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IV. FIRST ORDER TRANSITION WITHOUT DISCONTINUITY FIXED POINT IN THREE DIMENSIONS

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ABSTRACT

The Hamiltonian version of the three dimensional q-state Potts model is studied by the block transformation method on triangular and square lattices. The transition is found to be of first order when the number q is larger than a critical value. The first order transition however, is not controlled by a discontinuity fixed point.

The critical trajectory is attracted by a point, in which the transformation is discontinuous. The correlation length is finite and there is no time rescaling at the transition point, which represents a first order transition.

АННОТАЦИЯ

Методом блочного преобразования исследован гамильтоновский вариант трехмерной модели Поттса, находящейся в состоянии q, для триангулярной и квадратичной решеток. Показано, что наблюденный в модели фазовый переход является переходом первого рода, если значение q больше определенного критического значения, однако этот переход не контролируется дисконтинуальной фиксированной точкой. Критическая траектория притягивается точкой, при которой преобразование имеет разрыв. Длина корреляции является конечной и не возникает скалинг времени, характерный для переходов первого рода.

KIVONAT

A három dimenziós q-állapotu Potts modell Hamilton változatát tanulmányozzuk blokk transzformációs módszerrel háromszög- és négyzetrácson. Az átalakulást elsőrendünek találjuk, ha q egy kritikus értéket meghalad. Az átalakulást azonban nem egy diszkontinuitási fixpont kontrollálja.

A kritikus trajektóriát egy olyan pont vonzza, ahol a transzformáció szakadásos. A korrelációs hossz véges, és nincs idő skálázódás az átalakulási pontban, mely elsőrendü átalakulásokra jellemző.

I. Introduction.

The q-state Pottsmodel[1] is one of the most extensively studied models of statistical mechanics. In two dimensions (2D) there are many exact[2] and conjectured[3] results, but the properties of the model in three dimensions (3D) are much less known.

An interesting property of the model is that the nature of the phase transition depends on the number q. In d dimensions the transition if of first order, if $q > q_c(d)$, otherwise it is continuous. A mean-field calculation predicts $q_c(d) = 2$ independently of dimension. More refined methods however show that q_c does depend on dimension, and it is exactly known[2] that $q_c(2)=4$, and $q_c(4)=2$. In 3D there is no exact result, but some numerical calculations have been performed. Kogut and Sinclair[4] used the 1/q expansion and found $q_c(3) < 3$. The same conclusion was obtained by Nienhuis et al.[5] They applied the Kadanoff variational renormalization group (RG) for the Potts-lattice-gas model for dimensions 1.58, 2 and 2.32. By increasing the dimension a quickly decreasing q_c was found, and the result $q_c(3) < 3$ was obtained. The direct calculation in 3D (by the Migdal RG method), however, was not succesful in describing a first order transition. Our aim in this paper is to describe the first order transition in the 3D model by the RG method.

This work is the continuation of a series of papers[6], in which J.Solyom, P.Pfeuty and one of the present authors investigated the Hamiltonian version of the 2D Potts model by RG transformations. In the present paper the Hamiltonian version of the 3D model is studied. By performing the time-continuum limit[7] a 2D quantum problem is obtained, which is isomorphic with the 3D classical model. The critical properties of the model are studied by the block transformation[8], and a first order transition is found for $q > q_c$.

In our case however, the manifestation of the first order transition in the RG transformation is of a novel kind. A first order transition is generally described by a discontinuity fixed point[9] (DFP), in which one eigenvalue of the transformation is b^d (b is the rescaling factor). This fact results in a discontinuous behaviour of the order parameter, but some other properties of the transition controlled by the DFP are characteristic of continuous phase transitions, e.g. diverging correlation length, critical slowing down, etc. These problems are related to the fact that the DFP describes the transition with the appearance of an instability.

In our case the first order transition is not controlled by a fixed point in the usual way. The RG transformation has a special point which we call the discontinuity point (DP), which attracts the transition points separating the ordered and disordered phases. By approaching the DP, however, this point becomes infinitely repulsive in the perpendicular direction, which is due to a crossing of energy levels of the first two excited states of the cell Hamiltonian. At the transition point one obtains a finite mass gap, i.e. finite correlation length, and there is no critical slowing down. The thermodynamic quantities either show a jump at the transition point, or can else be described by critical exponents characteristic for first order transitions[10]. The mechanism bringing about the transition is in accordance with the physical picture describing the phase coexistence. The transition takes place before the DFP desribing instability of the ordered phase would appear, because the disordered phase becomes more favourable from the thermodynamic point of view.

The setup of the paper is as follows. In section II the Hamiltonian version of the 3D Potts model and the RG tranformation are presented. Section III contains the results of the calculation (structure of fixed points, critical

couplings and exponents) for square and triangular lattices. In section IV there is a discussion on the nature of the first order transition, while section V contains a summary.

