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ABSTRACT

The phase transition of the classical two-dimensional Potts model, in particular the order of the transition as the number of components q increases, is studied by constructing renormalization group transformations on the equivalent one-dimensional quantum problem. It is shown that the block transformation with two sites per cell indicates the existence of a critical q_c separating the small q and large q regions with different critical behaviours. The physically accessible fixed point for $q>q_c$ is a discontinuity fixed point where the specific heat exponent $\alpha=1$ and therefore the transition is of first order.

АННОТАЦИЯ

Изучаются фазовые переходы в классической двухмерной модели Поттса, частично зависимость порядка фазового перехода от числа компонентов q посредством исследования эквивалентной одномерной квантовой проблемы, применяя метод ренормализационной группы. Показано, что в проведенном преобразовании блоков, содержащих по два узла решетки, появляется критическое значение q_c, разделяющее две области, в каждой из которых критическое поведение различное. При $q > q_c$ достигается дисконтинуальная фиксированная точка, при которой показатель теплоемкости $\alpha = 1$, и поэтому происходит фазовый переход первого рода.

KIVONAT

A klasszikus kétdimenziós Potts model fázisátalakulásait, pontosabban az átalakulás rendjének a q komponensszámtól való függését tanulmányozzuk az ekvivalens egy dimenziós kvantum probléma renormálási csoportos vizsgálatával. Megmutatjuk, hogy a két rácspontot tartalmazó cellákon elvégzett blokk transzformációban megjelenik egy kritikus q_c mely különböző kritikus viselkedésü két tartományt választ el. $q>q_c$ esetén egy diszkontinuitási fix pontot érünk el, ahol a fajhő exponens $\alpha = 1$ és ezért az átalakulás elsőrendü.

1. INTRODUCTION

Recently there have been several attempts to describe the phase transition in the q-state Potts model[1]. This model is a possible generalization of the two-state Ising model to arbitrary number of states, but much less is known exactly. The critical temperature or critical coupling can be determined from a duality transformation. Baxter[2] has shown that the phase transition in the two-dimensional (2-d) Potts model is of second order if the number of components $q \leq 4$, but of first order for $q>4$. Except for special cases the critical exponents are not known exactly, although there are recent guesses both for the thermal[3] and magnetic[4] exponents.

We know even less about the model in three dimensions. There is evidence from high-temperature series[5] that the three-state Potts model has a first-order transition, there is, however, still no general agreement (see Refs. 6 and 7) whether the critical value q_c which separates the regions with second-order and first-order transitions, respectively, is between $q=2$ and $q=3$ or not. Even if the transition if of first-order, it is, at most, only weakly first order and therefore approximate treatments may easily fail to predict correctly the order of the transition.

In fact most approximate treatments do fail in describing the phase transitions in the Potts model. The mean-field theory[8] predicts first-order transition for the three-state Potts model in any dimensions. The renormalization group (RG) results which should improve upon the mean-field treatment are rather contro-

versial. The RG transformations performed on the continuum Ginzburg-Landau model versions of the Potts model[9,10] give first-order transition not only in ε-expansion around d=4 but also in d=3 and d=2. On the other hand the real space renormalization group transformation in its standard form[11,12] always gives second-order transition irrespective of the number of components.

The real-space RG transformations are not free from ambiguities. The mapping of the cell with several sites to a single Potts spin is rather arbitrary. It was this arbitrariness which allowed Nienhuis et al.[13] to choose that mapping which in its consequences comes closest to the known results of the 2-d Potts model. The mapping can generate vacancies in the lattice of Potts-spins if the Potts-spins in a cell are in different states. The generation of vacancies is more probable for large q (large number of states) than for small q and this gives rise to an abrupt change in the order of transition at a finite q_c. The fixed point of the RG transformation, which was accessible from the pure Potts model for $q \leq q_c$, is annihilated by another fixed point and the accessible fixed point for $q > q_c$ is a discontinuity fixed point.

It would be desirable to have RG transformations which have little arbitrariness in them and allow for systematic improvements. The zero-temperature renormalization groups for quantum systems[14-19] can be formulated in a way that a consistent perturbational calculation can be done in principle to any order. In this paper we present a first-order calculation for the Potts model using quantum RG transformations.

It is well known that d dimensional classical statistical mechanics problems can be related by the transfer matrix to d-1 dimensional quantum problems. In the particular case of the 2-d Ising model, the 1-d quantum equivalent is the Ising chain in transverse field. The Potts model being a generalization of the Ising model, the quantum version will similarly be a Potts chain with some kind of "transverse field". Since the quantum RG calculations do not give usually very good numbers for the critical exponents in the first approximation, it is not expected to get a separation of first-order and second-order transitions at $q_c = 4$, but at least we would like to get an indication that something happens at a finite q_c. In fact, as we will show, the quantum RG calculations reproduce the fixed point structure obtained by Nienhuis at al.[13], and a crossover from second-order to first-order transition is obtained at a finite q_c.

The outline of the paper is as follows. The 1-d Hamiltonian version of the 2-d Potts model is presented in Sec. II. The results of a self-dual RG transformation are given in Sec. III. Another transformation, a block transformation with two sites per cell is performed in Sec. IV. The critical exponents and the order of transition are studied in Sec. V. The discussion of the results is given in Sec. VI.

II. HAMILTONIAN VERSION OF THE POTTS MODEL

In the statistical mechanical formulation of the Potts model the Potts spin can be in q possible states at each site of the lattice. The energy of the configuration depends on whether the Potts spins are in the same or different state on neighboring sites. Denoting this energy difference by ε, the energy of a given configuration is given by

$$E = - \varepsilon \sum_{<ij>} \delta_{s_i, s_j} \tag{2.1}$$

where the Potts spin s_i at site i can have the values $s_i = 1,2,\ldots,q$, and the summation goes over nearest neighbors.

The transfer matrix of the Potts model was constructed by Mittag and Stephen[20]. Assuming different energies ε_1 and ε_2 for the vertical and horizontal nearest neighbors, they have shown that the transfer matrix is proportional to

$$T \sim \exp\left(- \frac{\varepsilon_2}{kT} A\right) \exp\left(- \left(\frac{\varepsilon_1}{kT}\right)^* B\right) \tag{2.2}$$

where $(\varepsilon_1/kT)^*$ is the dual of ε_1/kT,

$$A = \sum_{i=1}^{N} \sum_{k=1}^{q-1} \Omega_i^k \, \Omega_{i+1}^{q-k} , \tag{2.3}$$

and

$$B = \sum_{i=1}^{N} \sum_{k=1}^{q-1} M_i^k , \tag{2.4}$$

the summation over i goes along a row of the lattice, Ω is a diagonal matrix

$$\Omega = \begin{pmatrix} 1 & & & & \\ & \omega & & & \\ & & \omega^2 & & \\ & & & \ddots & \\ & & & & \omega^{q-1} \end{pmatrix}, \quad \omega = \exp\left(\frac{2\pi i}{q}\right) \tag{2.5}$$

while

$$M = \begin{pmatrix} 0 & 1 & 0 & \dots \\ 0 & 0 & 1 & \dots \\ \vdots & & & \\ 1 & 0 & 0 & \dots \end{pmatrix} . \tag{2.6}$$

Stephen and Mittag[21] have also shown that a simple pseudo--Hamiltonian, a linear operator that commutes with the transfer matrix, exists at the critical point of the Potts model which is at

$$(e^{-\frac{\varepsilon_1 q}{kT}} - 1)\,(e^{-\frac{\varepsilon_2 q}{kT}} - 1) = q , \tag{2.7}$$

and there the pseudo-Hamiltonian is proportional to A+B. A Hamiltonian formulation of the Potts model is therefore possible, strictly speaking, at the critical point only.

