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HAMILTONIAN STUDIES OF THE
TWO DIMENSIONAL N-COMPONENT
CUBIC MODEL, I.

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HAMILTONIAN STUDIES OF THE TWO DIMENSIONAL N-COMPONENT CUBIC MODEL, I.

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ABSTRACT

The Hamiltonian version of the two dimensional n -component cubic model is determined, and the phase diagram and the critical properties of the model are investigated. Judging from the results of simple limits, mean-field calculation and RG transformations, the phase diagram of the system is similar to that of the two dimensional model. Several RG transformations were used to investigate the critical properties using different cell sizes in the transformation. The coincidence of critical and tricritical fixed points and the presence of a marginal operator showed the formation of the Ashkin-Teller fixed line and the breaking of the universality. The cubic transition is found to be first order for $n > 2$.

АННОТАЦИЯ

Определен гамильтоновский вариант двумерной n -компонентной модели, исследованы ее критические свойства и фазовая диаграмма. Фазовая диаграмма гамильтоновского варианта, определенная на основе исследования простых предельных случаев, а также на основе применения среднего поля и трансформации группы ренормировок, является похожей на фазовую диаграмму двумерной системы. Для исследования критических свойств были применены разные трансформации группы ренормировок, и при этом были применены клетки возрастающих размеров. Совпадение критических и трикритических фиксированных точек и существование маргинального оператора указывает на формирование фиксированной линии Ашкина-Теллера и нарушение универсальности. В случае $n > 2$ кубический переход оказывается переходом первого рода.

KIVONAT

Meghatároztuk a két dimenziós n -komponensű köbös modell Hamilton változatát, és vizsgáltuk a modell fázisdiagramját és kritikus tulajdonságait. Az egyszerű határesetek vizsgálatából, mean-field számításokból és renormálási csoport transzformáció eredményéből meghatározott fázisdiagram hasonló a két dimenziós rendszer fázisdiagramjához. Különböző renormálási csoport transzformációkat használtunk a kritikus tulajdonságok vizsgálatához, és a transzformációról használt cella méretét növeltük. Kritikus és trikritikus fix pontok összeesése és marginális operátor létezése jelezte az Ashkin-Teller fix vonal formálódását és az univerzalitás sérülését. A köbös átalakulás $n > 2$ esetén elsőrendűnek adódott.

1. Introduction

The n -component cubic model represents a very general type of discrete lattice models and includes, in special cases, the Potts model (Potts 1952) and the Ashkin-Teller model (Ashkin and Teller 1943). Because of this the model shows many extraordinary aspects of critical behaviour. The nature of the phase transition changes with increasing number of spin components; as a result of competition the model is possessed of a multicritical point whose type also depends on n ; in two dimensions (2D) for $n=2$ there is a critical line in the system (the description of this line of fixed points by the usual renormalization-group (RG) transformation has not led to satisfactory results). However, by increasing the space of parameters by taking n to be a variable, and then extrapolating to $n = 2$, a satisfactory description is obtained (Nienhuis et al. 1983). This procedure will be followed in this paper, too.

The n -component cubic model was originally introduced as a means of modelling anisotropic magnetic systems (Kim et al. 1975, Aharony 1977), but it has many other applications. In 2D for example, the model describes some phase transitions of adsorbed monolayers (for a review see Schick 1983). The phase diagram of the model in 2D was determined by Domany and Riedel (1979), the critical properties were investigated by Nienhuis et al. (1983). In the latter paper the order of the phase transition was determined for different values of n by using the vacancy generating RG transformation (Nienhuis et al. 1979). Furthermore, by using

an exact mapping onto a solid on solid model for the $n = 2$ case, new interconnections were obtained among the class of cubic, Potts and Ashkin-Teller phase transition phenomena.

In this paper the phase transition properties of the Hamiltonian versions of the 2D model is investigated. By taking the time-continuum limit (Kogut 1979) the 2D model is mapped onto a 1D quantum problem. In most cases the anisotropy in the 2D models is irrelevant to the critical properties, and many approximate treatments are easier to apply in 1D.

The phase diagram of the system is determined by investigating simple limiting cases, by mean-field calculations, and by RG transformation. The critical properties of the system are investigated by several RG transformations. We use block transformation and decimation transformation and apply different sizes of the cell in the transformation, which together enable us to extrapolate the results.

According to the results, the topologies of the phase diagram and the critical properties of the $(1+1)D$ model and the 2D model are the same. The RG transformation give information on the change of the order of the phase transition with increasing n , and on the existence of the Ashkin-Teller fixed-line.

The paper is arranged as follows: §.2. contains the time-continuum limit, the different representations of the problem, and the analysis of different limiting cases. In §.3. the results of the mean-field calculation are presented, in §.4. the results of the RG transformation. §.5. presents a short discussion, the Appendix gives some details of the calculation.

2. Formalism

In the n -component cubic model there are spins on a lattice, each spin has $2n$ -states, denoted by $|1\rangle, |2\rangle, \dots |2n\rangle$. The energy of the system depends on the nearest neighbour configuration. The interaction energy between neighbouring spins is

$$H_\lambda |s_i s_{i+1}\rangle = \begin{cases} -\frac{\lambda_1}{2} |s_i s_{i+1}\rangle & , \text{ if } s_i = s_{i+1} \\ +\frac{\lambda_1}{2} |s_i s_{i+1}\rangle & , \text{ if } s_i = s_{i+1} + n \\ \frac{\lambda_2}{2} |s_i s_{i+1}\rangle & \text{ otherwise} \end{cases} \quad (2.1)$$

For $\lambda_1 = \lambda_2$, the model reduces to the $2n$ -state Potts model (Potts 1952), while for $n = 2$ it corresponds to the Ashkin-Teller model (Ashkin and Teller 1943). In the following the Hamiltonian version of this model will be determined.

The derivation of the Hamiltonian version of a classical, d -dimensional model is a well-known procedure (for a review see Kogut 1979). By taking the time-continuum limit, the model is mapped onto a $d-1$ -dimensional quantum problem, where external fields are introduced, and the strength of these fields plays the role of the temperature of the classical model. It is generally believed that the very high anisotropy does not affect the critical properties, and the type of singularity of the ground-state properties of the quantum problem is the same as for the free energy in the classical version. However, new types of singularity may occur, when the strength of the external fields is

negative, which would correspond to an imaginary temperature in the classical model.

The Hamiltonian version of the 2D n-component cubic model is a 1D chain with the classical (2.1) interaction in the presence of an external spin-flip field, which depends on two parameters h_1 and h_2 :

$$\langle s_i | H_h | s_j \rangle = \begin{cases} \delta_{ij} h_2 & , \quad \text{if } s_i = s_j \\ - \delta_{ij} h_2 & , \quad \text{if } s_i = s_j + n \\ - \delta_{ij} h_1 & \text{otherwise} \end{cases} \quad (2.2)$$

(In the following, we generally restrict ourselves to the subspace, where all the couplings are positive.)

In this representation the coupling part of the Hamiltonian (2.1) is diagonal, therefore it may be called the strong-coupling (or low temperature) representation. For the $h_1, h_2 \rightarrow 0$ limit, in the ground state all spins are in the same state which results in a $2n$ -fold degeneracy.

For the Ashkin-Teller model, as is well known, there exists an Ising spin representation (Fan 1972). Two sets of Ising spins are associated with every lattice site, and besides the usual two-spin interactions for each set of Ising spins, there is also a four-spin interaction between the two sublattices.

This procedure can be generalized to the n-component cubic model, if $2n = 2^k$. Now a k-set of Ising spins is associated with every lattice site, denoted by $\sigma_1(i), \sigma_2(i), \dots, \sigma_k(i)$ (i is the index of the site), to represent the $2n$ -possible states.

The assignment of Ising spins is the following. Every state has a different configuration of spins. Furthermore, if the state $|\ell\rangle$ is represented by the configuration $\sigma_1, \sigma_2, \dots, \sigma_k$, then the state $|\ell+n\rangle$ has the configuration $-\sigma_1, -\sigma_2, \dots, -\sigma_k$. For example for $k = 3$, the eight different states obtained by increasing the value of the spin can be represented by the values of the Ising spins: 1, 1, 1; 1, 1, -1; 1, -1, 1; 1, -1, -1; -1, -1, -1; -1, -1, 1; -1, 1, -1; and -1, 1, 1, respectively.

Now the coupling part of the Hamiltonian contains the two-, four-, ..., $2k$ -spin interactions between the sublattices, however, the $(2\ell-1)2$ and 4ℓ spin interactions have different couplings, viz. $-\frac{\lambda_1}{2n}$ and $-\frac{\lambda_2}{2n}$ respectively:

$$\begin{aligned}
 H_\lambda = & -\frac{\lambda_1}{2n} \sum_i \sum_{m=1}^{k_1} \sum_{1 \leq j_1 < j_2 < \dots < j_{2m-1} \leq k} \prod_{\ell=1}^{2m-1} \sigma_{j_\ell}^z(i) \sigma_{j_\ell}^z(i+1) \\
 & -\frac{\lambda_2}{2n} \sum_i \sum_{m=2}^{k_2} \sum_{1 \leq j_1 < j_2 < \dots < j_{2m} \leq k} \prod_{\ell=1}^{2m} \sigma_{j_\ell}^z(i) \sigma_{j_\ell}^z(i+1)
 \end{aligned}
 \tag{2.3/a}$$

Here $k-1 \leq 2k_1 + 1 \leq k$, $k-1 \leq 2k_2 \leq k$.

The spin-flip field can be expressed by the spin-flip operators $\sigma_j^x(i)$ in the following way:

$$\begin{aligned}
 H_h = & -h_1 \sum_i \sum_{m=1}^{k-1} \sum_{1 \leq j_1 < j_2 < \dots < j_m \leq k} \prod_{\ell=1}^m \sigma_{j_\ell}^x(i) - h_2 \sum_i \prod_{\ell=1}^k \sigma_{j_\ell}^x(i)
 \end{aligned}
 \tag{2.3/b}$$

Expressions (2.3/a, 2.3/b) show that only for $k = 2$, i.e. for the Ashkin-Teller model does there exist a decoupling point $\lambda_2 = h_2 = 0$, where the model reduces to two noninteracting Ising models. No such property holds for higher values of k .

Let us now turn to the weak coupling limit. Here it is more convenient to use the representation where the spin-flip field is diagonal. Let us introduce the following orthonormal set of vectors:

$$\begin{aligned}
 |1'\rangle &= \frac{1}{\sqrt{2n}} \{ |1\rangle + |2\rangle + \dots + |2n\rangle \} \\
 |2'\rangle &= \frac{1}{\sqrt{2n}} \{ |1\rangle + \omega |2\rangle + \dots + \omega^{2n-1} |2n\rangle \} \\
 &\vdots \\
 |(2n)'\rangle &= \frac{1}{\sqrt{2n}} \{ |1\rangle + \omega^{2n-1} |2\rangle + \dots + \omega^{(2n-1)^2} |2n\rangle \}
 \end{aligned} \tag{2.4}$$

where $\omega = \exp\left(\frac{2\pi i}{2n}\right)$.

Now the matrix elements of H_h depend on whether i' is one, even or odd:

$$\begin{aligned}
 H_h |1'\rangle &= -2(n-1)h_1 |1'\rangle \\
 H_h |(2k)'\rangle &= 2h_2 |(2k)'\rangle \quad k=1,2,\dots,n \\
 H_h |(2\ell-1)'\rangle &= 2h_1 |(2\ell-1)'\rangle \quad \ell=2,3,\dots,n
 \end{aligned}$$

In the (2.4) representation the coupling part of Hamiltonian, H_λ , flips neighbouring spins by increasing one of them and at the same time decreasing its neighbour by the same amount. (Due to the $Z(2n)$ symmetry of the model, $|\ell'\rangle = |\ell' + m \cdot 2n\rangle$,

$m = \text{integer.}$) Thus the effect of H_λ on the neighbouring spins $|k'l'\rangle$ is:

$$H_\lambda |k'l'\rangle = (n-1) \frac{\lambda_2}{2n} |k'l'\rangle - \frac{\lambda_1}{2n} |(k+1)'(\ell-1)'\rangle - \frac{\lambda_2}{2n} |(k+2)'(\ell-2)'\rangle - \frac{\lambda_1}{2n} |(k+3)'(\ell-3)'\rangle - \frac{\lambda_2}{2n} |(k+4)'(\ell-4)'\rangle - \dots - \frac{\lambda_1}{2n} |(k-1)'(\ell+1)'\rangle \quad (2.6/a)$$

So we can write:

$$\langle k'l' | H_\lambda | (k+m)'(\ell-m)' \rangle = \begin{cases} (n-1) \frac{\lambda_2}{2n} , & \text{if } m = 0 \\ - \frac{\lambda_2}{2n} , & \text{if } m = 2j \\ - \frac{\lambda_1}{2n} , & \text{if } m = 2j - 1 \end{cases} \quad (2.6/b)$$

where $j = 1, 2, \dots, n$.