II. Description of the method.

The interaction energy of the q-state Potts model[1] is

$$H_{int} = - \lambda \sum_{<ij>} \delta_{s_i s_j}$$

where $s_i = 1,2,\ldots,q$ and the summation goes over nearest neighbours. The (d-1)- dimensional quantum system whose groundstate properties are isomorphic with the thermodynamic properties of the d-dimensional classical system, can be obtained by making use of the time-continuum limit[7]. Its Hamiltonian can be written in the form:

$$H = H_{int} + H_{field}$$

where the external spin flip field is

$$H_{field} = - h \sum_{i} \sum_{k=1}^{q-1} M_i^k$$

M_i is the spin flip operator:

$$M = \begin{pmatrix} 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ \cdot & & & & \\ \cdot & & & & \\ \cdot & & & & \\ 1 & 0 & 0 & \ldots & 0 \end{pmatrix}$$

For some calculations it is more convenient to use the representation in which H_{field} is diagonal[6] :

$$H_{field} = - h \sum_{i} R_i$$

$$H_{int} = - \frac{\lambda}{q} \sum_{<ij>} \sum_{k=1}^{q-1} M_i^k M_j^{q-k}$$

where R is the nxn diagonal matrix:

$$R = \begin{pmatrix} q-1 & & & & \\ & -1 & & & \\ & & -1 & & \\ & & & \ddots & \\ & & & & -1 \end{pmatrix}$$

The order parameter of the system in the original representation is:

$$S = \delta_{1,\, s_i} - \frac{1}{q}$$

and has the form:

$$S = \frac{1}{q} \sum_{i}^{q-1} M_i^k$$

in the transformed basis.

The critical properties of the system are investigated by the block transformation method developed for quantum systems[8]. One of the present authors has shown that this method, which at first sight seems completely ad-hoc, is the zero temperature limit of a first order approximation to a free energy preserving mapping defined at finite temperature.[11]

In this method the lattice is divided into blocks labeled by an index α. For the triangular lattice the block was chosen as a triangle with three spins, while for the square lattice it is a square with four spins. Both blocks have the property that all sites of the cluster are equivalent. The Hamiltonian of the system is split into two parts. The unperturbed part contains all the field terms and the couplings within the blocks, while the perturbation contains the intra-block couplings. First the Hamiltonian of a cell is diagonalised exactly or numerically. The energy spectrum of the 2D blocks is similar to that obtained in 1D[6]: the ground state is non-degenerate (with energy E_1), while the first excited state is (q-1)-fold degenerate (with energy E_2). Thus

the first q states of the block are identified with the states of a block-spin, which has the original Potts symmetry, while the higher lying states of the block are omitted. The renormalized values of h are determined by the energy spectrum of the block. In the n^{th} step the transformation is:

$$h^{(n)} = \frac{E_2^{(n-1)} - E_1^{(n-1)}}{q}$$

At the same time the energy levels of the block shift by

$$\varepsilon^{(n)} = \frac{E_2^{(n-1)}\,(q-1) + E_1^{(n-1)}}{q}$$

in one renormalization step.

To obtain the renormalized values of the λ coupling, let us first investigate the transformation properties of the M_i operator. The matrix elements of M_i in the space of block-spin variables depend on the states. They are different, depending on whether the ground state is flipped, or the excited ones:

$$^{cell}\langle 1|\, M_i\,|\, q\rangle^{cell} = {}^{cell}\langle 2|\, M_i\,|\, 1\rangle^{cell} = \xi_1$$

$$^{cell}\langle 3|\, M_i\,|\, 2\rangle^{cell} = {}^{cell}\langle 4|\, M_i\,|\, 3\rangle^{cell} = \ldots = {}^{cell}\langle q|\, M_i\,|\, q-1\rangle^{cell} = \xi_2$$

As a consequence, the matrix elements of H_{int} also depend on the number of ground states flipped. It is λ_1/q, λ_2/q and λ_3/q if two, one or zero $|1\rangle^{cell}$ states are flipped, respectively. The three couplings are not independent, they can be expressed by $\xi_1^{(n)}$ and $\xi_2^{(n)}$:

$$\frac{\lambda_1^{(n)}}{q} = {}^{(n)}\langle 1\,2|\, H\,|\, 2\,1\rangle^{(n)} = 2(\xi_1^{(n)})^2$$

$$\frac{\lambda_2^{(n)}}{q} = {}^{(n)}\langle 1\,3|\, H\,|\, 2\,2\rangle^{(n)} = 2.\,\xi_1^{(n)}\xi_2^{(n)}$$

$$\frac{\lambda_3^{(n)}}{q} = {}^{(n)}\langle\, 2 \quad 3|\, H|\, 3 \quad 2 \,\rangle^{(n)} = 2(\xi_2^{(n)})^2$$

The factors 2 on the right hand side appear due to the fact that there are two couplings between blocks, both for triangular and square lattices. The subsequent renormalisation steps do not increase the number of different matrix elements. So in the n^{th} step they are:

$$\xi_1^{(n)} = a_{11}^{(n)}\, \xi_1^{(n-1)} + a_{12}^{(n)}\, \xi_2^{(n-1)}$$

$$\xi_2^{(n)} = a_{21}^{(n)}\, \xi_1^{(n-1)} + a_{22}^{(n)}\, \xi_2^{(n-1)} \qquad (2.2)$$

and

$$\xi_1^{(0)} = \xi_2^{(0)} = 1$$

We mention that the structure of the RG equations, as well as the type of the new couplings is the same as for the (1+1)D model[6]. In the following we use couplings λ, h, and $x=\xi_2/\xi_1$ to describe the state of the system. For the physical model x=1. The ground state energy of the physical system can be calculated from the shift of the block energy (2.1) along the flow trajectory:

$$E_o(\lambda/h) = \sum_{i=1}^{\infty} \frac{\varepsilon^{(i)}}{n_s^i}$$

where n_s is the number of spins in the block. The orderparameter can be calculated from the renormalisation of ξ_1 and ξ_2 (eqs.(2.2)) along the flow trajectory:

$$s = \lim_{n\to\infty} s^{(n)} \qquad (2.3)$$

where

$$s^{(n)} = \frac{q-1}{q^2}\left(\, 2.s_1^{(n)} + (q-2)\, s_2^{(n)} \,\right)$$

$$s_1^{(n)} = s_1^{(n-1)} \left(a_{11}^{(n)} + a_{21}^{(n)}\right)$$

$$s_2^{(n)} = s_2^{(n-1)} \left(a_{12}^{(n)} + a_{22}^{(n)}\right)$$

and

$$s_1^{(o)} = s_2^{(o)} = 1$$

III. Results.

The physical picture given by the RG equations is the same for the triangular and square lattices, and it is similar to that obtained for the (1+1)D model. The physical model (x=1) is ferromagnetically ordered for large values of λ/h and it is paramagnetic if λ/h is small. At the critical value of the coupling $(\lambda/h)_c$, there is a phase transition in the system. When

$$\lambda/h > (\lambda/h)_c \quad ; \quad h^{(n)} \underset{n\to\infty}{\to} 0 \ , \quad \lambda^{(n)} \underset{n\to\infty}{\to} \infty \quad \text{and} \quad x^{(n)} \underset{n\to\infty}{\to} 1$$

the ground state is q-times degenerate, ferromagnetically ordered.

When

$$\lambda/h < (\lambda/h)_c \quad ; \quad h^{(n)} \underset{n\to\infty}{\to} h^{\infty} \neq 0 \ , \quad \lambda^{(n)} \underset{n\to\infty}{\to} 0 \ \text{and} \ x^{(n)} \underset{n\to\infty}{\to} 0$$

the ground state is nondegenerate and paramagnetic.

At the critçial value of the coupling the properties of the transition are controlled by nontrivial fixed points. The structure of these is given in fig. 1. for $q < q_c$, i.e. when the transition is of second order. In this case the transition of the physical model is controlled by a critical fixed point, denoted by C1 in fig.1. The two nontrivial fixed points on the x=0 axis (C2 and T2) control the RG flow on this invariant line, but do not affect the critical properties of the physical model. There is another attractive point of the phase diagram at the position $x=\infty$, $\lambda/h=0$ but $(\lambda/h).x^2$ is finite. This point denoted by D in fig.1 is a DFP for q=3 on the triangular lattice, but for larger values of q and on the square lattice this point becomes a DP. While postponing the detailed analysis of the behaviour at point D to the next section, here we only mention that the point D in all cases can be seen as describing a first order transition in the system. The regions of first and second order transition points are separated by the tricritical fixed point T1.

By increasing the value of q, C1 and T1, as well as C2 and T2, move towards each other. At $q = q_c$ they annihilate each other, and the transition of the physical system is controlled by D, so it is of first order. The calculation can be performed only for integer values of q, therefore the mechanism of annihilation cannot be examined in such detail as in the (1+1) D model.[6] The transition is found to be of first order for $q > 5$ for the square lattice and for $q > 6$ for the triangular lattice. Both values for q_c are somewhat smaller than that obtained for the (1+1)D model in the simplest case (with two spins in a block) where $q_c(1+1) = 6.81$ was found[6]. These values however, are also rather far from the conjectured[4,5] $q_c \lesssim 3$.

The critical properties of the transition (critical coupling, correlation length critical exponent) for $q < q_c$ are given in table 1 both for triangular and square lattices. The series expansion results for the Ising model[12] (q=2) are given in brackets. One can see that the results for the square lattice seem to be more accurate, which can be ascribed to the fact, that in this case more spins are in a block, in comparison with the triangular lattice. The critical couplings as a function of q are given in figs.2.a and 2.b for triangular and square lattice, respectively. The result of the $1/q$ expansion[4] is also given in fig.2.b.

IV. Properties of the first order transition.

In this section we return to the question of the nature of the transition controlled by the point D in fig.1. Indeed this calculation is the first RG calculation which shows a point like the DP. Here we will give arguments why we believe it is possible that this point represents a first order transition.
When the point D is a DFP (for q=3 on the triangular lattice), the first order nature of the transition is signalled by the fact that the specific heat exponent $\alpha=1$. To calculate α we make use of the scaling relation for quantum systems:

$$2 - \alpha = (d-1+z)\,\nu$$

where z is the dynamical exponent, defined by

$$\lim_{n\to\infty} \frac{h^{(n+1)}}{h^{(n)}} = b^{-z}$$

In the DFP $h^{(n)} \underset{n\to\infty}{\to} 0$ and $z > 0$, which gives a diverging correlation length and critical slowing down at the transition point, characteristic also of continuous transitions.

By increasing the value of q, the DFP disappears, and the phase transition is attracted by a DP. To have a closer look at the nature of DP let us investigate the RG transformation in the neighbourhood of this point. Now it is more convenient to use the variables $1/x$ and $\lambda x^2/h$. The result of one RG step at the $1/x=0$ line for q=3 and q>3 are sketched schematically in fig.3.a and 3.b respectively. One can see in the figures that the RG transformation is discontinuous at this line due to a crossing of the energy levels of the first two excited states at a point denoted by CP. This discontinuity has no effect on the critical behavior for q=3, when the transformation still has a DFP. For q>3, however there

is no fixed point of the transformation, the phase transition trajectory is attracted by CP, which we call a discontinuity point (DP). We may still identify however an "imaginary" DFP (indicated between parentheses in fig.3.b), if the second excited state of the block is used in the RG transformation for $\lambda x^2/h<CP$. This "imaginary" DFP can be taken as the instability point of the ordered phase : the overheated system would melt at this point due to fluctuations.