Assuming, however, that the lattice anisotropy is irrelevant near the critical point, the discrete lattice can be made continuous in one direction. Identifying this direction as the time axis of the quantum model, a timecontinuum quantum version of

the Potts model can be derived[22] near the critical point in the form

$$H = -\frac{\lambda}{q} A - hB \quad , \tag{2.8}$$

and the critical point corresponds to $\lambda/q=h$.

The first part of the Hamiltonian is the usual Potts coupling between the neighboring sites (the energy is lower by $-\lambda$ if the neighbours are in the same state than if they are in different states). The second term is the analogue of the transverse field, it rotates any state into a linear combination of all other states.

It is sometimes more convenient to use a different representation, namely one in which the field part is diagonal. Denoting the states at site i in the representation where the Potts coupling is diagonal by $|k\rangle_i$, k=1,2,...,q, the states

$$|\ell'\rangle_i = \frac{1}{\sqrt{q}} \sum_{k=1}^{q} \omega^{(\ell-1)(k-1)} |k\rangle_i, \quad \ell = 1,2,...,q \tag{2.9}$$

are eigenstates of the transverse field with eigenvalue $-(q-1)h$ for $|1'\rangle$ and h for all the other states. In this representation

$$H = -\frac{\lambda}{q} \sum_{i=1}^{N} \sum_{k=1}^{q-1} M_i^k M_{i+1}^{q-k} - h \sum_{i=1}^{N} R_i \quad , \tag{2.10}$$

with

$$R = \begin{pmatrix} q-1 & & & & \\ & -1 & & & \\ & & -1 & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & -1 \end{pmatrix} . \tag{2.11}$$

This form of the Hamiltonian shows that in this representation the effect of the Potts coupling is to raise one spin and to lower the neighboring spin. The Potts spins are, however, not real spins. Raising the Potts spin when it is in its highest state $|q'\rangle$ brings it to its lowest state $|1'\rangle$.

III. A SELF-DUAL RENORMALIZATION GROUP TRANSFORMATION

The various realizations of the quantum RG transformations and their relationship is discussed in the accompanying paper[23]. Here we will present the results of a self-dual RG transformation and then in the next section another transformation will be considered.

Fernandez-Pacheco[18] proposed an RG transformation for the Ising model, which is self-dual and therefore gives the critical coupling exactly. In addition to that it gives also the ν exponent exactly for the Ising model. When using this method for the Potts model, the sites are groupped into clusters labelled by ℓ , each cluster having b sites. The spin-configuration is fixed on the first site of each cluster and the spins on the remaining sites are eliminated by taking their lowest energy configuration. The Hamiltonian given in Eqs. (2.8), (2.3) and (2.4) is split as

$$H = H_{\text{fixed spin}} + H_{\text{intermediate}} , \tag{3.1}$$

where

$$H_{\text{fixed spin}} = \sum_{\ell=1}^{N/b} H_{\ell} , \tag{3.2}$$

with

$$H_{\ell} = - \frac{\lambda}{q} \sum_{k=1}^{q-1} \Omega_{\ell,1}^{k} \Omega_{\ell,2}^{q-k} - h \sum_{k=1}^{q-1} M_{\ell,1}^{k} , \tag{3.3}$$

containes the single site term on site $(\ell,1)$, where the spin will be considered fixed, and the coupling of this spin to its

right neighbour, while

$$H_{\text{intermediate}} = \sum_{\ell=1}^{N/b} H_{\ell,\ell+1} \quad , \tag{3.4}$$

with

$$H_{\ell,\ell+1} = -\frac{\lambda}{q} \sum_{\alpha=2}^{b-1} \sum_{k=1}^{q-1} \Omega_{\ell,\alpha}^{k} \, \Omega_{\ell,\alpha+1}^{q-k} - \frac{\lambda}{q} \sum_{k=1}^{q-1} \Omega_{\ell,b}^{k} \, \Omega_{\ell+1,1}^{q-k} - h \sum_{\alpha=2}^{b} \sum_{k=1}^{q-1} M_{\ell,\alpha}^{k} \quad , \tag{3.5}$$

contains the field acting on the intermediate spins and all other couplings. This separation is such that both terms are self-dual and therefore the critical coupling will again be obtained exactly.

In the decimation transformation the spins are fixed on sites $(\ell,1)$, $\ell = 1,2 \ldots, N/b$. The thinning of the degrees of freedom is achieved by keeping for each configuration of the fixed spins a single configuration of the intermediate spins which has the lowest energy. Since $H_{\ell,\ell+1}$ does not contain the coupling to the site $(\ell,1)$, the cluster described by $H_{\ell,\ell+1}$ has b sites with one end spin fixed and the energy eigenvalues should be calculated for all possible end spin configurations. H_{ℓ} will be treated as perturbation, it will couple the clusters and will flip the spins which were until now fixed. As the simplest case, we will do the calculation with a scale factor $b=2$. The cluster part of the Hamiltonian is then

$$H_{\ell.\ell+1} = -\frac{\lambda}{q} \sum_{k=1}^{q-1} \Omega_{\ell,2}^{k} \, \Omega_{\ell+1,1}^{q-k} - h \sum_{k=1}^{q-1} M_{\ell,2}^{k} \quad , \tag{3.6}$$

i.e. the cluster has two spins coupled with a Potts coupling, the transverse field acts on one spin only, the other is held fixed. For any fixed state of the spin at $(\ell+1,1)$ the cluster has q states. The eigenstates of $H_{\ell,\ell+1}$ can be easily found. There is one lowest lying level with energy

$$E_o = -\frac{1}{2}[\lambda + (q-2)h] - \sqrt{\frac{1}{4}[\lambda - (q-2)h]^2 + (q-1)h^2}\ , \qquad (3.7)$$

q-2 degenerate levels with energy $E_1=h$, and another level at

$$E_2 = -\frac{1}{2}[\lambda + (q-2)h] + \sqrt{\frac{1}{4}[\lambda - (q-2)h]^2 + (q-1)h^2}\ . \qquad (3.8)$$