From eqs. (2.6) it follows that H_λ leaves invariant the sum of the spins along the chain, modulo $2n$. Therefore the eigenstates of the chain belong to $2n$ disjoint sectors that can be characterized by the functions: $|1'1' \dots 1'\rangle, |2'1' \dots 1'\rangle, \dots, |(2n)'1' \dots 1'\rangle$, and will be called the 1st, the 2nd and the 2nth subspace, respectively. From symmetry considerations it follows that the 1st subspace is non-degenerate, while the 2nd, 4th, ..., 2nth subspaces are n -fold degenerate, and the 3rd, 5th, ..., 2n-1th subspaces are $n-1$ -fold degenerate. At the thermodynamic limit, when the length of the chain tends to infinity, further degeneracies may occur. The type and the degeneracy of the ground state characterizes the different phases. To this question we shall return later.

Besides the weak and strong-coupling regions, characterized by the conditions $h_1, h_2 \ll \lambda_1, \lambda_2$ and $\lambda_1, \lambda_2 \ll h_1, h_2$ respectively, there exists another simple limiting case, when $\lambda_2, h_2 \gg \lambda_1, h_1$. (The fourth simple possibility, when $\lambda_2, h_2 \ll \lambda_1, h_1$, gives no simple ground state except for the Ashkin-Teller model - as we mentioned earlier in connection with the Ising spin representation.)

Let us now make use of the following combination of the states:

$$\begin{aligned}
 |1''\rangle &= \frac{1}{\sqrt{2}} (|1\rangle + |n+1\rangle) & |(n+1)''\rangle &= \frac{1}{\sqrt{2}} (|1\rangle - |n+1\rangle) \\
 |2''\rangle &= \frac{1}{\sqrt{2}} (|2\rangle + |n+2\rangle) & |(n+2)''\rangle &= \frac{1}{\sqrt{2}} (|2\rangle - |n+2\rangle) \\
 &\vdots & & \\
 &\vdots & & \\
 |n''\rangle &= \frac{1}{\sqrt{2}} (|n\rangle + |2n\rangle) & |(2n)''\rangle &= \frac{1}{\sqrt{2}} (|n\rangle - |2n\rangle)
 \end{aligned} \tag{2.7}$$

Now the part of the Hamiltonian, proportional to h_2 and λ_2 is diagonal. The effect of the Hamiltonian on the new states is:

$$\begin{aligned}
 H_h |1''\rangle &= -2h_1 (|2''\rangle + |3''\rangle + \dots + |n''\rangle) \\
 H_h |2''\rangle &= -2h_1 (|1''\rangle + |3''\rangle + \dots + |n''\rangle) \\
 &\vdots \\
 &\vdots \\
 H_h |n''\rangle &= -2h_1 (|1''\rangle + |2''\rangle + \dots + |(n-1)''\rangle) \\
 H_h |(n+1)''\rangle &= 2h_2 |(n+1)''\rangle \\
 H_h |(n+2)''\rangle &= 2h_2 |(n+2)''\rangle \\
 &\vdots \\
 &\vdots \\
 H_h |(2n)''\rangle &= 2h_2 |(2n)''\rangle
 \end{aligned} \tag{2.8/a}$$

The matrix elements of the H_λ -operator are:

$$\begin{aligned}
 H_\lambda |1"1"> &= -\frac{\lambda_1}{2} |(n+1)"(n+1)"> & H_\lambda |1"(n+1)"> &= -\frac{\lambda_1}{2} |(n+1)"1"> \\
 H_\lambda |2"2"> &= -\frac{\lambda_1}{2} |(n+2)"(n+2)"> & H_\lambda |2"(n+2)"> &= -\frac{\lambda_1}{2} |(n+2)"2"> \\
 &\vdots & &\vdots \\
 &\vdots & &\vdots \\
 H_\lambda |(2n)"(2n)"> &= -\frac{\lambda_1}{2} |n"n"> & H_\lambda |n"(2n)"> &= -\frac{\lambda_1}{2} |(2n)"n"> \\
 H_\lambda |i"j"> &= \frac{\lambda_2}{2} |i"j"> , & & \text{if } j \neq i, i+n \quad (2.8/b)
 \end{aligned}$$

Thus the H_λ operator flips the neighbouring spins by n if the neighbouring spins are in the same state or differ by n , otherwise H_λ does not change the spins.

The ground state of (2.8) at the limit $\lambda_2, h_2 \gg \lambda_1, h_1$ is n -fold degenerated: $|1"1" \dots 1">$, $|2"2" \dots 2">$, ... $|n"n" \dots n">$. The relevant excitations have a simple form either for $h_1 \ll \lambda_1$, or when $\lambda_1 \ll h_1$. In the first case the system can be represented by an Ising like state, each spin can be in two possible states, say $|1">$ and $|(n+1)">$. The form of the Hamiltonian reduces to:

$$H = -\frac{\lambda_1}{2} \sum_i \sigma_i^x \sigma_{i+1}^x - h_2 \sum_i (\sigma_i^z - 1) + O\left(\frac{h_1}{\lambda_2}\right) \quad (2.9)$$

where the σ_i^x, σ_i^z Pauli operators act on the states $|1">$ and $|(n+1)">$. At this limit eqs. (2.8) describe an Ising system. The phase transition takes place at:

$$\frac{h_2}{\lambda_1} = \frac{1}{2} \quad (2.10)$$

At the other limit, for $\lambda_1 \ll h_1$, the relevant excitations are, at each site, a combination of the states $|1\rangle$, $|2\rangle$, ... $|n\rangle$.

The Hamiltonian can be written as:

$$H = -\frac{\lambda_2}{2} \sum_i (\delta_{s_i s_{i+1}} - 1) - 2h_1 \sum_i \sum_{k=1}^n M_i^k + O\left(\frac{\lambda_1}{h_2}\right) \quad (2.11)$$

where $s_i = 1, 2, \dots, n$. M is an $n \times n$ matrix

$$M = \begin{bmatrix} 0 & 0 & \dots & 1 \\ 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & & 1 & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix}$$

acting on the states $|1\rangle$, $|2\rangle$, $|n\rangle$. Hamiltonian (2.11) describes the n -state Potts model. From the exact solution of Baxter (1973) it is known that the phase transition takes place at:

$$\frac{4nh_1}{\lambda_2} = 1 \quad (2.12)$$

furthermore it is first order for $n > 4$, and continuous for $n \leq 4$.

Now let us turn back to the original representation (2.8).

These have a set of solutions of the form

$$\psi_{af}(i_1, i_2, \dots, i_N) = |(n+i_1)\rangle, (n+i_2)\rangle, \dots (n+i_N)\rangle \quad (2.13)$$

where $1 \leq i_1, i_2, \dots, i_N \leq n$, and $i_j \neq i_{j+1}$. These states are $n(n-1)^{N-1}$ -fold degenerate having the energy:

$$E_{af} = N\left(\frac{\lambda_2}{2} + 2h_2\right) \quad (2.14)$$

The ψ_{af} states describe an n -state antiferromagnetic Potts model, and it is the ground state of the system for large negative values of λ_2 and h_2 . In closing the section let us briefly summarize the possible phases of the system. In the different representations of the Hamiltonian for special values of the couplings the different types of ground state, i.e. different phases, can be determined. For positive values of the couplings the system exhibits three phases. If the couplings are much greater than the external fields ($\lambda_1, \lambda_2 \gg h_1, h_2$) the system is ferromagnetically ordered, the ground state is $2n$ -fold degenerate. At the opposite limit, when the external fields are much stronger than the couplings ($h_1, h_2 \gg \lambda_1, \lambda_2$), the system is paramagnetic, the ground state is nondegenerate. Finally at the $\lambda_2, h_2 \gg \lambda_1, h_1$ limit, the system is partially ordered, the ground state is n -fold degenerate.

On the phase boundaries of the system the following can be determined. At the $2n$ -state Potts point ($\lambda_1 = \lambda_2$), and for $\lambda_1 < \lambda_2$ there is no partially ordered phase. By increasing the strength of the external fields the system goes in one step from the ferromagnetic phase to the paramagnetic phase. This is the cubic transition. By increasing the value of λ_2 the partially ordered phase appears and the cubic transition line bifurcates. At the $\lambda_2 \gg \lambda_1$ limit, according to eq. (2.9), the transition between the ferromagnetic and the partially ordered phase is equivalent to the transition in the Ising model. On the other hand, the transition between the partially ordered and the paramagnetic phase can be described by the n -state Potts model (eq. (2.11)).

Following the phase diagram further for negative values of λ_2 , we can say that the ferromagnetic and the paramagnetic phase extend to this region, too. However, for $-\lambda_2, -h_2 \gg |\lambda_1|, |h_1|$ the ground state of the system changes essentially. Here the ground state is described by eq. (2.13) and is equivalent to the n-state antiferromagnetic Potts model. The transition into this phase for $n = 2$ takes place through an xy-type phase (Kohmoto et al. 1981, Iglói and Solyom 1984). The existence of a phase like this for $n > 2$ is still an open question. In the following the phase structure of the system is investigated for positive values of the couplings.

3. Mean-field solution

At first the result of the mean-field calculation is presented. The simplest form is chosen for the trial wavefunction, this is the product of the one spin wavefunctions. For this calculation it is convenient to use the weak-coupling representation egs. (2.6).

$$\psi = \prod_i \psi_i \quad (3.1)$$

$$\psi_i = \frac{1}{\sqrt{1+(n-1)\alpha_1^2+n\alpha_2^2}} \{ |1'\rangle + \alpha_2 |2'\rangle + \alpha_1 |3'\rangle + \alpha_2 |4'\rangle + \dots + \alpha_2 |(2n)'\rangle \}$$

The parameters for every odd (except state $|1'\rangle$), and for every even state are the same from symmetry considerations. (Here we mention that better quantitative agreement may be expected if the trial wavefunction is written as a product of the wavefunction of larger clusters (Sólyom 1984). Renormalization group and finite-size scaling arguments may also be used for a series of mean-field results with different clusters.)

The energy per spin is given by:

$$\begin{aligned} E = \frac{1}{N} \langle \psi | H | \psi \rangle = & \frac{1}{1+(n-1)\alpha_1^2+n\alpha_2^2} \{ -2(n-1)h_1 + \\ & + \alpha_2 2nh_2 + \alpha_1^2 2(n-1)h_1 \} + \frac{1}{[1+(n-1)\alpha_1^2+n\alpha_2^2]^2} \{ -4n \frac{\lambda_1}{2n} \alpha_2^2 - \\ & - n^2(n-1) \frac{\lambda_2}{2n} \alpha_2^4 - 4(n-1) \frac{\lambda_2}{2n} \alpha_1^2 - 4(n-1)(n-2) \frac{\lambda_2}{2n} \alpha_1^3 - \\ & - (n-1)(n-2)^2 \frac{\lambda_2}{2n} \alpha_1^4 - 4n(n-1) (2 \frac{\lambda_1}{2n} + \frac{\lambda_2}{2n}) \alpha_1 \alpha_2^2 - \\ & - 2n(n-1) [2(n-1) \frac{\lambda_1}{2n} + (n-2) \frac{\lambda_2}{2n}] \alpha_1^2 \alpha_2^2 \} \end{aligned} \quad (3.2)$$

At given values of the couplings $h_1, h_2, \lambda_1, \lambda_2$ one should minimize the energy with respect to α_1 and α_2 . Equation (3.2) has three different types of minima, which characterize three different phases:

- I, $\alpha_1 = 0, \alpha_2 = 0$. Paramagnetic phase
- II, $\alpha_1 \neq 0, \alpha_2 = 0$. Partially ordered phase
- III, $\alpha_1 \neq 0, \alpha_2 \neq 0$. Ferromagnetically ordered phase

Expression (3.2) has no minima which would correspond to $\alpha_1 = 0, \alpha_2 \neq 0$.

The mean-field phase diagram is drawn in Fig. 1 for $n = 3$. The topology of the phase diagram is the same for all values of n , and is in accordance with those written in §.2. The order of the phase transitions obtained is different for $n = 2$ and for $n \geq 3$. The types of transitions between the different phases for $n = 2$, and for $n \geq 3$ are given in Table 1.