The transition of the physical system is controlled by the DP, so let us have a closer look at its properties. First we mention that the transition in this point has the physical picture of phase coexistence, characteristic of first order transitions. At the phase transition point, scaling to DP does not determine the properties of the system uniquely, since the ratio of the eigenvectors belonging to the same excitation energy of the block and so the ratio of the coexisting phases, are determined by external variables.

The scaling for $1/x > 0$ is continuous, because in this region hybridization of levels occurs instead of their crossing. The transformation properties of the RG equations close to DP, however, are special. Suppose that a point is at the position $h, 1/x$ and $\lambda_c(h,1/x) + \Delta\lambda_3$, i.e. $\Delta\lambda_3$ is the distance of the point from the phase transition trajectory in the $\lambda x^2=\lambda_3$ direction. This point transforms as:

$$h' = \mu_h \cdot h$$

$$(\frac{1}{x})' = \mu_x \cdot \frac{1}{x}$$

$$(\Delta\lambda_3)' = \mu_\lambda \cdot \Delta\lambda_3$$

where the eigenvalues are:

$$\mu_h \cong 1 - \frac{\text{const}}{x^2}$$

$$\mu_x = \text{const} < 1$$

$$\mu_\lambda \simeq \text{const}.x^{\delta}$$

$\delta=2$ for triangular lattice, and $\delta=3$ for the square lattice.

According to these equations we can state that the DP is attractive in the $1/x$ direction, but becomes infinitely repulsive in the perpendicular direction. Furthermore, on the phase transition trajectory[13]

$$h_{c\,n\to\infty}^{(n)} \to h_c^{\infty} > 0$$

Therefore the mass gap is finite at the transition point, which means finite correlation length. One can also see that there is no time rescaling (since $\mu_h \to 1$), so there is no critical slowing down at the transition. Thus we can conclude that the properties of the transformation at the DP are clearly characteristic of first order transitions. This discontinuous behaviour does not show up so clearly in the ground state properties of the system. Due to the approximations in the RG equations, the order parameter (eq.(2.3)) goes to zero at the transition point. However, the corresponding critical index β equals zero which according to the scaling hypotheses[10], is characteristic of first order transitions.

The DP therefore exhibits many properties characteristic of first order transitions. It is an interesting question whether the DP will remain present when larger cells are used, when we go to higher order[11,14], or when other RG schemes are used[15].

V. Summary.

In this paper the Hamiltonian version of the 3D Potts model was investigated by RG transformation, and it was found - for the first time for a 3D model - that the transition is of first order for $q>q_c$. In the simplest approximation $q_c=5$ was obtained for the square lattice, and $q_c=6$ for the triangular lattice. These values are rather far from the conjectured $q_c \lesssim 3$, but the quantum RG method generally gives rather approximate values[8,11].

The first order transition appeared in a novel way in our RG transformation. This transition is controlled by a discontinuity point (DP), by an attractive point, which is not a fixed point of the transformation. The transformation is discontinuous on the line containing DP, due to a crossing of the levels of the first two excited states. The phase transition controlled by the DP is found to be of first order, because at the transition point the correlation length is finite and there is no time rescaling.

Further investigation will have to show however whether the DP can be placed on the same footing as the DFP in describing first order transitions within RG theory.

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q	triangular lattice		square lattice	
	$(\lambda/h)_c$	ν	$(\lambda/h)_c$	ν
2	.381 (.400)	1.59 (.64)	.610 (.658)	1.20 (.66)
3	.805	1.65	1.210	1.03
4	1.303	1.55	1.896	0.84
5	1.908	1.29	2.630	0.66
6	2.526	1.04		

Table I

Table caption

Critical properties of the (2+1)D Pottsmodel obtained by RG transformation on triangular and square lattices.

$(\lambda/h)_c$ and ν denote the critical coupling and the correlation length critical exponent, respectively. The results of series expansion[12] for q=2 are given in parentheses.

Figure captions

fig. 1 : RG phase diagram of the (2+1)D Potts model for $q<q_c$. Empty circles and full dotts represent the trivial and nontrivial fixed points, respectively.

fig.2 : Critical coupling as a function of q for the (2+1)D Potts model:

a. On triangular lattice

b. On square lattice

For the square lattice the results of the 1/q expansion[4] are given by the full curve.

fig.3 : Renormalisation map in the limit 1/x=0 (schematic).

a.In the presence of a discontinuity fixed point

b.In the presence of a discontinuity point(see text)