The wave function of the lowest lying level, when the spin at $(\ell+1,1)$ is in state $|i\rangle_{\ell+1,1}$, is

$$\psi_i(\ell,\ell+1) = \frac{1}{\sqrt{1+(q-1)a^2}}\{a|1\rangle_{\ell,2} + a|2\rangle_{\ell,2}+\ldots+a|i-1\rangle_{\ell,2}+|i\rangle_{\ell,2}+a|i+1\rangle_{\ell,2}+\ldots$$

$$+ a|q\rangle_{\ell,2}\}|i\rangle_{\ell+1,1} = \chi_i(\ell,\ell+1)\ |i\rangle_{\ell+1,1}\ , \qquad (3.9)$$

with

$$a = \frac{1}{(q-1)h}\{-\frac{1}{2}[\lambda - (q-2)h] + \sqrt{\frac{1}{4}[\lambda - (q-2)h]^2 + (q-1)h^2}\}. \qquad (3.10)$$

Keeping only this lowest energy state, the reduced space of states will be

$$|i_1\rangle_{\ell,1}\,\chi_{i_2}(1,2)|i_2\rangle_{2,1}\ldots|i_\ell\rangle_{\ell,1}\chi_{i_{\ell+1}}(\ell,\ell+1)\ |i_{\ell+1}\rangle_{\ell+1,1}\cdots\ , \qquad (3.11)$$

and it will be mapped onto the state

$$|i_1\rangle_{1\ \text{cell}}\ |i_2\rangle_{2\ \text{cell}} \cdots |i_\ell\rangle_{\ell\ \text{cell}}\ |i_{\ell+1}\rangle_{\ell+1\ \text{cell}} \cdots \qquad (3.12)$$

where $|i_\ell\rangle_{\text{cell}}$ is the i_ℓ state of the ℓ^{th} cell. The Potts coupling between the renormalized states is obtained by calculating the energy difference when the neighboring spins are in the same or different states and we get

$$\lambda_{\text{cell}} = \lambda \frac{1-a^2}{1+(q-1)a^2} \quad . \qquad (3.13)$$

The renormalized value of the transverse field is given by the matrix element between two states differing by a spin flip.

$$h_{\text{cell}} = h \frac{2a+(q-2)a^2}{1+(q-1)a^2} \quad . \qquad (3.14)$$

Repeating this RG transformation n times, the recursion relation for the ratio λ/h is

$$\frac{\lambda_{n+1}}{h_{n+1}} = \frac{\lambda_n}{h_n} \frac{1-a_n^2}{2a_n+(q-2)a_n^2} \qquad (3.15)$$

where a_n is obtained from Eq. (3.10) by using λ_n and h_n in it. The ratio is used because one of the couplings can be used to set the energy scale.

Apart from the trivial fixed points $(\lambda/h)^* = 0$ ($\lambda = 0$, h finite) and $(\lambda/h)^* = \infty$ (λ finite, $h = 0$), there is one non-trivial fixed point at $(\lambda/h)_c = q$, which is the exact result for the critical coupling. Linearizing around the fixed point, the "thermal" eigenvalue is

$$y_t = \frac{q+2\sqrt{q}+2}{\sqrt{q}+2} \qquad (3.16)$$

and the critical exponent ν is obtained from

$$\nu = \frac{\log 2}{\log y_t} \quad . \tag{3.17}$$

An exponent ν_Δ can also be defined from the behavior of the energy gap. In the weak coupling case, when $\lambda/h < (\lambda/h)_c = q$, λ renormalizes to zero, but h goes to a constant value, proportional to the energy gap. Near the critical coupling, the gap Δ behaves as

$$\Delta \sim h \sim \left((\frac{\lambda}{h})_c - \frac{\lambda}{h} \right)^{\nu_\Delta} \quad . \tag{3.18}$$

The exponent ν_Δ can be obtained by following the renormalization of h or using the scaling arguments of Fradkin and Raby[19]. We get

$$\nu_\Delta = \frac{\log Z_h^{-1}((\frac{\lambda}{h})_c)}{\log y_t} \tag{3.19}$$

where Z_h is the multiplicative factor in the renormalization of h,

$$Z_h = \frac{2a+(q-2)a^2}{1+(q-1)a^2} \quad . \tag{3.20}$$

When evaluated at the critical coupling, it gives

$$Z_h^{-1}\left((\frac{\lambda}{h})_c\right) = \frac{2\sqrt{q}+2}{\sqrt{q}+2} \quad . \tag{3.21}$$

As was shown by Jullien et al.[15] the dynamical exponent z can be obtained from the renormalization of the absolute energy spacing, namely

$$b^{-z} = \frac{\lambda_{n+1}}{\lambda_n} = \frac{h_{n+1}}{h_n} \tag{3.22}$$

when these ratios are evaluated at the fixed point value of λ/h. This means that for b=2

$$z = \frac{\log z_h^{-1}((\frac{\lambda}{h})_c)}{\log 2} \tag{3.23}$$

Comparison of Eqs. (3.17), (3.19) and (3.23) gives

$$\nu_\Delta = z\nu \tag{3.24}$$

We have also calculated the eigenvalue for a magnetic perturbation of the form

$$H_{magn} = -\mu \sum_i \delta_{s_i,1} . \tag{3.25}$$

The recursion relation for the perturbation μ is

$$\mu_{n+1} = \mu_n \frac{2+(q-2)\ a_n^2}{1+(q-1)\ a_n^2} \tag{3.26}$$

and the eigenvalue at the fixed point is

$$y_m = \frac{3\sqrt{q} + 4}{2\sqrt{q} + 2} \tag{3.27}$$

The β magnetic exponent has been calculated from

$$\beta/\nu = d - \frac{\log y_m}{\log 2} . \tag{3.28}$$

Finally the specific heat exponent has been obtained using the scaling law

$$2 - \alpha = (1+z)\nu . \tag{3.29}$$

Usually the corresponding scaling law for the static critical exponents is written in the form $2 - \alpha = d\nu$. In the present

quantum case the dimensionality is 1+1, but the time or energy dimension is scaled differently from the spatial dimension. This leads to the factor 1+z instead of d.

The numerical values for the critical exponents are given in Table I. for some values of q. Since very few exact results are known for the Potts model, these numbers should be compared with the conjectured values and will be contrasted to the results of the next sections. The tendency in the variation of the eigenvalues and exponents with q is correct for small q. The exact value of ν for q=2 seems, however, to be an accident. No other exponents are obtained exactly and there is no indication that the order of transition changes as q increases. The transition obtained by this method is always a second order phase transition.