This simple method is not able to account for some unusual critical properties of the Ashkin-Teller model, and it probably fails to predict the order of the I \rightarrow II transition for $n = 3$ and $n = 4$. Furthermore the phase boundaries are approximate. However, by increasing the value of n , we may hope for better quantitative agreement. This tendency is generally true for models where either the number of components of the spin or the range of interactions goes to infinity. In our case this statement is only partially fulfilled. The phase diagram for $n \rightarrow \infty$ is shown in Fig. 2 in the following plane:

$$\begin{aligned}\frac{\lambda_1}{2n} &= 1 \\ h &= \frac{2nh_1}{\lambda_1} = \frac{2nh_2}{\lambda_2} \\ \lambda &= \frac{\lambda_2}{\lambda_1} = \frac{h_2}{h_1}\end{aligned}\tag{3.3}$$

Upon the importance of this subspace we will touch in the second part of this paper (Paper II, Iglói 1984). Here we use it for better representation.

The mean-field phase diagram is exact for the cubic transition line, as we can state in comparing it to the result of the $1/n$ expansion (Paper II). A further possibility to check this is to compare the phase diagram with the asymptotic transition lines (eqs. (2.09) and (2.11)). In this way the paramagnetic-partially ordered transition coincides with eq. (2.09) whereas the partially ordered-ferromagnetic transition does not agree with the asymptotic line (2.11).

To conclude this section, we comment on the method of Livi et al. (1983) who determined the order of the phase transition by using a mean-field calculation. The mean-field calculation, due to its approximate character, generally overestimates the transition temperature, and results rather in a first order transition, then a second order one. In some cases the mean-field calculation also describes a second order transition from a metastable state at lower temperature, than where the first order transition took place. According to the method of Livi et al. (1983), this second order transition is taken to be the real type of

transition of the system, if its transition temperature is not higher than its exactly or numerically known value. For our model this procedure has limited use since an underlying second order transition takes place only for $n = 2$. The phase transition is predicted to be second order for $\lambda \geq 1$; and at $\lambda = 1$ predicts the exact crossover value of n . For $\lambda < 1$, however, even for $n = 2$ this method does not alter the findings of the mean-field calculation.

4. Renormalization-group calculation

In order to obtain more accurate phase diagram and critical properties of the model, in this Section we make several RG transformations. Our aim is also to investigate the break-down of universality and the crossover of the transition from second order to first order by increasing values of n . Our earlier study on the Ashkin-Teller model (Iglói and Sólyom 1984) did not give clear evidence on the existence of a line of fixed points. Now our hope is, that by increasing the space of parameters as taking n to be a variable, the line of fixed points will show up in the calculation.

Recently Nienhuis et al. (1983) performed an RG calculation for the classical 2D model. By using the vacancy generating RG technique (Nienhuis et al. 1979) a complex description was given on many extraordinary features of the critical properties of the model. Our RG calculation has a different starting point based on the success of Sólyom and Pfeuty (1981) in explaining the first order phase transition in the 2D Hamiltonian Potts model. Otherwise, the structure of fixed points and the evaluation of these with increasing value of n is, in our calculation, like those obtained by Nienhuis et al. (1983). This is not really surprising since after all the two RG methods have the same spirit (Iglói and Sólyom 1983b).

In the RG transformation of quantum spin systems (for a review see Pfeuty et al. 1982), the Hamiltonian of the system is split into an unperturbed part containing noninteracting

cells of spins, and a perturbation which contains the intra-cell couplings. The solution of the unperturbed part is a product of the states of the cells. In the RG transformation the low lying levels of a cell are mapped onto the states of a new spin, which will be the new cell variable. For the n -component cubic model this new spin, obtained after the RG transformation, has the symmetry of the original spin for ferromagnetic value of the couplings. Furthermore, this sector is invariant under the RG transformation therefore we restrict our investigation to the ferromagnetic region.

Depending on the choice how the Hamiltonian is split, different RG transformations can be defined. In this paper we consider three of them. To determine the phase-structure a decimation transformation is used, which was originally proposed by Fernandez-Pacheco (1979) for the Ising model. The critical properties of the model are investigated by block transformation and by decimation transformation. The latter two methods are equivalent for self-dual models (Sólyom 1981), but in our case supply different information. In these methods, we used different sizes of the cells in the transformation, in order to make extrapolations.

4.1 The phase diagram

A decimation transformation is used in this section. This transformation was proposed for the Ising model by Fernandez-Pacheco (1979) and was later used for the Potts model by Horn et al. (1980), Hu (1980), Sólyom and Pfeuty (1981), Iglói and

Sólyom (1983a); and for the Ashkin-Teller model by Iglói and Sólyom (1984). The transformation generally gives the exact phase transition points for self-dual models so it is often called the self-dual RG method (SDRG) or duality concerning decimation. This method seems to give quite accurate results even for non-self-dual models for the phase diagram, however, the critical properties obtained by this method are less valuable.

Now let us briefly discuss the method for the simplest case with two spins in a cell. The non-interacting cells are chosen such that every other spin is fixed in a given state and it interacts with its left neighbour only. The non-fixed spins are eliminated by the RG procedure. The derivation of the RG transformation as well as the structure of the fixed points is like those obtained for the Ashkin-Teller model (Iglói and Sólyom 1984). The RG transformation does not generate new couplings, and the recursion relations have three types of trivial fixed point solution yielding three different phases. The region of attraction of these fixed points is shown in Fig. 3 for $n = 2$. It is mentioned that the structure of the phase diagram obtained by this transformation does not depend on the value of n , it is only that the boundaries of the phases are changing.

The different phases can be characterized as follows:

I/ Paramagnetic phase - the couplings scale to $h_1 =$
 $=$ arbitrary, $h_2 =$ arbitrary, $\lambda_1 = 0$, $\lambda_2 = 0$.

II/ Partially ordered phase - the couplings scale to
 $h_1 = 0$, $h_2 =$ arbitrary, $\lambda_1 = 0$, $\lambda_2 =$ arbitrary.

III/ Ferromagnetically ordered phase - the couplings scale
to $h_1 = 0$, $h_2 = 0$, $\lambda_1 =$ arbitrary, $\lambda_2 =$ arbitrary.

The critical surfaces, which separate the different phases, are characterized by the following nontrivial fixed-points:

i) The points of the surface separating the paramagnetic and the ferromagnetic region scale to: $h_1 = 0$, $h_2 = 0$, $\lambda_1 = 0$, $\lambda_2 = 0$, with however,

$$\frac{2nh_1}{\lambda_1} = \text{finite} \quad , \quad \frac{h_2}{\lambda_1} = 0 \quad , \quad \frac{\lambda_2}{\lambda_1} = 0 .$$

This fixed point is denoted by $I(n)$ in Fig. 3. (The notation is explained by the fact that for $n = 2$ it is an Ising-like fixed point.) The position of the fixed point as well as the eigenvalues of the linearized RG transformation at the fixed point are given in Table 2.

ii) The points of the critical surface separating the paramagnetic and the partially ordered region scale to: $h_1 = 0$, $\lambda_1 = 0$, $\lambda_2 = 0$, $h_2 = \text{arbitrary}$, with, however,

$$\frac{2nh_1}{\lambda_2} = \frac{1}{2} \quad , \quad \frac{\lambda_1}{\lambda_2} = 0$$

This is the fixed point of the n -state Potts model, denoted by $P(n)$. The thermal eigenvalue is $(n + 2\sqrt{n} + 2)/(\sqrt{n} + 2)$.

iii) The points of the surface separating the ferromagnetic region and the partially ordered region scale to:

$h_1 = 0$, $h_2 = 0$, $\lambda_1 = 0$, $\lambda_2 = \text{arbitrary}$, with, however,

$$\frac{h_1}{\lambda_1} = 0, \quad \frac{h_2}{\lambda_1} = 1/2.$$

This is an Ising-like fixed point denoted by I , the thermal eigenvalue is 2, the critical exponent ν is 1.

iiii) The points of the line where the three phases coexist scale to: $h_1 = 0, h_2 = 0, \lambda_1 = 0, \lambda_2 = 0$, with, however,

$$\frac{2nh_1}{\lambda_1} = 1, \quad \frac{2nh_2}{\lambda_1} = 1, \quad \frac{\lambda_2}{\lambda_1} = 1 .$$

This is the critical point of the $2n$ -state Potts model, denoted by $P(2n)$. The eigenvalues at this point are

$$\lambda_1^T = \frac{2n + 2\sqrt{2n} + 2}{\sqrt{2n} + 2}$$

$$\lambda_2^T = 1 + \frac{2}{(\sqrt{2n} + 1) \left(1 + \frac{\sqrt{2n}}{2}\right)}$$

$$\lambda_3^T = 1$$

This renormalization-group procedure accurately describes the phase boundaries in the region between the $I(n)$ and $P(2n)$ fixed points, as is shown in Paper II by comparing the results with series expansion. However, in some respects it gives a rather crude description. First of all, the phase transition are determined to be second order for any values of n , in contrast to the fact that transitions described by the $I(n)$, $P(2n)$, $P(n)$ fixed points should be of first order for large values of n . Otherwise the bifurcation line always goes through the $2n$ -state Potts point, although it should move to higher values of λ_2 and h_2 , as is shown by series expansion results (Paper II).

In order to get a more reliable description of the critical properties, in the next section we use the block transformation and the usual decimation transformation.

4.2 Critical properties

In the block transformation (BT) and in the decimation transformation (DT) more couplings are included in the unperturbed part of the Hamiltonian compared with SDRG, and generally they result in a more reliable description of the critical properties of models. By using both transformations on the n-component cubic model, it turned out that the two methods result in the same qualitative description of the critical properties. Let us now outline the two transformations.

In BT the unperturbed part of the Hamiltonian contains all the field terms and the intra-block couplings. The unperturbed part of DT contains all coupling terms and the field terms within the cells, while the perturbation is the field acting on the edges of the cells, i.e. on the non-decimated spins. In both transformations starting with the Hamiltonian with four couplings, the RG transformation generates three new ones, but further renormalization steps do not increase the number of couplings. Derivations of the RG equations for the two transformations are given in the Appendix.

Both transformations describe a similar phase-diagram consisting of three phases:

I/ Paramagnetic phase - the couplings scale to:

$$h_1 = \text{arbitrary}, h_2 = \text{arbitrary}, \lambda_1 = 0, \lambda_2 = 0, x=y=z=c_1,$$

where $c_1 = 0$ for BT and $c_1 = 1$ for DT.

II/ Partially ordered phase - the couplings scale to:

$$h_1 = 0, h_2 = \text{arbitrary}, \lambda_1 = 0, \lambda_2 = \text{arbitrary}, x=y=z=1.$$

III/ Ferromagnetically ordered phase - the couplings scale to:

$h_1 = 0, h_2 = 0, \lambda_1 = \text{arbitrary}, \lambda_2 = \text{arbitrary}, x=y=z=c_3,$
where $c_3 = 1$ for BT, and $c_3 = 0$ for DT.

The surfaces separating the different phases are characterized by nontrivial fixed points. In these transformations, there are more nontrivial fixed points compared with the SDRG, and the picture given by these transformations on the nature of the phase transition is also richer. A schematic picture on the RG phase diagram in the extended space of couplings is given in Fig. 4 for different values of n . The third axis, pointing perpendicularly to the physical plane, serves to represent all new couplings, and therefore somehow plays the role of the dilution in the 2D classical model. Figure 4 shows that the structure of nontrivial fixed points is similar to that obtained by Nienhuis et al. (1983) for the 2D cubic lattice-gas model. The figure demonstrates that the number of nontrivial fixed points as well as the nature of the transition depends on the value of n . In the following, we summarize the properties of the nontrivial fixed points.

i) The critical surface separating the paramagnetic and the ferromagnetic region is controlled in the most general case by three fixed points denoted by $I^c(n)$, $I^t(n)$ and $I^d(n)$; these are called the critical, tricritical and the discontinuity fixed point, respectively. These fixed points are characterized by:

$$h_1 = 0, h_2 = 0, \lambda_1 = 0, \lambda_2 = 0, \quad \text{but, however,}$$

$$\frac{\lambda_2}{\lambda_1} = 0, \quad \frac{h_1}{\lambda_1} = \text{finite}, \quad \frac{h_2}{\lambda_1} = \text{finite}, \quad X = \text{finite}$$

for BT, and

$$\frac{\lambda_2}{\lambda_1} = \text{finite}, \quad \frac{h_1}{\lambda_1} = \text{finite}, \quad \frac{h_2}{\lambda_1} = 0, \quad y = \text{finite}, \quad z = \text{finite}$$

for DT.

The critical fixed point is one-fold unstable, describes second order transition and controls the cubic transition of the physical model. The thermal exponent - as a function of n at this fixed point - is given in Fig. 5 for DT when the size of the cell (B) is 2 and 3. The discontinuity fixed point is one-fold instable and describes first order transition since the specific heat exponent is $\alpha = 1$ at this fixed point.