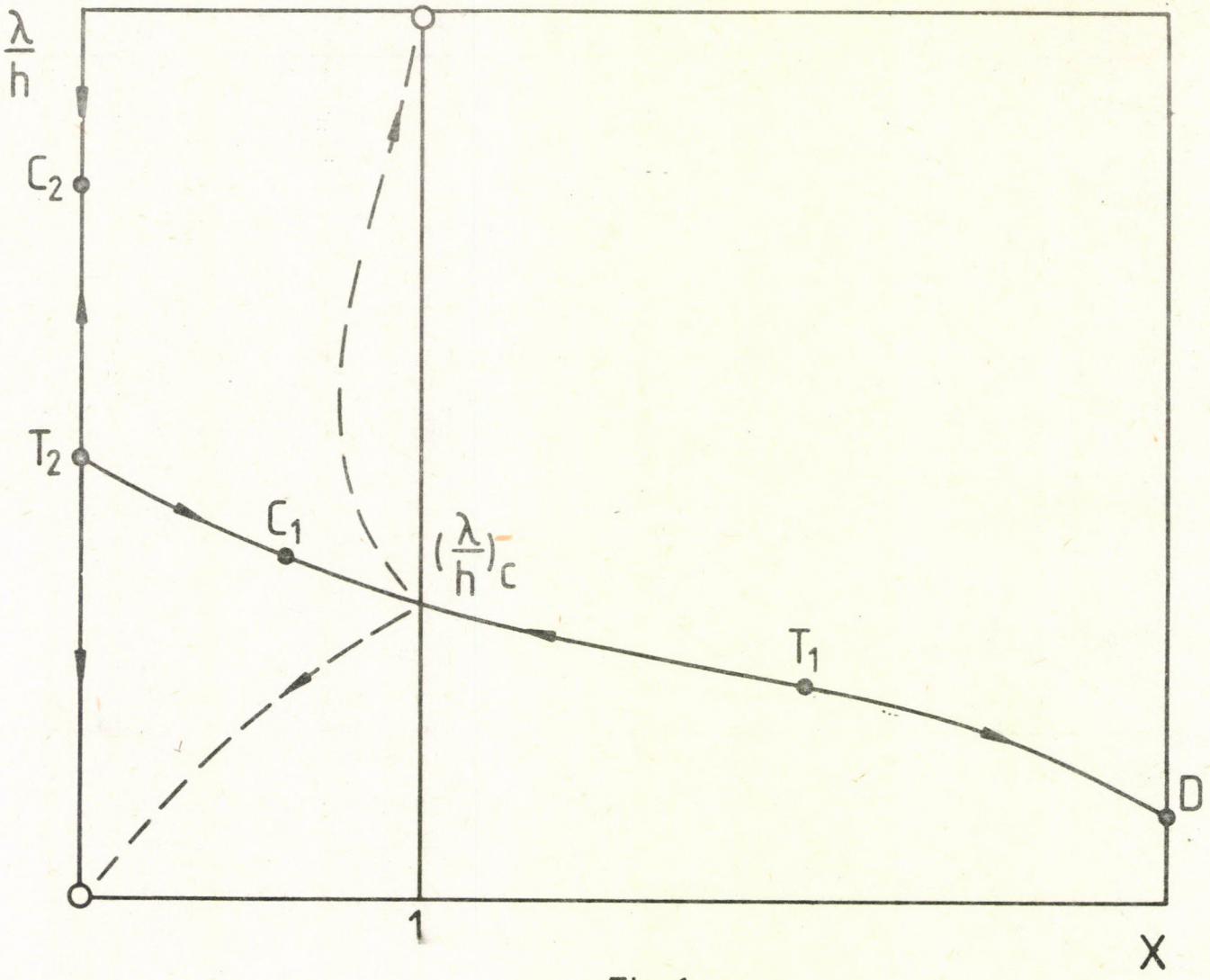

Fig.1

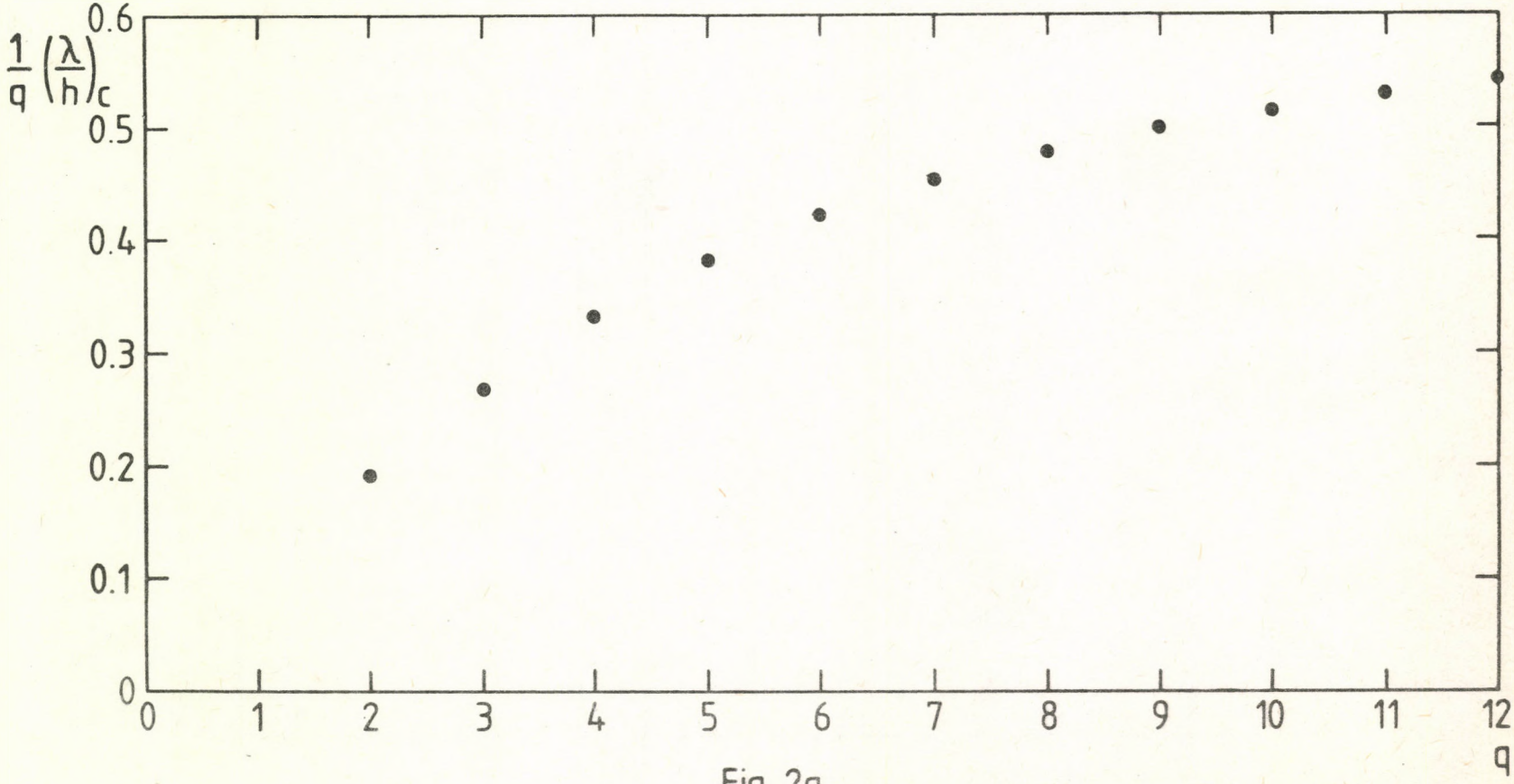
$\frac{1}{q}\left(\frac{\lambda}{h}\right)_c$
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
7
8
9
10
11
12
q