This result is not very surprising after all. The model has only one relevant coupling, λ/h, the ordered and disordered phases are separated by a usual fixed point. A first-order transition can be expected to occur only in a model, where the space of couplings is enlarged, as in the Potts lattice gas version[13] of the Potts model. We will show in the next Section that the generation of new couplings naturally happens in the other versions of the quantum RG transformation.

IV. SCALING EQUATIONS OF THE BLOCK TRANSFORMATION

We will consider now the usual block transformation[14-17] with two sites per cell. The Hamiltonian is split into intracell and intercell parts

$$H = H_{intra} + H_{inter} \quad , \tag{4.1}$$

where the intracell part is

$$H_{intra} = \sum_{\ell=1}^{N/2} H_\ell \quad . \tag{4.2}$$

with

$$H_\ell = -\frac{\lambda}{q} \sum_{k=1}^{q-1} \Omega_{\ell,1}^{k} \Omega_{\ell,2}^{q-k} - h \sum_{\alpha=1}^{2} \sum_{k=1}^{q-1} M_{\ell,\alpha}^{k} \quad , \tag{4.3}$$

while the intercell coupling is

$$H_{inter} = \sum_{\ell=1}^{N/2} H_{\ell,\ell+1} \tag{4.4}$$

with

$$H_{\ell,\ell+1} = -\frac{\lambda}{q} \sum_{k=1}^{q-1} \Omega_{\ell,2}^{k} \Omega_{\ell+1,1}^{q-k} \quad . \tag{4.5}$$

As a first step of the RG transformation, the eigenfunctions and eigenvalues of a single cell have to be determined. A cell of two spins has q^2 states. This eigenvalue problem can be conveniently solved in the representation given in Eq. (2.10) where the eigenstates of the transverse field are used as a basis. In this representation the Hamiltonian of a cell is

$$H_\ell = -\frac{\lambda}{q} \sum_{k=1}^{q-1} M_{\ell,1}^{k} M_{\ell,2}^{q-k} - h \sum_{\alpha=1}^{2} R_{\ell,\alpha} \quad . \tag{4.6}$$

Since the Potts coupling corresponds now to raising and lowering, respectively, the neighboring spins, the q^2 states of the cell fall into q subgroups which are not mixed by H_ℓ. The state $|1'1'>$, when both spins are in the state $|1'>$ (see Eq. (2.9)), is mixed to $|2'q'>$, $|3'\ (q-1)'>$ ... and $|q'2'>$. Looking for the eigenvalues of H_ℓ in the form

$$\psi = a_1 |1'1'> + a_2|2'q'> + \ldots + a_q|q'2'> \tag{4.7}$$

a straightforward diagonalization gives the following wave functions and energies:

$$\psi_1 = \frac{1}{\sqrt{1+(q-1)a^2}} \{|1'1'> + a|2'q'> + a|3'(q-1)'> + \ldots + a|q'2'>\} , \tag{4.8}$$

where

$$a = \frac{q}{(q-1)\lambda} \{ -qh + \frac{q-2}{2q}\lambda + \sqrt{(qh - \frac{q-2}{2q}\lambda)^2 + \frac{q-1}{q^2}\lambda^2} \} , \tag{4.9}$$

is a non-degenerate lowest lying level with energy

$$E_1 = -(q-2)h - \frac{(q-2)}{2q}\lambda - \sqrt{(qh - \frac{q-2}{2q}\lambda)^2 + \frac{q-1}{q^2}\lambda^2} \quad . \tag{4.10}$$

There is a (q-2)-fold degenerate level at a higher energy

$$E_2 = 2h + \frac{\lambda}{q} \quad , \tag{4.11}$$

with wave functions

$$\begin{aligned}
\psi_2^{(1)} &= \frac{1}{\sqrt{q-1}} \{|2'q'> + \varepsilon|3'(q-1)'> + \varepsilon^2|4'(q-2)'> + \ldots + \varepsilon^{q-2}|q'2'> , \\
\psi_2^{(2)} &= \frac{1}{\sqrt{q-1}} \{|2'q'> + \varepsilon^2|3'(q-1)'> + \varepsilon^4|4'(q-2)'> + \ldots + \varepsilon^{2(q-2)}|q'2'>\} , \\
&\vdots \\
\psi_2^{(q-2)} &= \frac{1}{\sqrt{q-1}} \{|2'q'> + \varepsilon^{q-2}|3'(q-1)'> + \varepsilon^{2(q-2)}|4'(q-2)'> + \ldots + \varepsilon^{(q-2)^2}|q'2'>\}
\end{aligned} \tag{4.12}$$

where $\varepsilon = \exp\left(\frac{2\pi i}{q-1}\right)$.

Finally there is another non-degenerate level

$$\psi_3 = \frac{1}{\sqrt{(q-1)^2a^2+q-1}} \{ -(q-1)a|1'1'> + |2'q'> + |3'(q-1)'> + \ldots + |q'2'> \} , \tag{4.13}$$

with energy

$$E_3 = -(q-2)h - \frac{q-2}{2q}\lambda + \sqrt{(qh - \frac{(q-2)}{2q}\lambda)^2 + \frac{q-1}{q^2}\lambda^2} \tag{4.14}$$

Another set of states can be obtained by looking at the state $|1'2'>$ and the states mixed to it. By symmetry similar sets can be obtained by starting from $|1'3'>, \ldots, |1'q'>$ and the energy spectrum will be the same. Seeking the eigenstates in the form

$$\phi = b_1 |1'2'> + b_2 |2'1'> + b_3 |3'q'> + \ldots + b_q |q'3'> , \tag{4.15}$$

the Hamiltonian H_ℓ can again be diagonalized exactly and we get for the eigenfunctions of the lowest lying levels:

$$\begin{aligned}
\phi_1^{(1)} &= \frac{1}{\sqrt{q-2+2b^2}} \{ b|1'2'> + b|2'1'> + |3'q'> + |4'(q-1)'> + \ldots + |q'3'> \} \\
\phi_1^{(2)} &= \frac{1}{\sqrt{q-2+2b^2}} \{ b|1'3'> + |2'2'> + b|3'1'> + |4'q'> + \ldots + |q'4'> \} , \\
&\vdots \\
\phi_1^{(q-1)} &= \frac{1}{\sqrt{q-2+2b^2}} \{ b|1'q'> + |2'(q-1)'> + |3'(q-2)'> + \ldots + b|q'1'> \} ,
\end{aligned} \tag{4.16}$$

with

$$b = \frac{q}{2\lambda} \{ \frac{q}{2}h - \frac{q-4}{2q}\lambda + \sqrt{(\frac{q}{2}h - \frac{q-4}{2q}\lambda)^2 + \frac{2(q-2)}{q^2}\lambda^2} \} , \tag{4.17}$$

and the energy of this (q-1)-fold degenerate level is

$$E_1' = -\frac{q-4}{2}\,h - \frac{q-2}{2q}\,\lambda - \sqrt{\left(\frac{q}{2}\,h - \frac{q-4}{2q}\,\lambda\right)^2 + \frac{2(q-2)}{q^2}\,\lambda^2}\quad . \tag{4.18}$$