The tricritical fixed point is two-fold unstable, and separates the second order and first order transition regions of the surface. The thermal exponents at this fixed point are also given in Fig. 5.

Evaluation of the fixed points with increasing value of n is similar to that of the Potts model obtained by Solyom and Pfeuty (1981). The critical and tricritical fixed points move towards each other. At $n = n_c^I$ they coincide, the next to leading eigenvalue of the linearized RG equations at the fixed point is 1, another eigenvalue is very close to 1. If the value of n is further increased the two fixed points annihilate each other, and the cubic transition in the physical system is controlled by the discontinuity fixed point, i.e. it is of first order. The annihilations of n for the different transitions and different sizes of the cells are given in Table 3.

ii) The points of the critical surface separating the paramagnetic and the partially ordered region scale to:

$$h_1 = 0, h_2 = \text{arbitrary}, \lambda_1 = 0, \lambda_2 = 0, \text{ with, however,}$$

$$\frac{h_1}{\lambda_2} = \text{finite}, \quad \frac{\lambda_1}{\lambda_2} = 0, \quad z = \text{finite}, \quad y = 0 \quad \text{for BT, and}$$

$$\frac{h_1}{\lambda_2} = \text{finite}, \quad \frac{\lambda_1}{\lambda_2} = 0, \quad x=y=z=\text{finite} \quad \text{for DT.}$$

At this point the recursion equations are the same as that of the n-state Potts model, in accordance with eq. (2.11), since the model reduces to the n-state Potts model at this limit. From the results of the RG-transformation on the Potts model (Sólyom and Pfeuty 1981, Iglói and Sólyom 1983b), it is known that critical, tricritical and discontinuity fixed points exist, denoted respectively by $P^c(n)$, $P^t(n)$ and $P^d(n)$. They are one-fold, two-fold and one-fold unstable, respectively. The evaluation of the fixed-point structure is the same as was mentioned for the $I(n)$ fixed points. The annihilation value for n can be obtained from Table 3, they are $2n_C^P$.

iii) The points of the surface separating the ferromagnetic region and the partially ordered region scale to:

$$h_1 = 0, \quad h_2 = 0, \quad \lambda_1 = 0, \quad \lambda_2 = \text{finite} \quad \text{with, however,}$$

$$\frac{h_1}{\lambda_1} = 0, \quad \frac{h_2}{\lambda_1} = \text{finite}, \quad x=y=z=1 \quad \text{for BT, and}$$

$$\frac{h_1}{\lambda_1} = 0, \quad \frac{h_2}{\lambda_1} = \text{finite}, \quad z = \text{finite}, \quad x = 0 \quad \text{for DT.}$$

This is an Ising-type fixed point, denoted by I in Fig. 4.

iiii) The points of the line where the three phases coexist scale to: $h_1 = 0, h_2 = 0, \lambda_1 = 0, \lambda_2 = 0$, but, however,

$$\frac{h_1}{h_2} = 1, \quad \frac{\lambda_1}{\lambda_2} = 1, \quad \frac{h_1}{\lambda_1} = \text{finite}, \quad x=y=z$$

for both BT and DT, since it is the $2n$ -state Potts point, where the model is self-dual. The critical, tricritical and discontinuity fixed points are denoted by $P^C(2n)$, $P^t(2n)$ and $P^d(2n)$, and are two-fold, three-fold and two-fold unstable, respectively. The thermal exponents at the critical and tricritical fixed points are given in Fig. 6 for different sizes of the cell, together with the exact values (den Nijs 1979). The annihilation procedure takes place at this point too; the annihilation values $n = n_C^p$ are given in Table 3 for different sizes of the cell.

Here we mention that the $B = 2$ case (when two spins are in the cell) behaves somewhat differently for DT and BT.

In this case, as one can see in Table 3, the $I^C(n)$ fixed point becomes two-fold unstable before the annihilation takes place and the $I^t(n)$ tricritical fixed point becomes three-fold unstable in the same way. When the order of instability of the fixed points changes, new fixed points appear from which the one-fold unstable controls the cubic transition whereas the two-fold unstable plays the role of the tricritical fixed point. If we increase the value of n these new fixed points move towards the $2n$ -state Potts fixed points. When $P^C(2n)$ and $P^t(2n)$ change stability, these new fixed points and their counterparts for

$\lambda_2 > \lambda_1$ coincide with the Potts fixed points, and the moving fixed points annihilate each other. The moving fixed points for $\lambda_2 > \lambda_1$ for smaller n values have no physical meaning because they have complex eigenvalues.

By using larger cells in the transformation these moving fixed points do not appear therefore their appearance for $B = 2$ is attributed to the effect of approximation.

From the results of the different RG transformation the following physical picture emerges on the phase transition in the 2D n -component cubic model. The cubic transition is of second-order for $n < n_C^I$, and controlled by one fixed point, i.e. it is universal. For $n > n_C^I$, the cubic transition is controlled by one discontinuity fixed point therefore it is of first order. This breaking of the universal behaviour occurs when $n = n_C^I$. The series of n_C^I values in Table 3 seems to tend to 2. This is supported by the fact that at $n = 2$ the transition is of second order, and the inequality $n_C^I < n_C^D$ holds for all calculated sizes of the cell in the transformation, and n_C^D tends to 2. At $n = n_C^I$, one eigenvalue of the linearized RG equation is 1, and another is very close to this value. The same situation is true for the $2n$ -state Potts fixed point. These facts signal the presence of a marginal operator and a line of fixed points with continuously varying critical exponents, i.e. the Ashkin-Teller fixed line. Therefore, in this case, the breaking of universality on the cubic transition line takes place in two steps for increasing value of n :

- i) At $n = 2$ the critical indices of the second order transition depend on the coupling.

ii) for $n > 2$ the transition is of first order, the latent heat depends on the coupling.

Finally we would mention that the neighbourhood of the multicritical point cannot be investigated satisfactorily by these RG transformations for $n > 2$. With these calculations, similarly to the SDRG, the multicritical point and the $2n$ -state Potts point are found to be the same, which is in contrast to the result of the $1/n$ expansion (Paper II). The nature of the multicritical point is still unsolved, even for the 2D classical model.

5. Summary

In this paper the phase diagram and the critical properties of the Hamiltonian version of the 2D n -component cubic model were determined by different methods. Analysis of simple limiting cases and the results of mean-field calculation and RG transformations have shown that the phase diagram of the $(1+1)D$ model is similar to that of the 2D model. Furthermore, the critical behaviour of the two models turned out to be the same.

The critical properties of the model were investigated by different RG transformations. By using different sizes of the cell in the transformation it was possible to extrapolate the results. The calculation gave an account on the line of fixed points in the Ashkin-Teller model, and on the first order transition on the cubic transition line for $n > 2$. The properties of this first order transition will be investigated by expansion methods in Paper II.

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Appendix 1.

Recursion equations in the block transformation

In this method, it is convenient to use the weak-coupling representation (2.4). As was mentioned earlier, in this representation the spectrum of the Hamiltonian splits into $2n$ disjoint sectors. Furthermore it turned out that for ferromagnetic values of the couplings, the $2n$ lowest eigenstates of the Hamiltonian belong to different sectors, and possess maximal symmetry. In the following we write down these states for the simplest case with two spins in a block.

The lowest eigenstate can be written in the form:

$$\varphi_1 = a_0 \psi_0^1 + a_1 \psi_1^1 + a_2 \psi_2^1$$

where

$$\psi_0^1 = |1'1'\rangle$$

$$\psi_1^1 = |3'(2n-1)'\rangle + |5'(2n-3)'\rangle + \dots + |(2n-1)'3'\rangle$$

$$\psi_2^1 = |2'(2n)\rangle + |4'(2n-2)'\rangle + \dots + |(2n)'2'\rangle$$

and a_0, a_1, a_2 are the components of the normalized eigenvector, belonging to the lowest eigenvalue (E_1) of the following matrix:

$$\begin{pmatrix} -4(n-1)h_1 & -\frac{\lambda_2}{2n}\sqrt{n-1} & -\frac{\lambda_1}{2n}\sqrt{n} \\ -\frac{\lambda_2}{2n}\sqrt{n-1} & 4h_1 - \frac{\lambda_7}{2n}(n-2) & -\frac{\lambda_3}{2n}\sqrt{n(n-1)} \\ -\frac{\lambda_1}{2n}\sqrt{n} & -\frac{\lambda_3}{2n}\sqrt{n(n-1)} & 4h_2 - \frac{\lambda_4}{2n}(n-1) \end{pmatrix}$$

In this formula, for simplicity, the matrix is expressed in terms of the generated new couplings, the definition of those will be given later (A1).

The next energy level is n-fold degenerate. One of those can be written as:

$$\varphi_2 = b_0 \psi_0^2 + b_1 \psi_1^2$$

Here:

$$\psi_0^2 = |1'2'\rangle + |2'1'\rangle$$

$$\psi_1^2 = |3'(2n)'\rangle + |4'(2n-1)'\rangle + \dots + |(2n)'3'\rangle$$

and b_0 and b_1 are the components of the normalized eigenvector, belonging to the lowest eigenvalue (E_2) of the following matrix:

$$\begin{pmatrix} -2(n-1)h_1 + 2h_2 - \frac{\lambda_1}{2n} & - \left(\frac{\lambda_6}{2n} + \frac{\lambda_5}{2n} \right) \sqrt{n-1} \\ - \left(\frac{\lambda_6}{2n} + \frac{\lambda_5}{2n} \right) \sqrt{n-1} & 2h_1 + 2h_2 - \frac{\lambda_8}{2n} (n-2) - \frac{\lambda_3}{2n} (n-1) \end{pmatrix}$$

The other degenerate states can be obtained from the states $|1'4'\rangle, \dots, |1'(2n)'\rangle$, and will be denoted by $\varphi_4, \varphi_6, \dots, \varphi_{2n}$, respectively.

The third low lying level is (n-1)-fold degenerate. One of these can be written as:

$$\varphi_3 = c_0 \psi_0^3 + c_1 \psi_1^3 + c_2 \psi_2^3$$

Here:

$$\psi_0^3 = |1'3'\rangle + |3'1'\rangle$$

$$\psi_1^3 = |2'2'\rangle + |4'(2n)'\rangle + \dots + |(2n)'4'\rangle$$

$$\psi_2^3 = |5'(2n-1)'\rangle + |7'(2n-3)'\rangle + \dots + |(2n-1)'5'\rangle$$

and c_0, c_1, c_2 are the components of the normalized eigenvector, belonging to the lowest eigenvalue (E_3) of the following matrix:

$$\begin{pmatrix} -2(n-2)h_1 - \frac{\lambda_2}{2n} & -\frac{\lambda_5}{2n} \sqrt{2n} & -\frac{\lambda_9}{2n} \sqrt{2(n-2)} \\ -\frac{\lambda_5}{2n} \sqrt{2n} & 4h_2 - \frac{4}{2n} (n-1) & -\frac{\lambda_3}{2n} \sqrt{n(n-2)} \\ -\frac{\lambda_9}{2n} \sqrt{2(n-2)} & -\frac{\lambda_3}{2n} \sqrt{n(n-2)} & 4h_1 - \frac{\lambda_7}{2n} (n-3) \end{pmatrix}$$

The other degenerate states can be obtained from the states $|1'5'\rangle, \dots, |1'(2n-1)'\rangle$, and will be denoted $\phi_5, \dots, \phi_{2n-1}$ respectively. The renormalized values of the couplings can be obtained from the condition that the matrix elements have to be the same before and after the transformation.