Fig. 2a

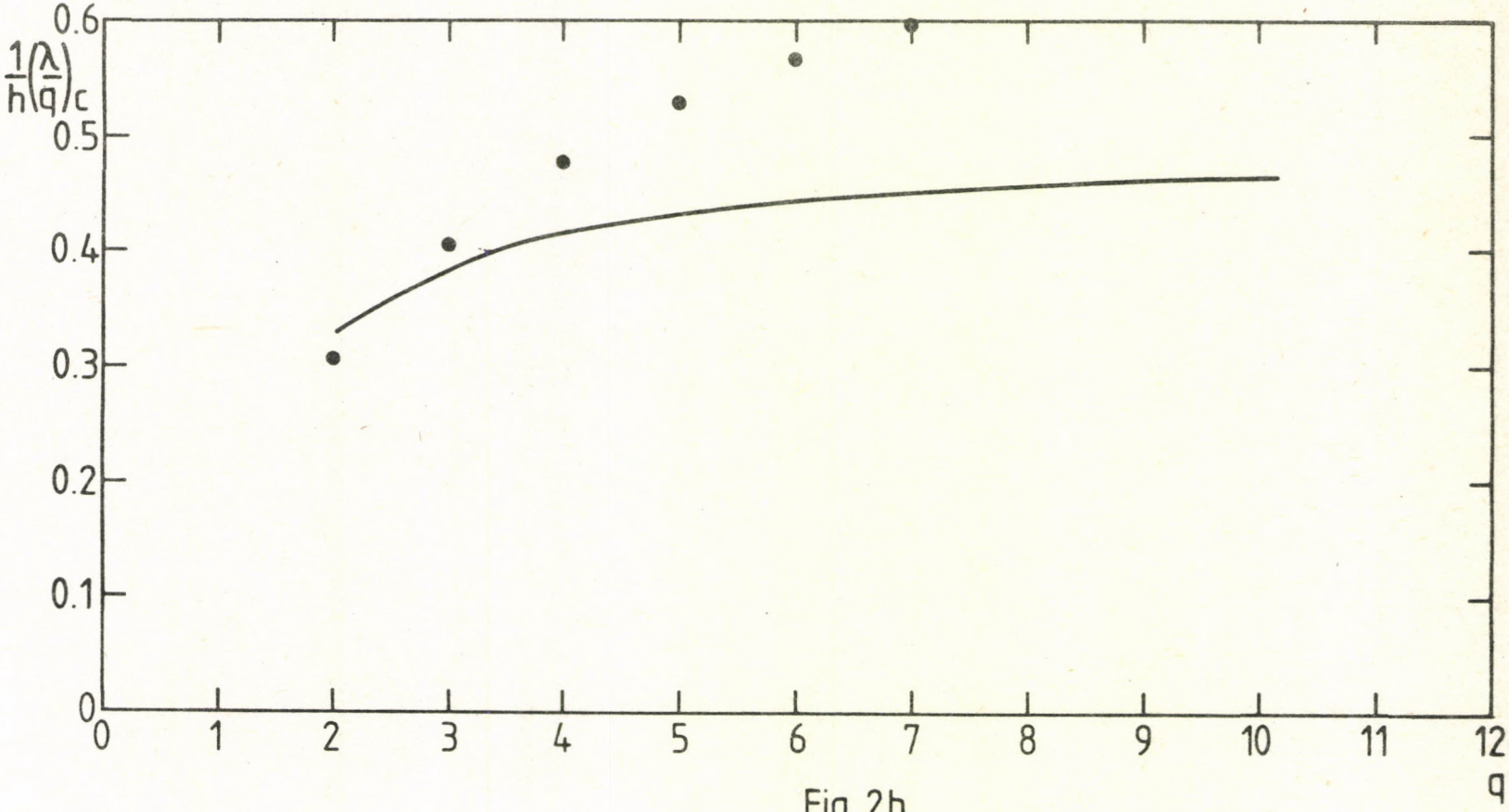
$\frac{1}{h}\left(\frac{\lambda}{q}\right)_c$
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
7
8
9
10
11
12
q