There is a higher lying level at

$$E_2' = 2h + \frac{\lambda}{q}\quad , \tag{4.19}$$

which is (q-1)(q-3)-fold degenerate. The wave functions are

$$\begin{aligned}
\phi_2^{(1,1)} &= \frac{1}{\sqrt{q-2}}\,\{|3'q'\rangle + \eta\,|4'(q-1)'\rangle + \eta^2|5'(q-2)'\rangle + \ldots + \eta^{q-3}|q'3'\rangle\}\ ,\\
\phi_2^{(1,2)} &= \frac{1}{\sqrt{q-2}}\,\{|3'q'\rangle + \eta^2|4'(q-1)'\rangle + \eta^4|5'(q-2)'\rangle + \ldots + \eta^{2(q-3)}|q'3'\rangle\}\ ,\\
&\vdots\\
\phi_2^{(1,q-3)} &= \frac{1}{\sqrt{q-2}}\,\{|3'q'\rangle + \eta^{q-3}|4'(q-1)'\rangle + \eta^{2(q-3)}|5'(q-2)'\rangle + \ldots + \eta^{(q-3)^2}|q'3'\rangle\},\\
\phi_2^{(2,1)} &= \frac{1}{\sqrt{q-2}}\,\{|2'2'\rangle + \eta|4'q'\rangle + \eta^2|5'(q-1)'\rangle + \ldots + \eta^{q-3}|q'4'\rangle\}\ ,\\
\phi_2^{(2,2)} &= \frac{1}{\sqrt{q-2}}\,\{|2'2'\rangle + \eta^2|4'q'\rangle + \eta^4|5'(q-1)'\rangle + \ldots + \eta^{2(q-3)}|q'4'\rangle\}\quad ,\\
&\vdots\\
\phi_2^{(2,q-3)} &= \frac{1}{\sqrt{q-2}}\,\{|2'2'\rangle + \eta^{q-3}|4'q'\rangle + \eta^{2(q-2)}|5'(q-1)'\rangle + \ldots + \eta^{(q-3)^2}|q'4'\rangle\}
\end{aligned} \tag{4.20}$$

and similar functions, where $\eta = \exp(2\pi i/(q-2))$.

Finally, the highest lying level at

$$E_3' = -\frac{q-4}{2}\,h - \frac{q-2}{2q}\,\lambda + \sqrt{\left(\frac{q}{2}\,h - \frac{q-4}{2q}\,\lambda\right)^2 + \frac{2(q-2)}{q^2}\,\lambda^2} \tag{4.21}$$

is again (q-1)-times degenerate and the wave functions are:

$$\phi_3^{(1)} = \sqrt{\frac{(q-2)/2}{q-2+2b^2}}\{|1'2'> + |2'1'> - \frac{2}{q-2}b|3'q'> -...- \frac{2}{q-2}b|q'3'>\} ,$$

$$\phi_3^{(2)} = \sqrt{\frac{(q-2)/2}{q-2+2b^2}}\{|1'3'> - \frac{2}{q-2}b|2'2'> +|3'1'> -...- \frac{2}{q-2}b|q'4'>\}$$

$$\vdots$$

$$\phi_3^{(q-1)} = \sqrt{\frac{(q-2)/2}{q-2+2b^2}}\{|1'q'> - \frac{2}{q-2}b|2'(q-1)'> - \frac{2}{q-2}b|3'(q-2)'>-...+|q'1'>\} .$$

(4.22)

The energy spectrum is such that E_1 is the lowest lying level, the next is the (q-1)-times degenerate E_1' level. E_2 and E_2' lie higher and are again degenerate. E_3 and E_3' lie even higher. Keeping the two lowest lying levels with q states, these states could be mapped onto the states of a cell spin with the identification.

$$\psi_1 \rightarrow |1'>_{cell} , \quad \phi_1^{(i)} \rightarrow |(i+1)'>_{cell} , \quad i = 1,2,...,q-1 . \quad (4.23)$$

The effective transverse field acting on the cell spin can be obtained from the energy splitting of the cell spin states

$$qh_{cell} = E_1' - E_1 . \quad (4.24)$$

The Potts coupling between the cell spins can be calculated from the matrix elements between the cell states $|i'>_{\ell cell}|j'>_{\ell+1 cell}$ and $|(i+1)'>_{\ell\ cell}\ |(j-1)'>_{\ell+1 cell}$. Since the wave function of the lowest lying cell state $|1'>_{cell}$ is different in structure from the higher lying (q-1) degenerate states, the matrix element will be different whether all the states $|i'>_{cell}$, $|j'>_{cell}$, $|(i+1)'>_{cell}$ and $|(j-1)'>_{cell}$ are among the degenerate states, or $|1'>_{cell}$ appears

once or twice. This indicates that the RG transformation generates new couplings. For a consistent calculation we will enlarge the space of couplings. Instead of having one Potts coupling, λ, we will introduce three, λ_1, λ_2 and λ_3. They are most conveniently defined by the matrix elements:

$$
\begin{aligned}
-\frac{\lambda_1}{q} &= {}_{\ell+1}\langle 1'|_{\ell}\langle 1'|H|2'\rangle_{\ell}|q'\rangle_{\ell+1} = {}_{\ell+1}\langle 1'|_{\ell}\langle 2'|H|1'\rangle_{\ell}|2'\rangle_{\ell+1} \ , \\
-\frac{\lambda_2}{q} &= {}_{\ell+1}\langle (i-1)'|_{\ell}\langle 2'|H|\,1'\rangle_{\ell}|i'\rangle_{\ell+1} \ , \quad i' = 3',4',\ldots,q' \ , \qquad (4.25) \\
-\frac{\lambda_3}{q} &= {}_{\ell+1}\langle (j-1)'|_{\ell}\langle (i+1)'|H|i'\rangle_{\ell}|j'\rangle_{\ell+1} \ , \ i'= 2',\ldots,(q-1)', \ j'= 3',\ldots q'.
\end{aligned}
$$

