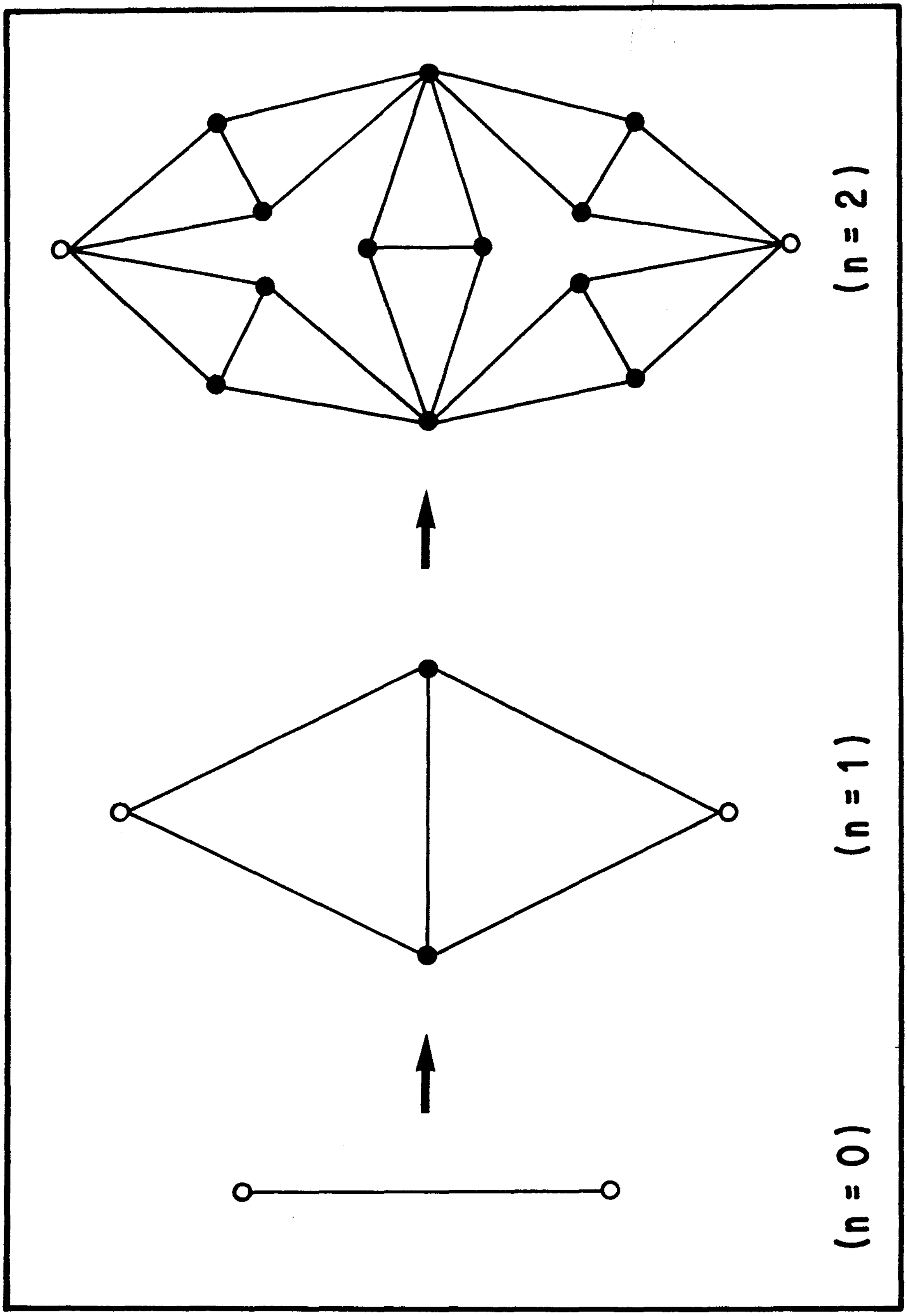

FIG.2