Fig. 2b

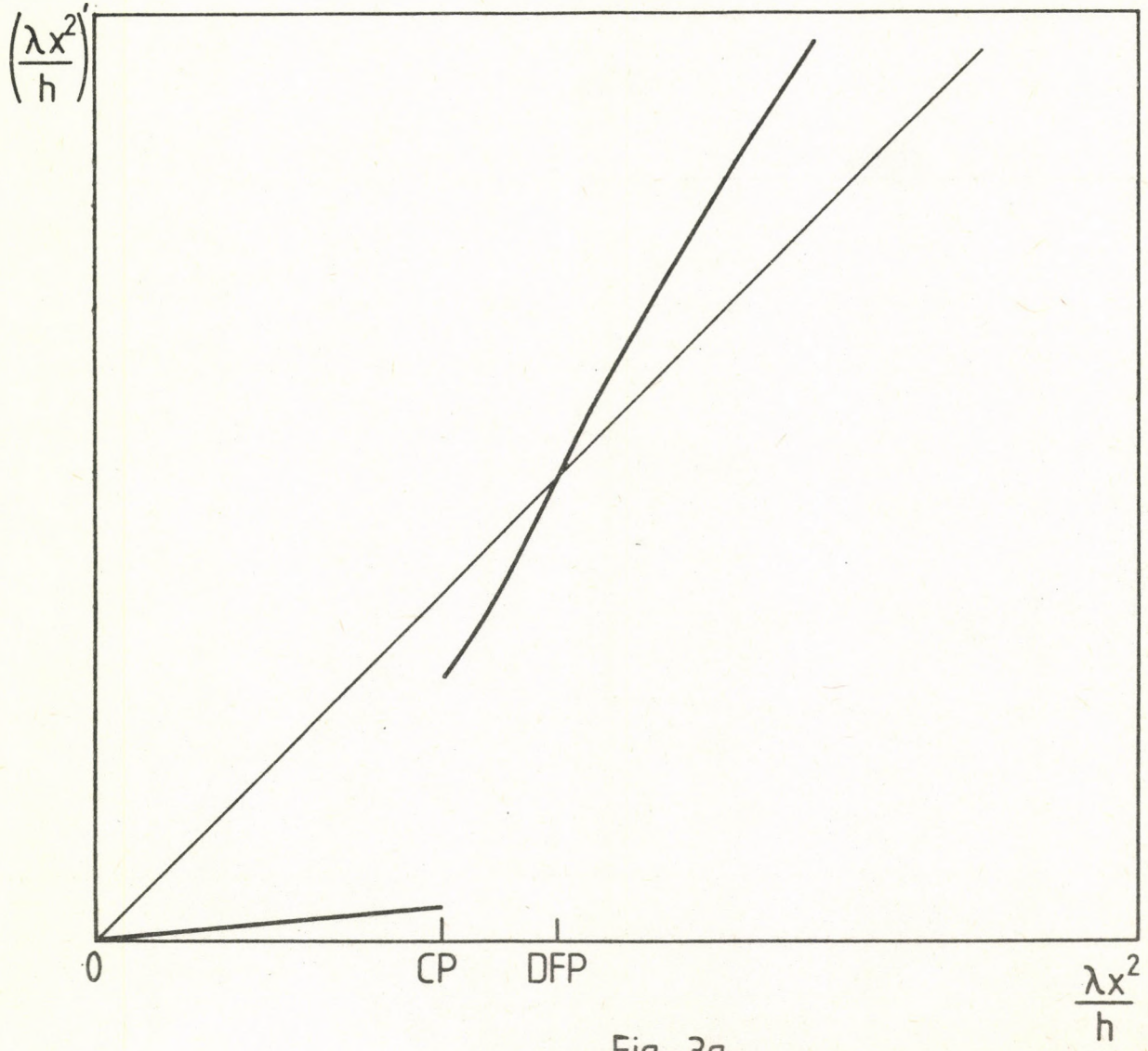

Fig. 3a

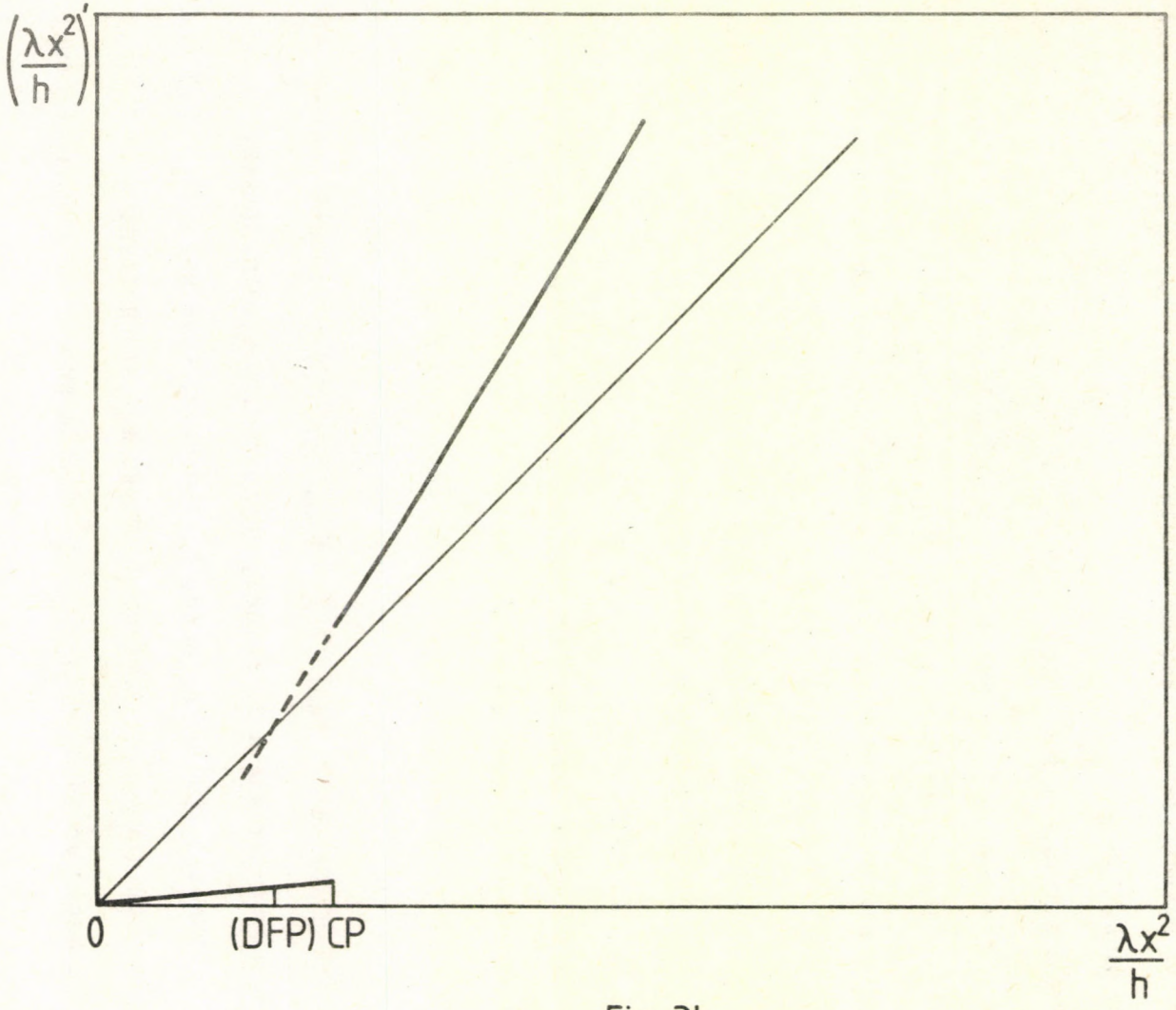

Fig. 3b

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$\lim_{n\to\infty} (\mu_h^{(n+1)} - 1)/(\mu_h^{(n)} - 1) = (\mu_x)^2 < 1$