The energy spectrum of a single cell can be calculated for this general model in the same way. The parameters a and b in the wave functions are modified

$$
a = \frac{q}{(q-1)\lambda_1}\left\{ -qh + \frac{q-2}{2q}\lambda_3 + \sqrt{\left(qh - \frac{q-2}{2q}\lambda_3\right)^2 + \frac{q-1}{q^2}\lambda_1^2} \right\} , \qquad (4.26)
$$

$$
b = \frac{q}{2\lambda_2}\left\{ \frac{q}{2}h + \frac{\lambda_1-(q-3)\lambda_3}{2q} + \sqrt{\left(\frac{q}{2}h + \frac{\lambda_1-(q-3)\lambda_3}{2q}\right)^2 + \frac{2(q-2)}{q^2}\lambda_2^2} \right\}
$$

and the energies of the two interesting levels are shifted to

$$
\begin{aligned}
E_1 &= -(q-2)h - \frac{q-2}{2q}\lambda_3 - \sqrt{\left(qh - \frac{q-2}{2q}\lambda_3\right)^2 + \frac{q-1}{q^2}\lambda_1^2} \ , \qquad (4.27) \\
E_1' &= -\frac{q-4}{2}h - \frac{\lambda_1+(q-3)\lambda_3}{2q} - \sqrt{\left(\frac{q}{2}h + \frac{\lambda_1-(q-3)\lambda_3}{2q}\right)^2 + \frac{2(q-2)}{q^2}\lambda_2^2}
\end{aligned}
$$

The effective field acting on the cell spins is still given by

the energy splitting of the cell states, as in Eq. (4.24). The λ_1, λ_2 and λ_3 type couplings between the cells are given by the appropriate matrix elements between the cell states.

$$\lambda_{1\ \text{cell}} = \frac{1}{[1+(q-1)a^2][q-2+2b^2]} \{\lambda_1(1+a)^2b^2 + 2(q-2)\lambda_2(1+a)ab + (q-2)^2\lambda_3 a^2\} ,$$

$$\lambda_{2\ \text{cell}} = \frac{1}{\sqrt{1+(q-1)a^2}\ (q-2+2b^2)^{3/2}} \{2\lambda_1(1+a)b^2 + \lambda_2[1+a)b(q-3+b^2) +$$

$$+ 2(q-2)ab] + (q-2)\lambda_3 a(q-3+b^2)\} , \qquad (4.28)$$

$$\lambda_{3\ \text{cell}} = \frac{1}{(q-2+2b^2)^2} \{4\lambda_1 b^2 + 4\lambda_2 b(q-3+b^2) + \lambda_3(q-3+b^2)^2\} .$$

Further iterations of these recursion relations do not lead to new couplings. Since in the original Potts model $\lambda_1 = \lambda_2 = \lambda_3$, it is easy to show that the choice

$$\lambda_2 = x\lambda_1 , \quad \lambda_3 = x^2\lambda_1 \qquad (4.30)$$

reproduces itself. Starting from an arbitrary λ_1 and x, which originally is equal to unity, the renormalized values for a cell are

$$\lambda_{1\ \text{cell}} = \frac{\lambda_1}{[1+(q-1)a^2]\ [q-2+2b^2]} [(1+a)b + x(q-2)a]^2 ,$$

$$x_{\text{cell}} = \frac{\sqrt{1+(q-1)a^2}}{\sqrt{q-2+2b^2}} \quad \frac{[2b+x(q-3+b^2)]}{[(1+a)b+x(q-2)a]} . \qquad (4.31)$$

As mentioned earlier, the quantum decimation transformation[19] is dual to this block transformation. Instead of introducing new

nearest neighbor interactions, there three-spin couplings would appear. The effect of the transverse field would depend on the states of the neighboring spins.

These recursion relations have two trivial fixed points. Starting from the weak field case, $h << \lambda_1 = \lambda_2 = \lambda_3$, the field renormalizes to smaller values, λ_1, λ_2 and λ_3 renormalizes to different values (x gets different from unity), but at the fixed point x=1 again and $h^*=0$, while $\lambda_1^* = \lambda_2^* = \lambda_3^*$ can be arbitrary.

On the other hand, the renormalization of the strong field case, $h >> \lambda_1 = \lambda_2 = \lambda_3$ leads to a fixed point, where h^* can be arbitrary and the Potts couplings vanish, $\lambda_1^* = \lambda_2^* = \lambda_3^* = 0$, but λ_3 and λ_2 vanish faster than λ_1 and $x^* = 0$.

The two regions are separated by the critical value of the couplings, which from duality transformation is known exactly and should be at $h = \lambda/q$. The critical couplings obtained in the present approximation are given in Table II for a few values of q. As it is seen from there, the numbers are better for larger q values and there they give the critical coupling to about 10 % accuracy. Since this is a first-order calculation, it is hoped that next corrections can give quite accurate result.

Starting from the critical coupling and from x = 1, a non--trivial fixed point is reached. The couplings at this fixed point are also given in Table II. The position of the fixed point moves continuously with increasing q up to $q_c = 6.81$, where it jumps to $h/\lambda = \infty$, $x = \infty$.

A closer look at the recursion relations shows that this non-trivial fixed point is not the only one. For $q < 4 + \sqrt{3}$ there is no other fixed point, for $q \geq 4 + \sqrt{3}$, however, two new fixed points appear. A convenient representation is to plot the fixed point values of $h/\lambda x^2$ and $1/x$ for various values of q (see Fig.1). One set of fixed points is always on the line $1/x = 0$ with

$$\frac{h}{\lambda_1 x^2} = \frac{(q-2)^2(q-3)}{q^2(q^2-2q-1)} \tag{4.32}$$

The other set of fixed points moves away to finite x values and merges with the physically accessible fixed points of the Potts model at $q_c \sim 6.81$ and the two fixed points annihilate each other. For larger q values the fixed point at $x = \infty$ becomes physically accessible.

This fixed point structure is very similar to that obtained by Nienhuis et al.[13] for their vacancy model. Their q_c is closer to the $q_c = 4$ exactly known number, but again this may be due to our first approximation. In the next section we will analyze whether the transition for large q is in fact a first-order transition or not.

V. ANALYSIS OF THE CRITICAL BEHAVIOR

Second-order phase transitions are usually described in the framework of the renormalization group calculations in terms of fixed points which are accessible on the critical surface. The situation is not so clear for first-order transitions. There is a large class of magnetic systems[24,25], where the first-order transition has been attributed to the absence of stable fixed points within the domain of stability of the model. This does not apply here, since there is always an accessible fixed point for any value of q.

Nienhuis and Nauenberg[26] have introduced an important new concept, the discontinuity fixed point. There are systems where the first-order transition can be described in terms of the behavior around a special fixed point. A sufficient condition to get a discontinuity in the order parameter or other derivatives of the free energy is to have a fixed point, where the thermal and magnetic eigenvalues of the RG transformation are equal to b^d, where b is the scale factor in the RG transformation and d is the dimensionality. A fixed point where the eigenvalues are equal to b^d is called discontinuity fixed point.

The calculated values of the eigenvalues are given in Table II. As one can see both the thermal and magnetic eigenvalues tend to 2 as $q \to \infty$ but they are not equal to b^d for any finite value of q. Nevertheless one can argue, that the fixed points, which become accessible for $q>q_c$, are discontinuity fixed point and describe a first-order transition.