The renormalized values of the fields are obtained from the energy spectrum of the renormalized states:

$$h_1^{\text{cell}} = \frac{E_3 - E_1}{2n}$$

$$h_2^{\text{cell}} = \frac{nE_2 - (n-1)E_3 - E_1}{2n}$$

The renormalization procedure for the coupling terms, however, generates new couplings, whose definitions are the following:

$$\frac{\lambda_0}{2n} = \langle i'j' | H_\lambda | i'j' \rangle$$

$$\frac{\lambda_1}{2n} = - \langle 1'1' | H_\lambda | (2i)'(2n-2i+2)' \rangle$$

$$\frac{\lambda_2}{2n} = - \langle 1'1' | H_\lambda | (2k+1)'(2n-2k+1)' \rangle$$

$$\frac{\lambda_3}{2n} = - \langle (2i)'(2j)' | H_\lambda | (2i-2k-1)'(2j+2k+1)' \rangle$$

$$\frac{\lambda_4}{2n} = - \langle (2i)'(2j)' | H_\lambda | (2i-2k)'(2i+2k)' \rangle \quad (A1)$$

$$\frac{\lambda_5}{2n} = - \langle 1'(2i)' | H_\lambda | (2k)'(2i-2k+1)' \rangle$$

$$\frac{\lambda_6}{2n} = - \langle 1'(2i)' | H_\lambda | (2i-2k+1)'(2k)' \rangle$$

$$\frac{\lambda_7}{2n} = - \langle (2i+1)'(2j+1)' | H_\lambda | (2i-2k+1)'(2j+2k+1)' \rangle$$

$$\frac{\lambda_8}{2n} = - \langle (2i+1)'(2j)' | H_\lambda | (2i-2k+1)'(2j+2k)' \rangle$$

$$\frac{\lambda_9}{2n} = - \langle 1'(2i+1)' | H_\lambda | (2j+1)'(2i-2j+1)' \rangle$$

By shifting the zero of the energy, the diagonal term, λ_0 is taken to be zero. Furthermore the matrix elements have the property:

$$\langle ab | H_\lambda | cd \rangle = \langle da | H_\lambda | bc \rangle = \langle cd | H_\lambda | ab \rangle = \langle bc | H_\lambda | da \rangle$$

Starting from the physical model:

$$\lambda_1 = \lambda_3 = \lambda_5 = \lambda_7 = \lambda_8 = \lambda_9, \quad \lambda_2 = \lambda_4 = \lambda_6$$

after the renormalization the generated couplings are not independent. They may be expressed by three new parameters, x , y , and z in following way:

$$\lambda_3 = x^2 \lambda_1, \quad \lambda_5 = x \lambda_1$$

$$\lambda_4 = y^2 \lambda_2, \quad \lambda_6 = y \lambda_2, \quad \lambda_7 = z^2 \lambda_2, \quad \lambda_8 = zy \lambda_2, \quad \lambda_9 = z \lambda_2.$$

The recursion equations for the coupling terms read as:

$$\lambda_1^{\text{cell}} = \lambda_1 [(a_0 + a_2)b_0 + x b_1 (a_2 + a_1)(n-1)]^2$$

$$\lambda_3^{\text{cell}} = \lambda_1 \{ (b_0 c_1 + b_1 c_0) + x [b_0 c_0 + (n-2)b_1 c_2 + (n-1)b_1 c_1] \}^2$$

$$x^{\text{cell}} = (\lambda_3^{\text{cell}} / \lambda_1^{\text{cell}})^{1/2}$$

$$\lambda_2^{\text{cell}} = \lambda_2 [(c_0 a_1 + c_1 a_0) + y n c_1 a_2 + z (n-2) a_1 c_2]^2$$

$$\lambda_4^{\text{cell}} = \lambda_2 [2b_0 b_1 + y [b_0^2 + (n-1)b_1^2] + z (n-2)b_1^2]^2$$

$$y^{\text{cell}} = (\lambda_4^{\text{cell}} / \lambda_2^{\text{cell}})^{1/2}$$

$$\lambda_7^{\text{cell}} = \lambda_2 \{ 2c_0 c_2 + y n c_1^2 + z [(n-3)c_2^2 + c_0^2] \}^2$$

$$z^{\text{cell}} = (\lambda_7^{\text{cell}} / \lambda_2^{\text{cell}})^{1/2}$$

It should be noted that the subsequent renormalization steps do not increase the number of new couplings.

By using larger cells, the same new couplings are generated by the RG transformation, and the structure of the RG equations remains the same. The lowest energy levels of the cells belong to different subspaces, and are maximally symmetrical. In the case of three spins in a cell, the dimensions of the eigenvalue matrices are 8, 13 and 12.

Appendix 2.

Recursion equations in the decimation transformation

It is convenient to use the strong-coupling representation eqs. (2.1), (2.2) in the calculation. In the simplest case every second spin is fixed in a given state, i.e. the field term does not act on these spins. The state of the cell containing three spins depends on the relative positions of the edge spins, and in this way three different cases can be distinguished:

- i. the fixed spins are in the same state
- ii. the fixed spins differ by n
- iii. the difference of the fixed spins is neither zero nor n .

i. When the fixed spins are in the same state, say ℓ , the lowest state of the cell can be written as:

$$\psi_{\ell, \ell} = |\ell\rangle |a_0| \ell\rangle + a_1 |\ell+n\rangle + a_2 [|1\rangle + \dots + |\ell-1\rangle + |\ell+1\rangle + \dots + |\ell+n-1\rangle + |\ell+n+1\rangle + \dots + |2n\rangle] |\ell\rangle$$

where a_0 , a_1 and $\sqrt{2(n-1)}a_2$ are the components of the normalized eigenvector belonging to the lowest eigenvalue (E_1) of the matrix:

$$\begin{pmatrix} -\lambda_1 & -h_2 & -\sqrt{2(n-1)}h_1 \\ -h_2 & \lambda_1 & -\sqrt{2(n-1)}h_7 \\ -\sqrt{2(n-1)}h_1 & -\sqrt{2(n-1)}h_7 & \lambda_2 - h_4 - 2(n-2)h_3 \end{pmatrix}$$

This matrix, for simplicity, is expressed in the space of the generated new couplings (A2).

ii. When the fixed spins differ by n, the lowest state of the cell can be expressed as:

$$\psi_{\ell, \ell+n} = |\ell\rangle \{ c_0 (|\ell\rangle + |\ell+n\rangle) + c_1 (|1\rangle + \dots + |\ell-1\rangle + |\ell+1\rangle + \dots + |\ell+n-1\rangle + |\ell+n+1\rangle + \dots + |2n\rangle) \} |\ell+n\rangle$$

Here $c_0\sqrt{2}$ and $c_1\sqrt{2(n-1)}$ are the components of the normalized eigenvector belonging to the lowest eigenvalue (E_3) of the matrix:

$$\begin{pmatrix} -h_2 & -h_9 2\sqrt{n-1} \\ -h_9 2\sqrt{n-1} & \lambda_2 - h_4 - h_3^2(n-2) \end{pmatrix}$$

iii. When the fixed spins are not in the above mentioned two special positions, then the lowest eigenstate is the following:

$$\psi_{\ell, k} = |\ell\rangle \{ b_0 (|\ell\rangle + |k\rangle) + b_1 (|\ell+n\rangle + |k+n\rangle) + b_2 (|2\rangle + \dots + |\ell-1\rangle + |\ell+1\rangle + \dots + |k-1\rangle + |k+1\rangle + \dots + |\ell+n-1\rangle + |\ell+n+1\rangle + \dots + |k+n-1\rangle + |k+n+1\rangle + \dots + |2n\rangle) \} |k\rangle$$

Here $b_0\sqrt{2}$, $b_1\sqrt{2}$ and $b_2\sqrt{2(n-2)}$ are the components of the normalized eigenvector belonging to the lowest eigenvalue (E_2) of the following matrix:

$$\begin{pmatrix} -\frac{\lambda_1}{2} + \frac{\lambda_2}{2} - h_1 & -h_6 - h_9 & -h_5 2\sqrt{n-2} \\ -h_6 - h_9 & \frac{\lambda_1}{2} + \frac{\lambda_2}{2} - h_7 & -h_8 2\sqrt{n-2} \\ -2\sqrt{n-2}h_5 & -2\sqrt{n-2}h_8 & \lambda_2 - h_4 - h_3^2(n-3) \end{pmatrix}$$

For a given value of $|\ell\rangle$ the other spin $|k\rangle$ has $2(n-1)$ possible states.

The renormalized values of the couplings can be derived from the lowest energy levels of the cells:

$$\lambda_1^{\text{ren}} = E_3 - E_1$$

$$\lambda_2^{\text{ren}} = 2E_2 - E_1 - E_3$$

The renormalization procedure generates new field terms, depending on the state of the neighbouring spins. Thus:

$$\begin{aligned} h_1 &= - \langle \ell, \ell, \ell | H_h | \ell, k, \ell \rangle = - \langle \ell, \ell, k | H_h | k, k, \ell \rangle \\ h_2 &= - \langle \ell, \ell, \ell | H_h | \ell, \ell+n, \ell \rangle = - \langle \ell, \ell, \ell+n | H_h | \ell+n, \ell+n, \ell \rangle \\ h_3 &= - \langle k, \ell, m | H_h | m, p, k \rangle \\ h_4 &= - \langle k, \ell, m | H_h | m, \ell+n, k \rangle \\ h_5 &= - \langle \ell, \ell, m | H_h | m, k, \ell \rangle \\ h_6 &= - \langle \ell, \ell, m | H_h | m, \ell+n, \ell \rangle \\ h_7 &= - \langle \ell+n, \ell, \ell+n | H_h | \ell+n, k, \ell+n \rangle \\ h_8 &= - \langle \ell+n, \ell, m | H_h | m, k, \ell+n \rangle \\ h_9 &= - \langle \ell, \ell, \ell+n | H_h | \ell+n, k, \ell \rangle \end{aligned} \tag{A2}$$

The generated couplings are not independent of each other, they may be expressed with the help of three new variables, x , y and z :

$$\begin{aligned} h_3 &= h_1 y^2, \quad h_5 = h_1 y, \quad h_7 = h_1 z^2, \quad h_8 = h_1 z y, \quad h_9 = h_1 z \\ h_4 &= h_2 x^2, \quad h_6 = h_2 x. \end{aligned}$$

The recursion equations for the spin flip field are the following:

$$h_1^{\text{ren}} = h_1 [b_0(a_0+a_2) + zb_1(a_1+a_2) + y^2(n-2)a_2b_2]^2$$

$$h_3^{\text{ren}} = h_1 [2b_0b_2 + z^2b_1b_2 + y(b_0^2 + b_1^2 + 2(n-3)b_2^2)]^2$$

$$y^{\text{ren}} = (h_3^{\text{ren}}/h_1^{\text{ren}})^{1/2}$$

$$h_7^{\text{ren}} = h_1 [c_0b_1 + b_0c_1 + z(c_0b_0 + b_1c_1) + y^2(n-2)b_2c_1]^2$$

$$z^{\text{ren}} = (h_7^{\text{ren}}/h_1^{\text{ren}})^{1/2}$$

$$h_2^{\text{ren}} = h_2 [c_0(a_1 + a_0) + xa_2c_1^2(n-1)]^2$$

$$h_4^{\text{ren}} = h_2 [2b_0b_1 + x(b_0^2 + b_1^2 + 2(n-2)b_2^2)]^2$$

$$x^{\text{ren}} = (h_4^{\text{ren}}/h_2^{\text{ren}})^{1/2}$$

Finally we mention that the structure of the RG equations, and the number of new couplings remain the same, by using a larger cell in the calculation. The dimensions of the eigenvalue matrices will be 8, 8, 17 for $B=3$ and 33, 28, 84 for $B=4$.

References

- Aharony A. 1977 J.Phys. A 10 389
- Ashkin J. and Teller E. 1943 Phys.Rev. 64 178
- Baxter R.J. 1973 J.Phys. C 6 L445
- Domany E. and Riedel E.K. 1979 Phys.Rev. B 19 5817
- Fan C. 1972 Phys.Lett. 39A 136
- Fernandez-Pacheco A. 1979 Phys.Rev. B 19 3173
- Horn D., Karliner M. and Jankielowicz S. 1980 Nucl.Phys. B 170
FS1 467
- Hu B. 1980 J.Phys. A 13 L321
- Iglói F. 1984 J.Phys.A (following paper)
- Iglói F. and Sólyom J. 1983a Phys.Rev. B 28 2785
- Iglói F. and Sólyom J. 1983b Phys.Rev. B 28 2792
- Iglói F. and Sólyom J. 1984 J.Phys. A 17 1531
- Iglói F., Kapor D.V., Škrinjar M. and Sólyom J. 1983 J.Phys.
A 16 4067
- Kim D., Levy P.M. and Uffer L.F. 1975 Phys.Rev. B 12 989
- Kogut J. 1979 Rev.Mod.Phys. 51 659
- Kohmoto M., den Nijs M. and Kadanoff L.P. 1981 Phys.Rev.
B 24 5229
- Livi R., Maritan A., Ruffo S. and Stella A.L. 1983 Phys.Rev.Lett.
50 459
- Nienhuis B., Berker A.N., Riedel E.K. and Schick M. 1979
Phys.Rev.Lett. 43 737
- Nienhuis B., Riedel E.K. and Schick M. 1983 Phys.Rev. B 27 5625

den Nijs MPM 1979 J.Phys. A 12 1857

Pfeuty P., Jullien R. and Penson K.A. 1982 Real Space

Renormalization ed. T.W. Burkhardt and J.M.J. van Leeuwen
(Berlin: Springer) p.119

Potts R.B. 1952 Proc. Cambridge Philos. Soc. 48 106

Schick M. 1983 Surf.Sci. 125 94

Sólyom J. 1981 Phys.Rev. B 24 230

Sólyom J. 1984 unpublished

Sólyom J. and Pfeuty P. 1981 Phys.Rev. B 24 218

Table captions

Table 1. Nature of transitions in the mean-field calculation. I, II and III denote the same regions as in Fig. 1.