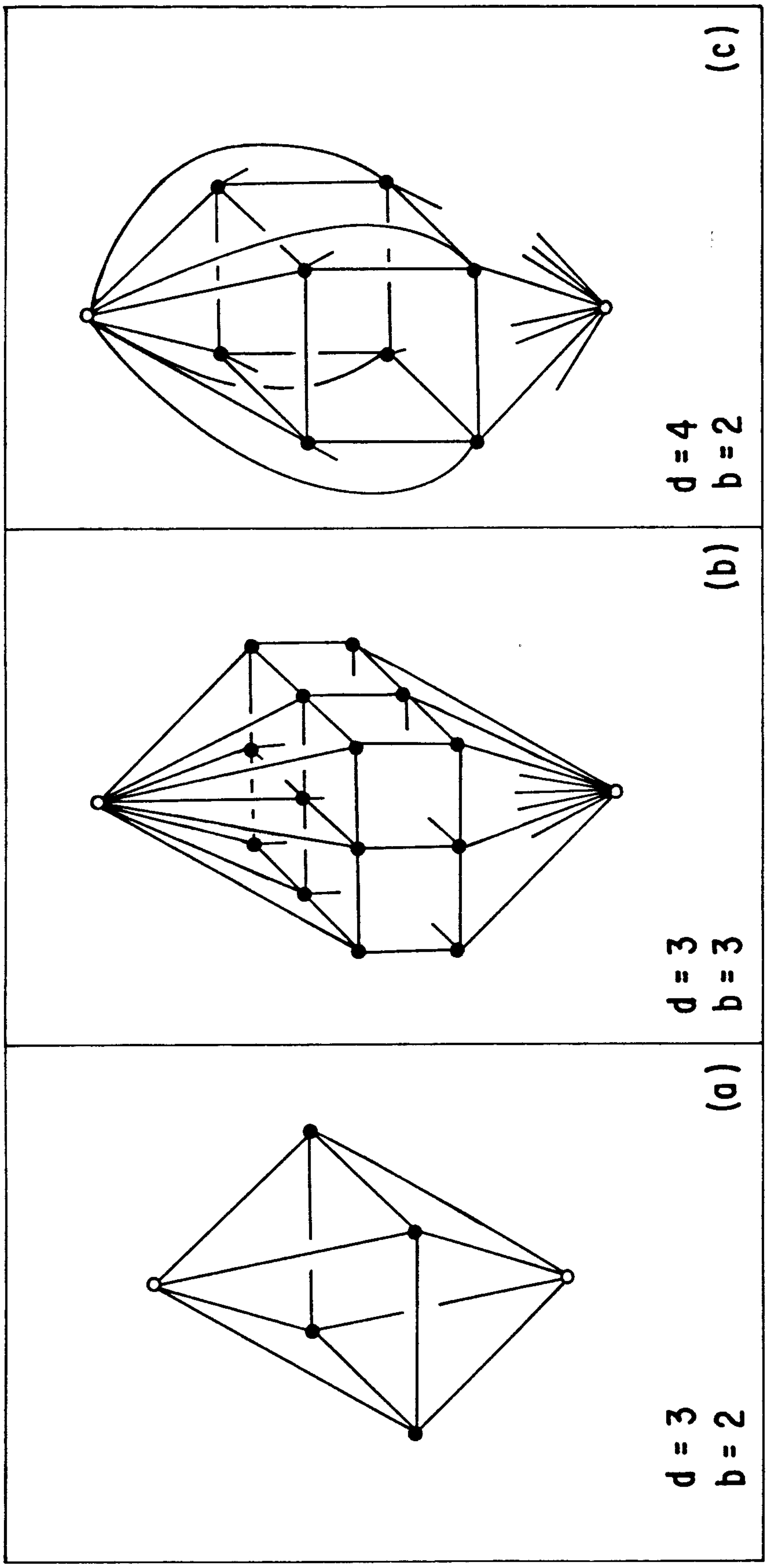

FIG. 3