We have calculated the critical exponents ν, z, β and α in the same way as in Sec. III., while ν_Δ has been determined numerically from the behavior of the gap. For $q = 7, 8, 9$ we could not calculate the gap exponent for computational reasons. We could not reach the trajectories which would come close enough to the fixed point, to see the asymptotic behavior. The values of the critical exponents are given in Table III.

It is seen that the numerically calculated ν_Δ satisfies the scaling law given in Eq. (3.24). Furthermore $2\beta/\nu = z$ is also satisfied.

For $q > q_c$ the thermal and magnetic eigenvalues are

$$y_t = 2\,\frac{(q-2)^2}{(q-3)^2} \quad , \tag{5.1}$$

$$y_m = 2\,\frac{q-3}{q-2} \quad , \tag{5.2}$$

and the dynamical exponent z is obtained from

$$2^{-z} = \frac{\lambda_i^{(n+1)}}{\lambda_i^{(n)}}\bigg|_{(\frac{h}{\lambda})^*} = \frac{h^{(n+1)}}{h^{(n)}}\bigg|_{(\frac{h}{\lambda})^*} = \frac{(q-3)^2}{(q-2)^2} \quad . \tag{5.3}$$

It follows from these expressions and from Eq. (3.17) that

$$(1 + z)\,\nu = 1$$

and therefore Eq. (3.25) gives $\alpha = 1$. We argue that $\alpha = 1$ is the indication that the fixed points for $q > q_c$ are discontinuity fixed points, they describe first-order transition.

When $q \to q_c$, the specific heat exponent $\alpha \to 1$. This means that the critical exponent for the entropy goes to zero, i.e. the entropy gets a step function like temperature dependence, a discontinuity, when q_c is reached. This discontinuity persists for any $q > q_c$.

VI. DISCUSSION

In this paper we have presented a RG treatment of the quantum version of the 2-d Potts model. Our RG calculation gives a crossover from second-order to first-order transition as the number of components increases, in agreement with the known exact results. The fixed point structure of our RG transformation is very similar to that obtained by Nienhuis et al.[13]. The renormalized Hamiltonian has two couplings, h/λ and x, the latter one being generated during the renormalization only. Below a certain critical value of the number of components, q_c, there are three fixed points, two of them at finite values of the couplings, one at infinity. The two fixed points at finite values merge at q_c and annihilate each other and thereby the infinite fixed point becomes physically accessible. At this fixed point the specific heat exponent $\alpha = 1$ and we argued that this is an indication of the first-order nature of the transition. We want to emphasize that our RG transformation is a standard one and no ambiguity was built in, contrary to the modified majority rule of the vacancy model of Nienhuis et al.[13].

Our renormalization group transformation generated a new coupling $x \neq 1$. The coupling was introduced in the representation defined by the states of Eq. (2.9). In terms of the original Potts states the new coupling will flip simultaneously two neighbouring spins. One can try to construct a classical 2-d model whose transfer matrix would correspond to our renormalized Hamiltonian. This classical model will contain four-spin

coupling on a plaquette, but the strengths of the possible four-spin terms are all related to each other. It seems that the introduction of the four-spin couplings has the same effect as the introduction of vacancy variables and allows to describe the crossover from second-order to first-order transition.

The value obtained for q_c , $q_c = 6.81$, is somewhat far from the exact result $q_c = 4$. This is the consequence of taking two sites per cell and keeping for each cell the q lowest lying states only. Improvements could be obtained either by taking larger cells or by taking into account the higher lying states in a perturbational way as proposed for the Ising model by Um[16] and Hirsch and Mazenko[17]. In the first case diagonalization of large matrices would be needed, while in the second case an extremely large number of new couplings would be generated. We feel that both methods would give a slight improvement of q_c, leaving our conclusion on the crossover from second-order transition to first-order intact.

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FIGURE CAPTION

Fig. 1. Locations of the fixed points on the $h/\lambda x^2$ versus $1/x$ plot. q is a parameter of the curves. Fixed points on the straight lines can be reached from the $x = 1$ Potts line. The fixed points on the dotted lines are accessible for a more general model only.

CAPTION OF TABLES

Table I. The thermal and magnetic eigenvalues of the RG transformation and the critical exponents of the q-state Potts model, obtained by a self-dual RG transformation.

Table II. The critical and fixed-point values of the couplings obtained with a block transformation for several q values and the thermal and magnetic eigenvalues of the RG transformation.

Table III. The critical exponents obtained with a block transformation with two sites per block.