Table 2. Position of the I(n) fixed point and the eigenvalues of the SDRG transformation for different values of n.

Table 3. Critical values of n, where the critical and tricritical fixed points annihilate each other.

Subscripts I and P refer to the I(n) and P(2n) fixed points, respectively; $n_c^I(\text{BT})$ and $n_c^I(\text{DT})$ were calculated by block transformation and by decimation transformation, respectively. The values in parentheses are the next to leading eigenvalues of the RG transformations when the critical and tricritical fixed points coincide.

Table 1.

Transition	n	Type of transition
I → III	2	2 nd -order, 1 st -order, tricritical points
	≥3	1 st -order
I → II	2	2 nd -order
	≥3	1 st -order
II → III	2	2 nd -order
	≥3	2 nd -order

Table 2.

n	$\frac{2nh_1}{\lambda_1}$	λ_1^T	λ_2^T	λ_3^T
2	1.	2.	.707	.707
3	.733	2.476	.814	.737
4	.650	2.870	.861	.761
5	.611	3.212	.888	.779
10	.547	4.532	.942	.829
100	.504	14.214	.993	.936
∞	$.5 + \frac{8}{2n}$	$\sqrt{2n}$	1.	1.

Table 3.

B	n_C^I (BT)		n_C^I (DT)		n_C^P	
2	3.24	(1.009)	3.34	(1.010)	3.41	(0.993)
3	3.04	(0.972)	3.08	(0.980)	3.12	(1.014)
4			2.99		3.02	(1.040)
5					2.92	
∞	2.	(1.)	2.	(1.)	2.	(1.)

Figure captions

Fig. 1. Mean-field phase diagram for $n = 3$. The model is paramagnetic in region I, partially ordered in region II, and ferromagnetic in region III.

Fig. 2. Mean-field phase diagram for $n \rightarrow \infty$. The II \rightarrow III transition takes place on the line: $\frac{h_1}{\lambda_1} = \left(\frac{\lambda_2}{\lambda_1}\right)^{-1}$.

Fig. 3. Phase diagram for $n = 2$ obtained by SDRG. $I(n)$, $P(2n)$, $P(n)$ and I denote the nontrivial fixed points.

Fig. 4. Schematic renormalization-group phase diagrams obtained by decimation transformation and by block transformation. The $\{h_i\}$ axis serves to represent all new couplings generated by the transformations. a, $n < 2$ b, $n = 2$ (Ashkin-Teller model) c, $n > 4$. Dots represent nontrivial fixed points, the double line for $n = 2$ is the Ashkin-Teller fixed line.

Fig. 5. Critical and tricritical thermal exponents at the $I(n)$ fixed point calculated by decimation transformation for $B = 2$ and 3 . The square denotes the exactly known value for the Ising model.

Fig. 6. Critical and tricritical thermal exponents at the $2n$ -state Potts point by using different sizes of the cell in the transformation. The exact values (den Nijs 1979) are represented by dashed line.

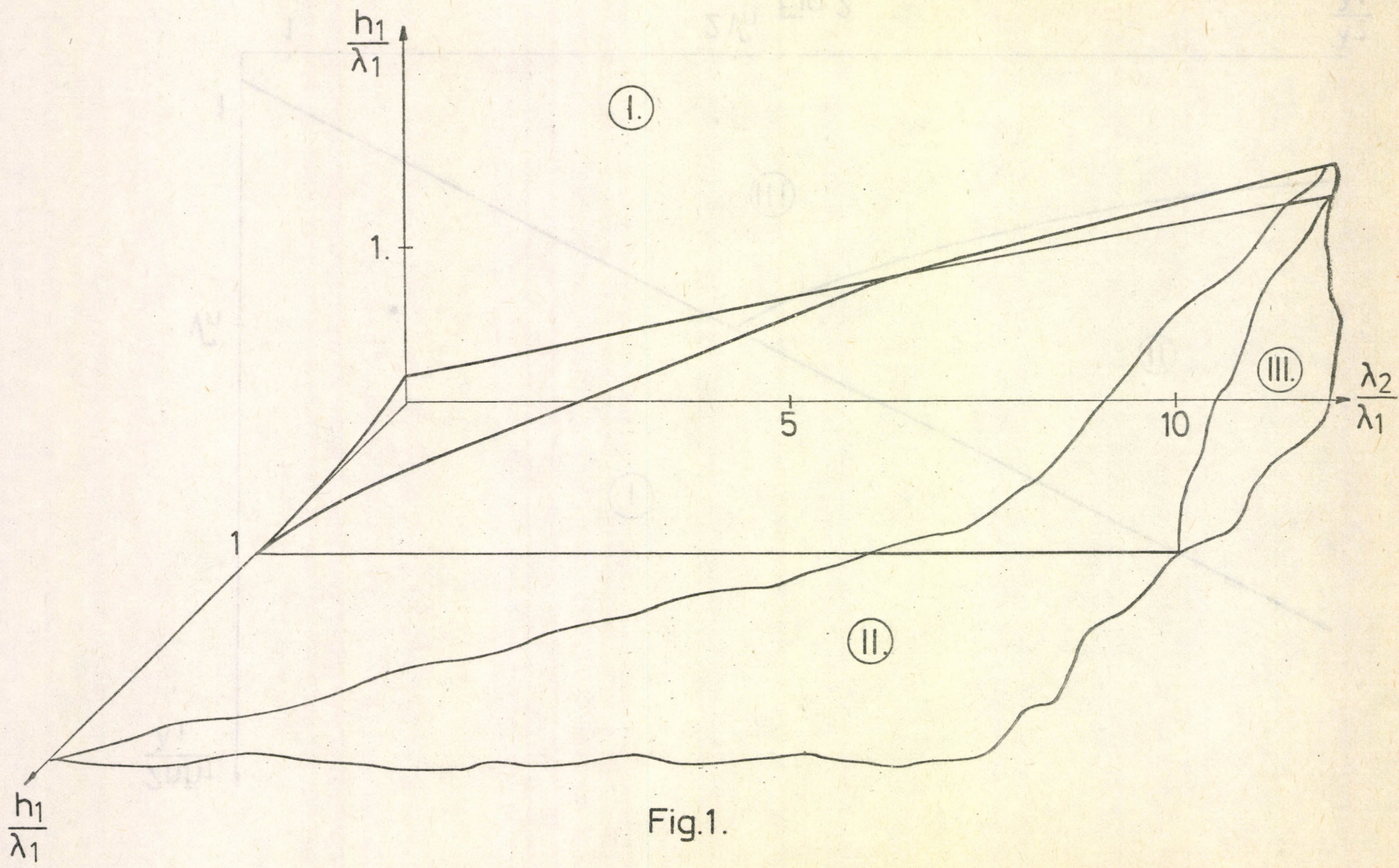


Fig.1.

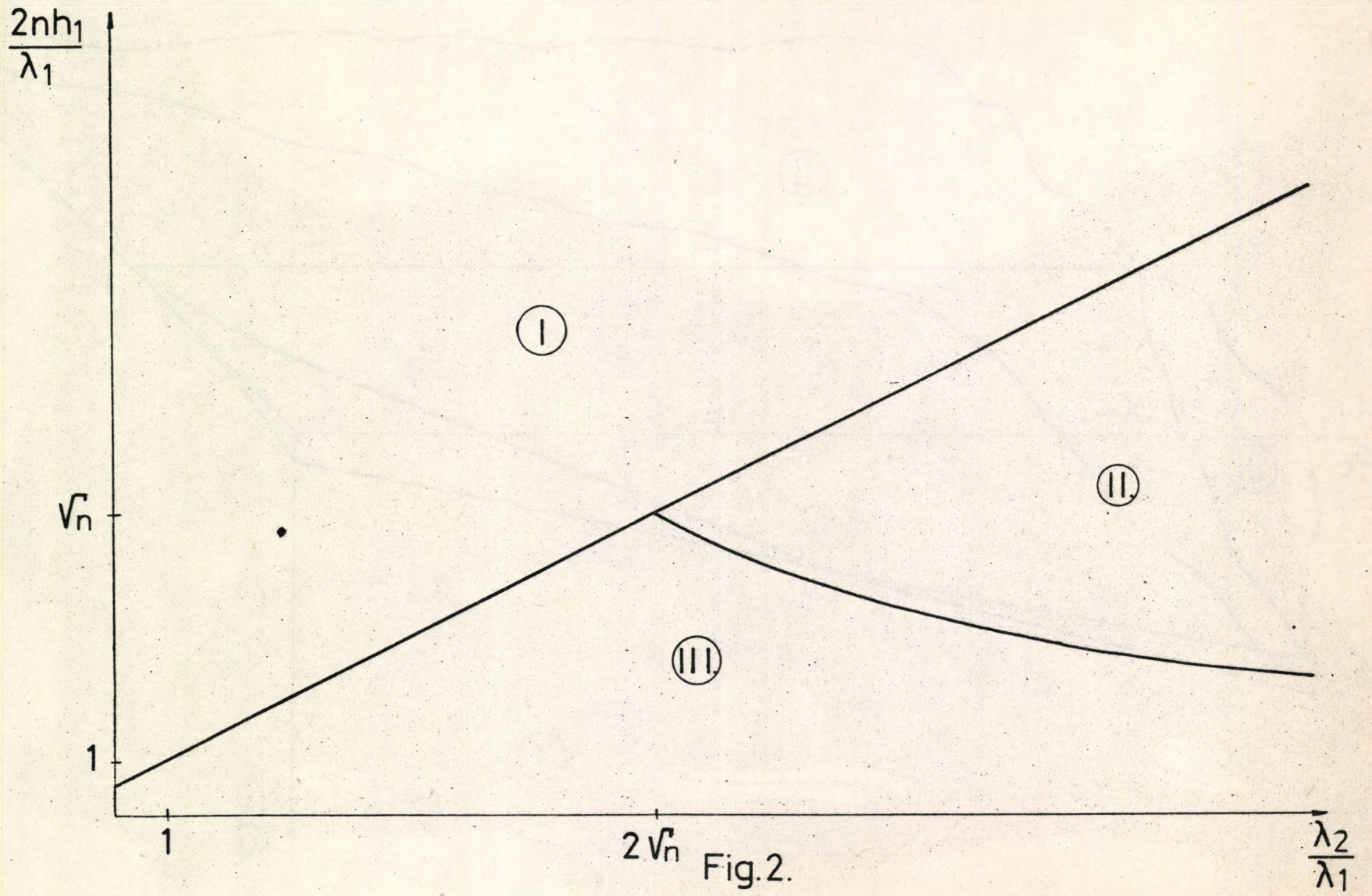


Fig. 2.