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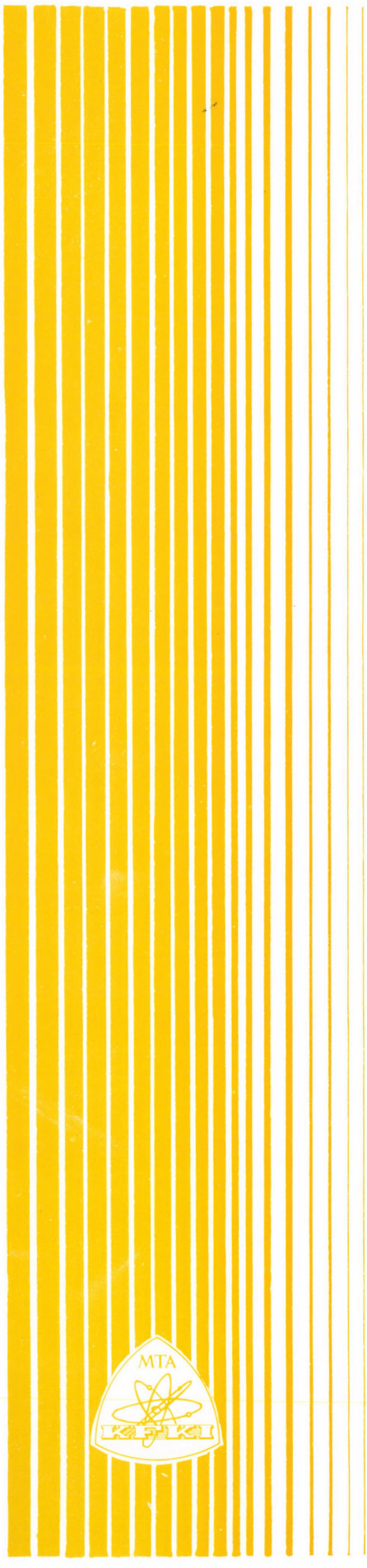

Kiadja a Központi Fizikai Kutató Intézet
Felelős kiadó: Kroó Norbert
Szakmai lektor: Fazekas Patrik
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