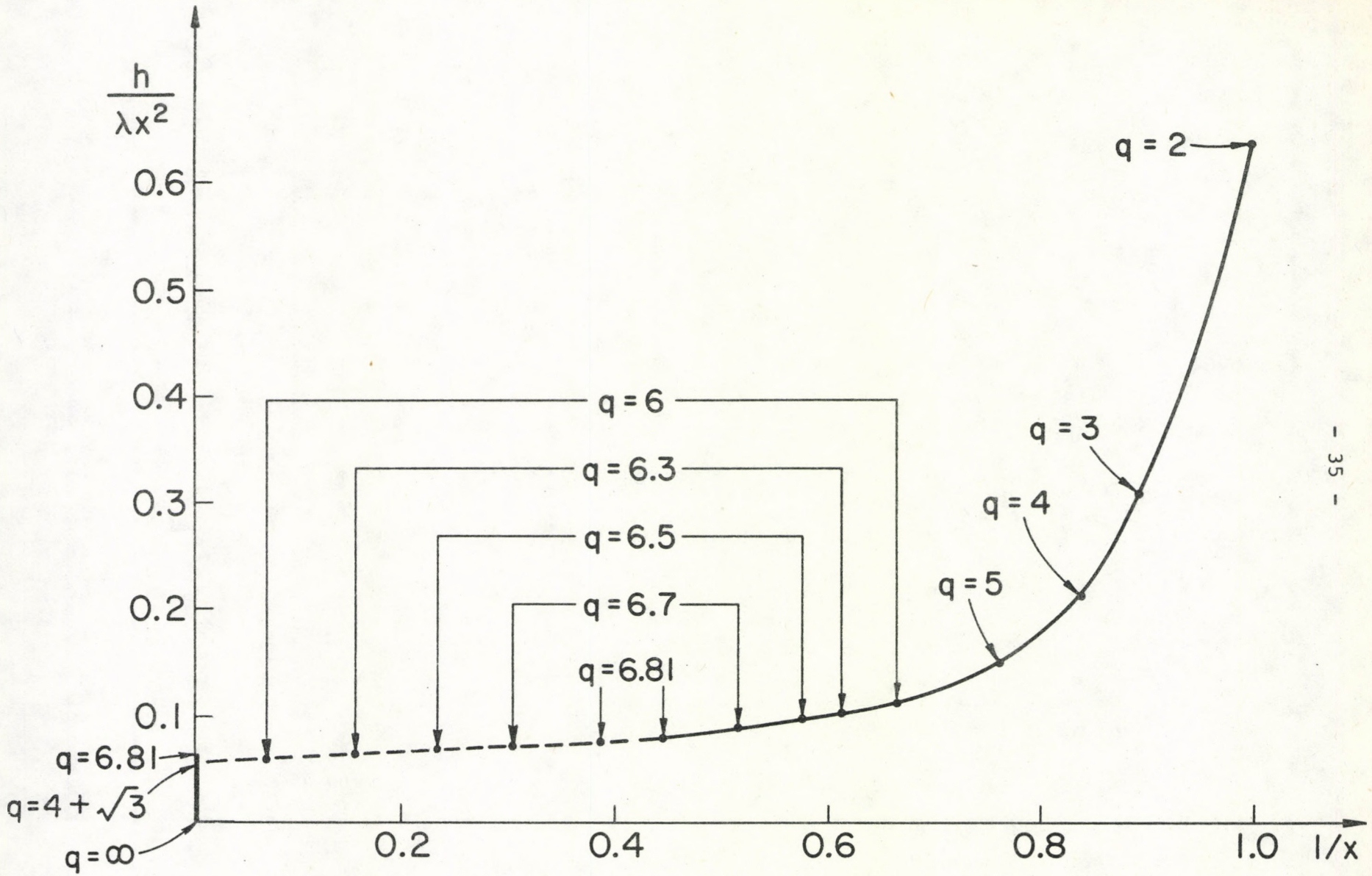

h/λx²
0.6
0.5
0.4
0.3
0.2
0.1
q=6.81
q=4+√3
q=∞
q = 6
q=6.3
q=6.5
q=6.7
q=6.81
q = 2
q = 3
q = 4
q = 5
0.2
0.4
0.6
0.8
1.0
1/x

Fig. 1.

Table I.

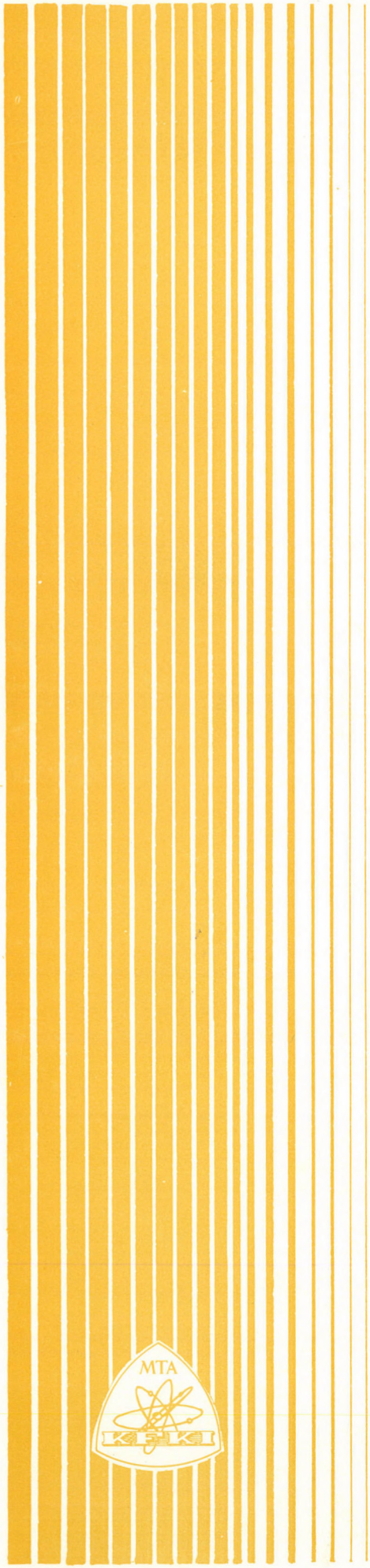
q	eigenvalues		critical exponents					
	thermal λ_t	magnetic λ_m	ν	z	$z\nu=\nu_\Delta$	β	β/ν	α
2	2	1.707	1	0.5	0.5	0.228	0.228	0.5
3	2.268	1.683	0.846	0.550	0.465	0.211	0.249	0.689
4	2.500	1.667	0.756	0.585	0.442	0.199	0.263	0.802
5	2.708	1.655	0.696	0.612	0.426	0.190	0.274	0.878
6	2.899	1.645	0.651	0.633	0.412	0.184	0.282	0.937
7	3.076	1.637	0.617	0.650	0.401	0.178	0.289	0.982
8	3.243	1.631	0.589	0.665	0.392	0.174	0.295	1.019
9	3.400	1.625	0.566	0.678	0.384	0.170	0.300	1.050
10	3.550	1.620	0.547	0.689	0.377	0.166	0.304	1.076
∞	∞	1.500	0	1	0	0	0.415	2

Table II.

q	critical coupling $\frac{h}{\lambda}$	fixed point $\mu = \frac{h}{\lambda_1}$	fixed point x	fixed point $\frac{\mu}{x^2} = \frac{h}{\lambda_1 x^2}$	eigenvalues thermal λ_t	eigenvalues magnetic λ_m
2	0.638	0.638	1.000	0.638	1.596	1.652
3	0.373	0.392	1.115	0.315	1.778	1.635
4	0.260	0.297	1.193	0.209	1.966	1.621
5	0.199	0.258	1.307	0.151	2.177	1.607
6	0.161	0.257	1.513	0.113	2.455	1.592
6.81	0.139	0.407	2.253	0.080	3.020	1.567
6.82	0.139	∞	∞	0.060	3.184	1.585
7	0.135	∞	∞	0.060	3.125	1.600
8	0.116	∞	∞	0.060	2.880	1.666
9	0.102	∞	∞	0.059	2.722	1.714
10	0.091	∞	∞	0.057	2.612	1.750
∞		∞	∞	0	2	2

Table III.

q	ν	$y = \nu^{-1}$	z	$z\nu$	ν_Δ	β/ν	β	α
2	1.483	0.674	0.551	0.818	0.82	0.276	0.409	- 0.301
3	1.205	0.830	0.581	0.700	0.70	0.291	0.350	0.095
4	1.025	0.975	0.607	0.622	0.62	0.303	0.311	0.353
5	0.891	1.122	0.631	0.563	0.56	0.316	0.281	0.546
6	0.772	1.295	0.659	0.508	0.51	0.329	0.254	0.720
6.81	0.627	1.594	0.705	0.442	0.47	0.352	0.221	0.931
6.82	0.598	1.671	0.671	0.401		0.336	0.201	1
7	0.608	1.645	0.644	0.392		0.322	0.196	1
8	0.655	1.527	0.526	0.344		0.264	0.172	1
9	0.692	1.445	0.445	0.308		0.223	0.154	1
10	0.722	1.385	0.385	0.278	0.26	0.193	0.139	1
∞	1	1	0	0		0	0	1



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