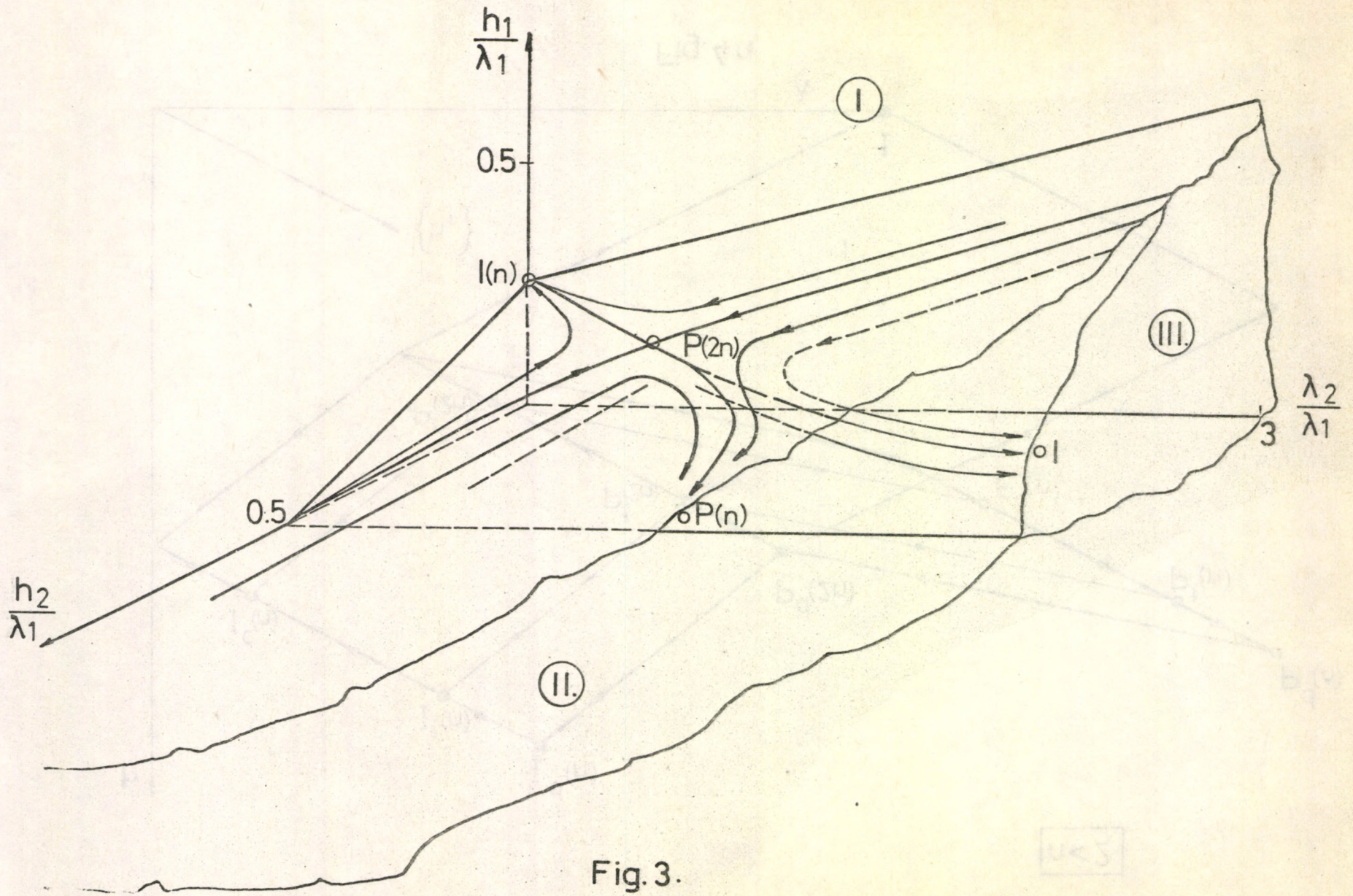


Fig. 3.

$n < 2$

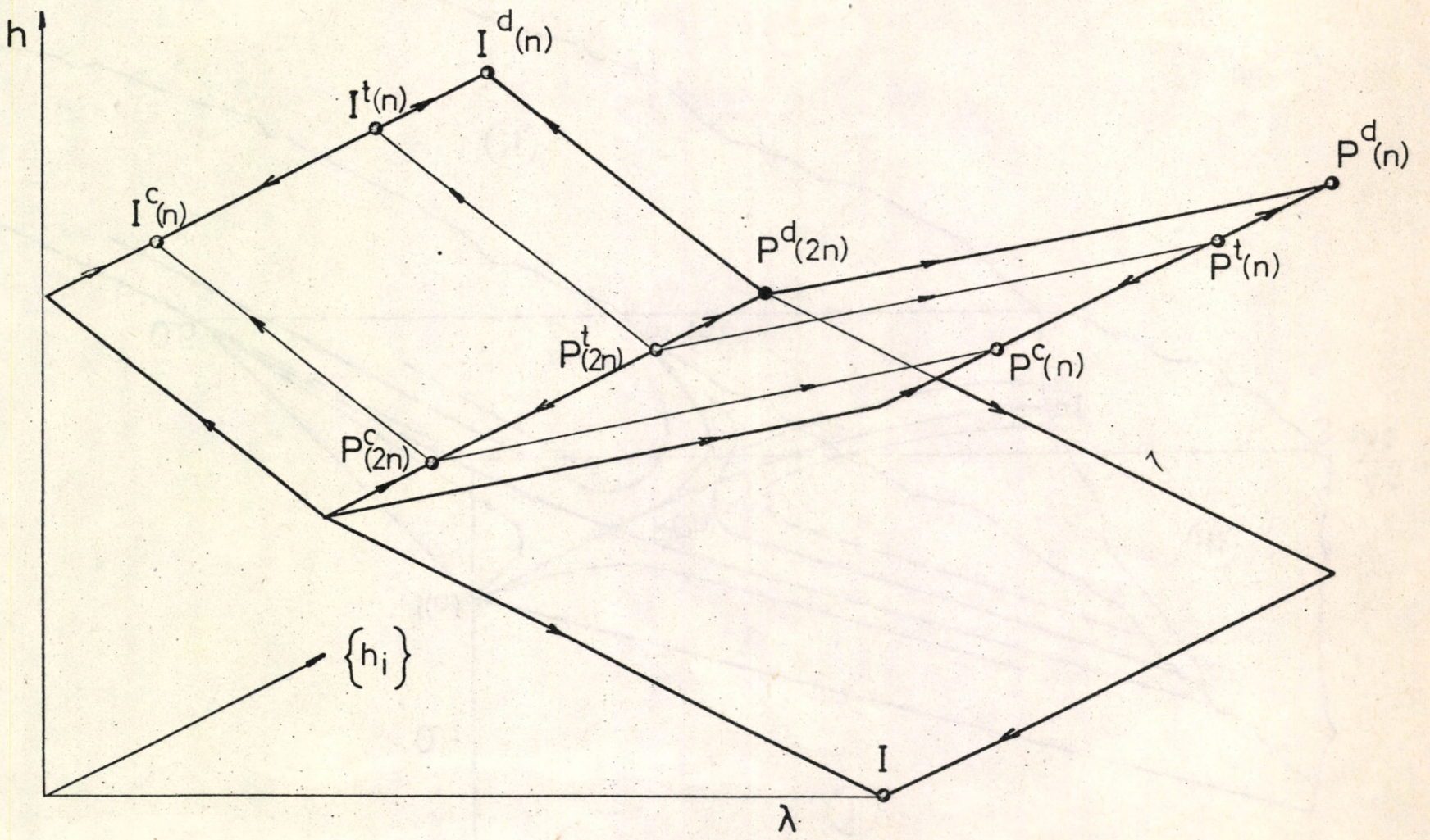


Fig.4a

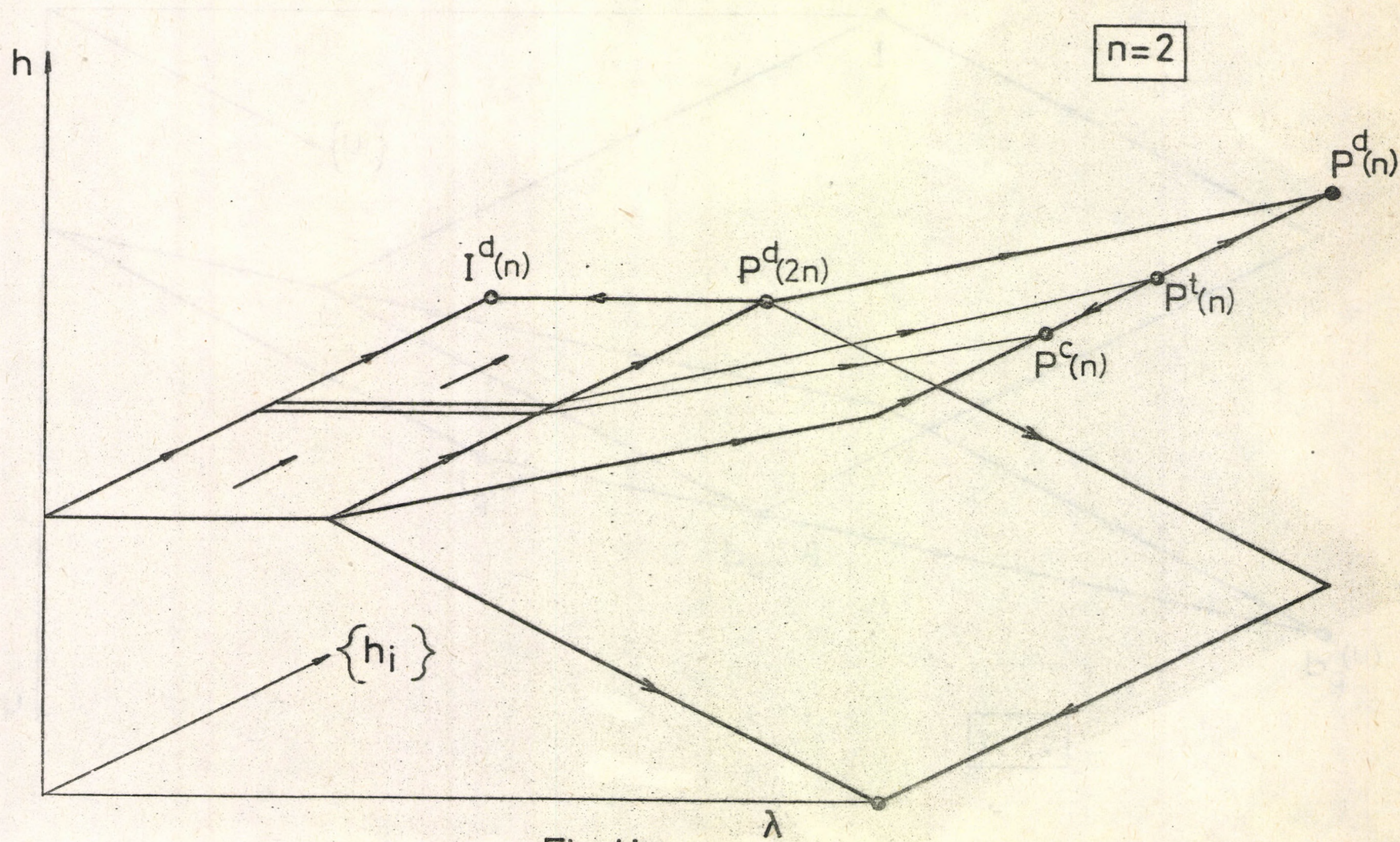


Fig.4b.

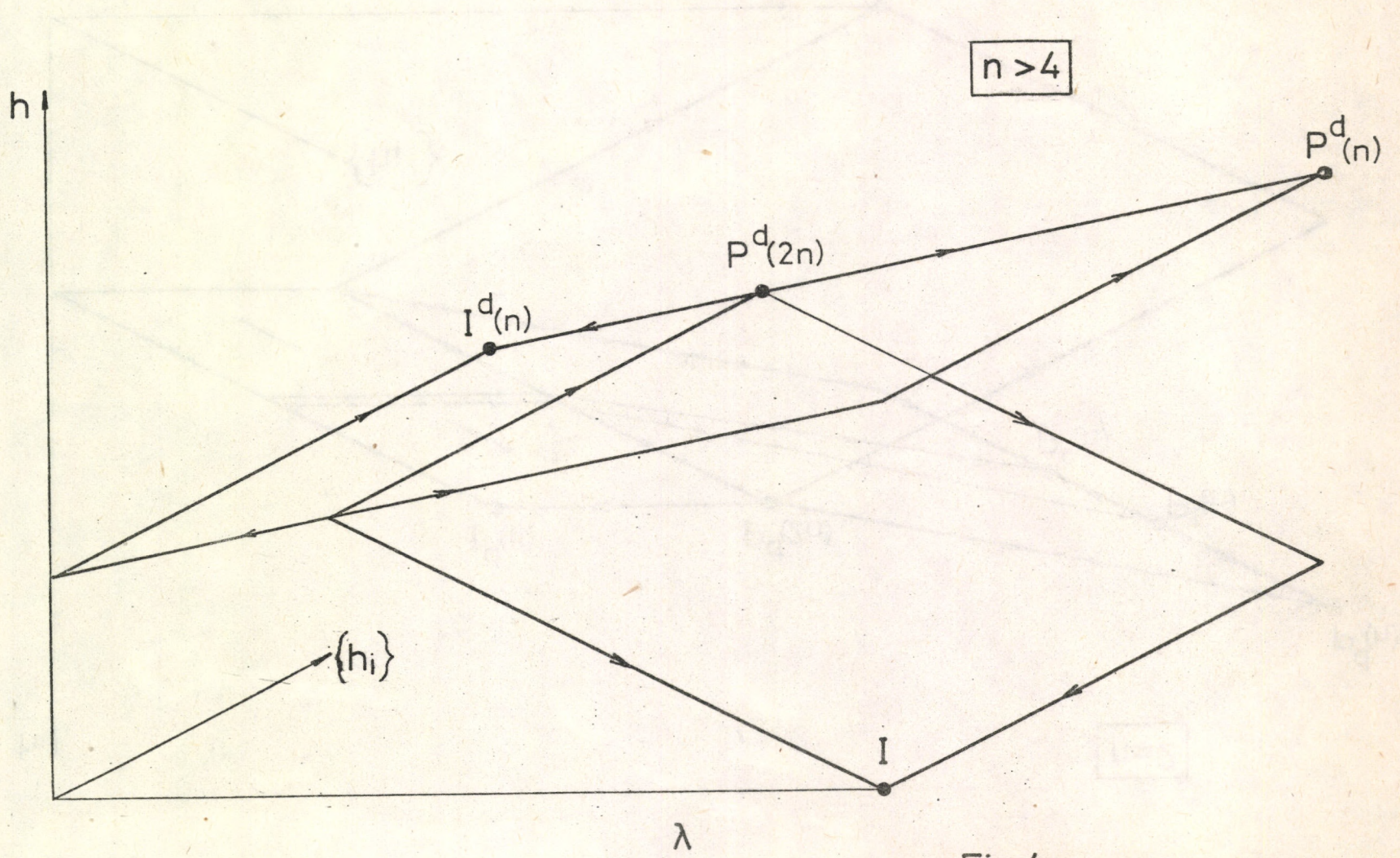


Fig.4c

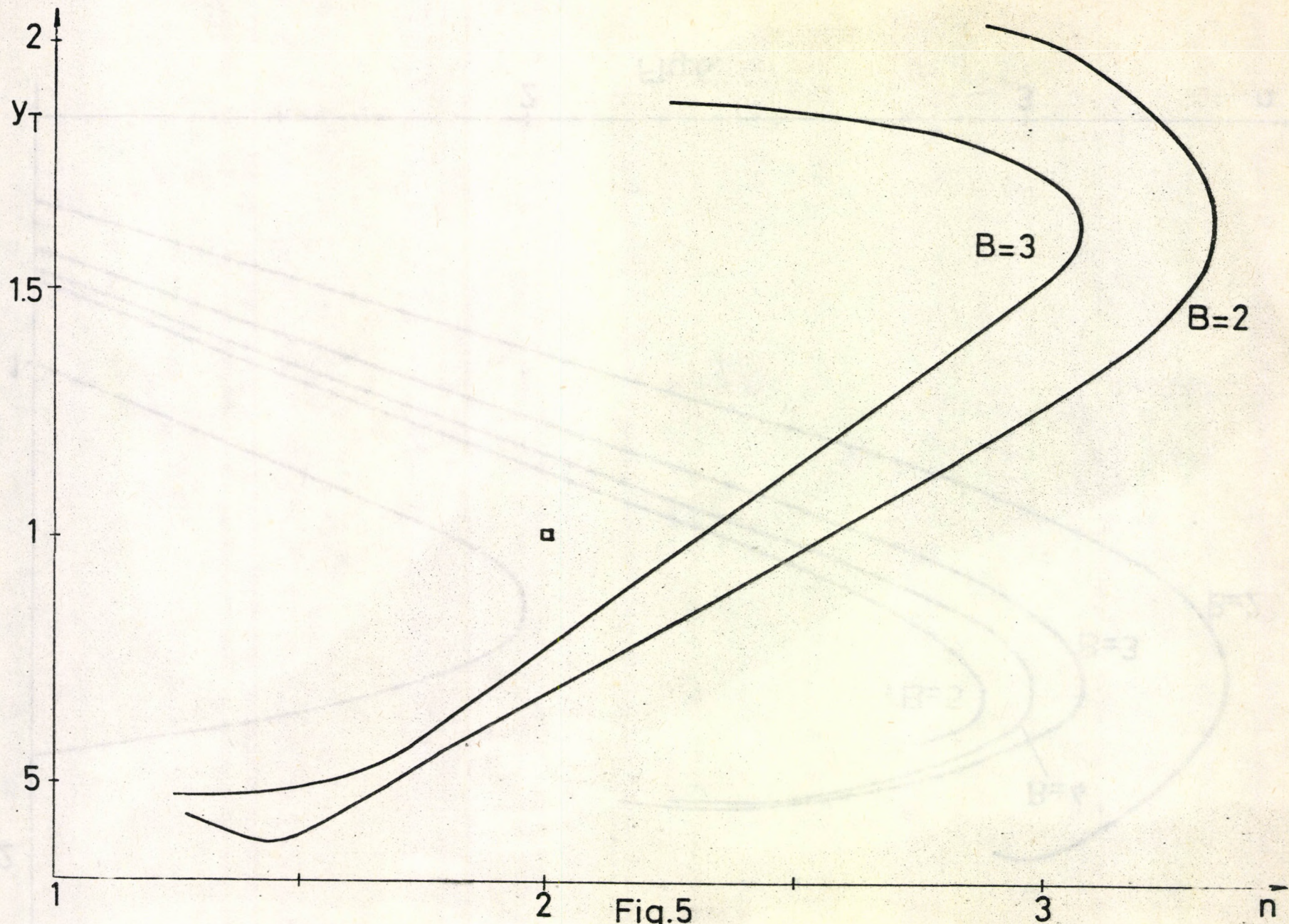


Fig.5

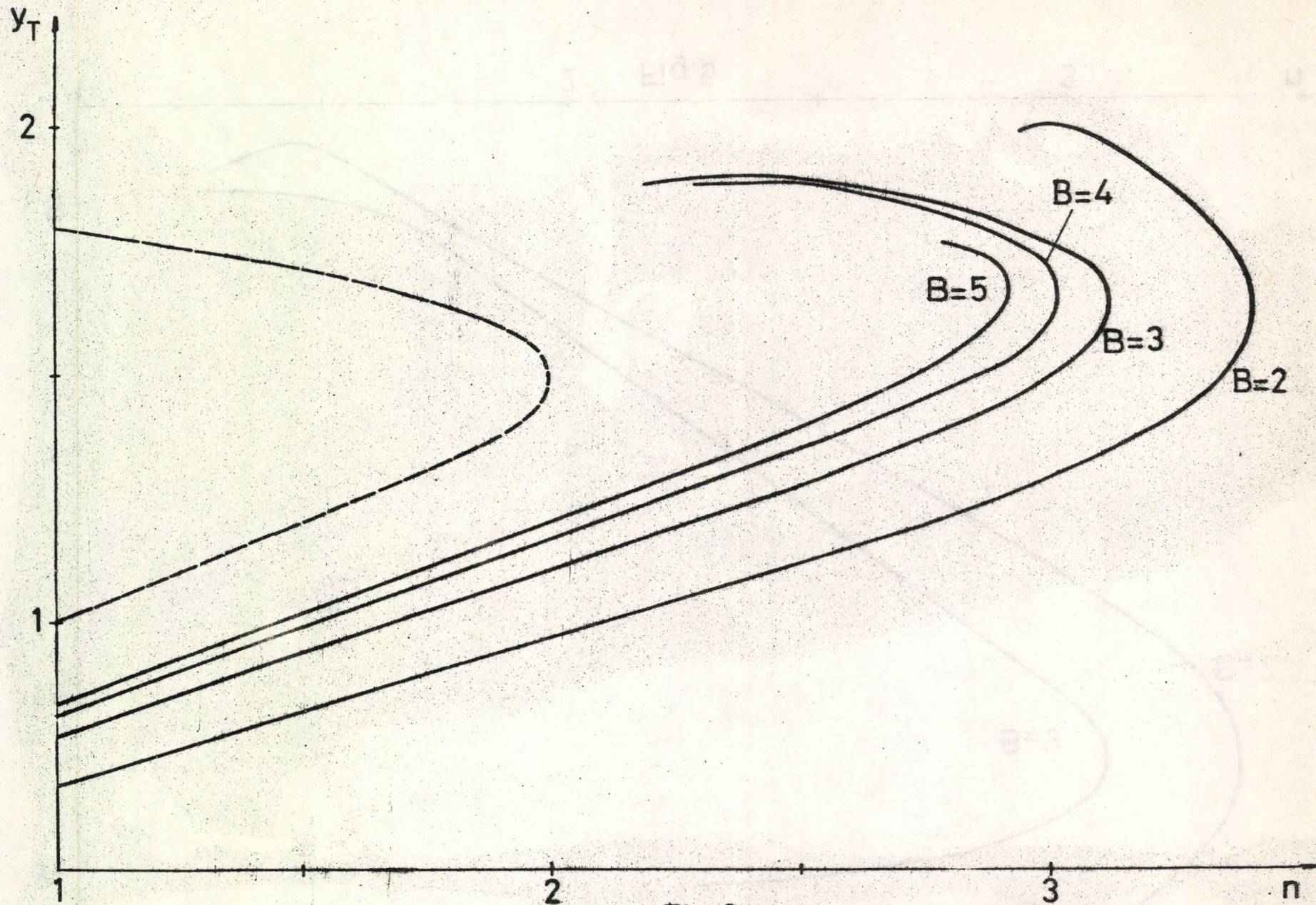
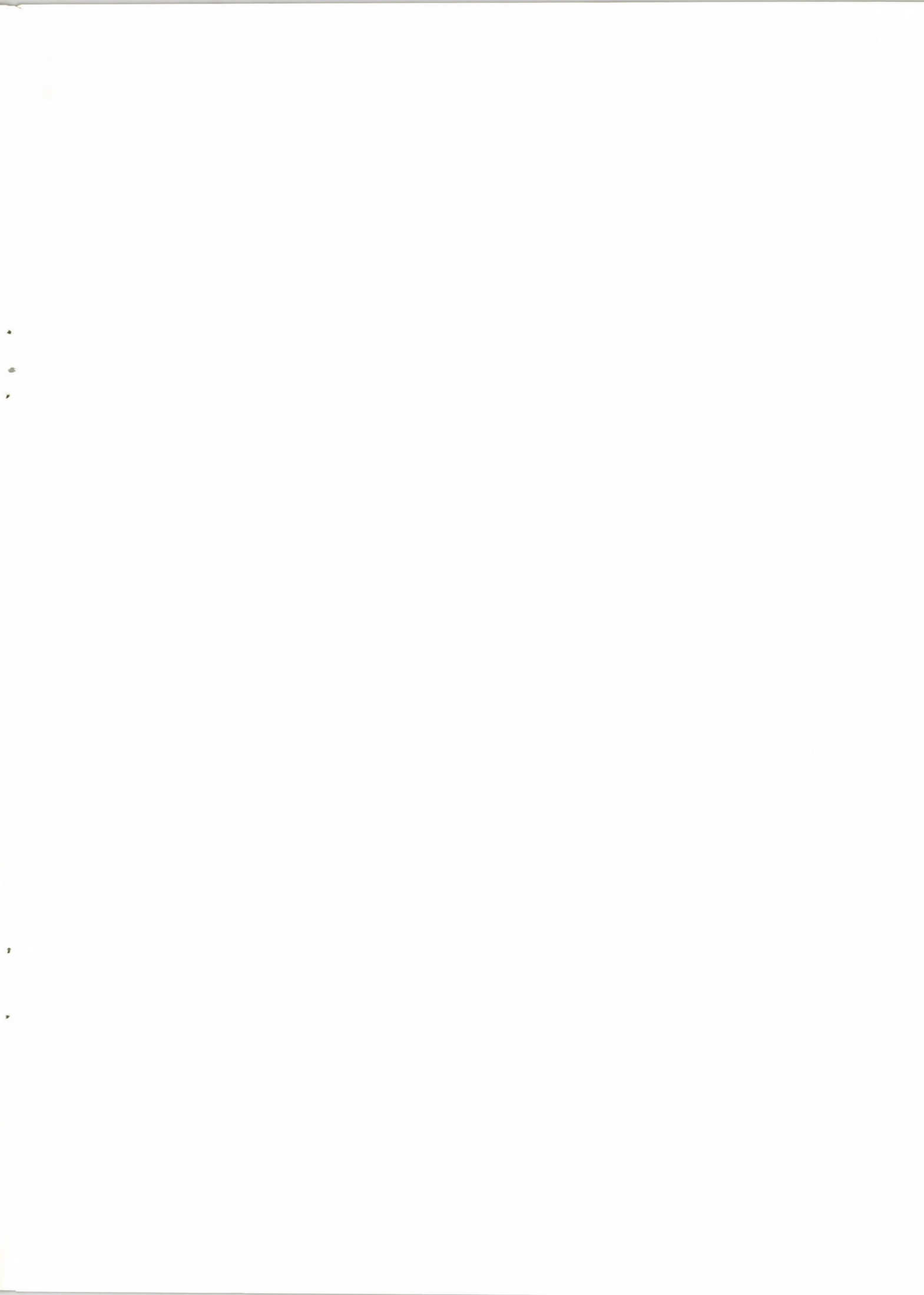


Fig.6.



67.623



Kiadja a Központi Fizikai Kutató Intézet
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