Physica **92A** (1978) 323–342 © *North-Holland Publishing Co.*

VARIATIONAL PRINCIPLES IN RENORMALIZATION THEORY

W. VAN SAARLOOS, J.M.J. VAN LEEUWEN

Delft Technological University, Lab. voor Technische Natuurkunde der TH, P.O. Box 5046, 2600 GA – Delft, The Netherlands

and

A.M.M. PRUISKEN

Brown University, Department of Physics, Providence, Rhode Island 02912, USA

Received 9 January 1978

The variational principles introduced by Kadanoff et al in the renormalization theory are analyzed. It is shown that the values for the specific heat critical exponent α which can be found by a variational method are restricted to $\alpha < 0$ or $\alpha = 1$ (first order transition). The reason is the confluence of the singularities in the free energy and in the variational parameters. A full implementation of the variational principle changes for the square Ising lattice the earlier obtained $\alpha = 0.001756$ to $\alpha = -0.123413$.

0. Introduction

The renormalization theory for critical phenomena has provided the means to calculate the critical exponents. The first attempts[1,2]) to obtain accurate exponents by a position space method involved a considerable amount of computational effort. In the search for a simple and accurate method the variational approach of Kadanoff, Houghton and Yalabik (KHY)[3]) seems to be a breakthrough and it has been applied to a variety of models[4]).

The idea of KHY is to use the freedom in defining a renormalization transformation to optimize the free energy. They showed that approximate renormalization transformations can be defined generating a free energy which is a rigorous upper or lower bound to the true free energy. Then the free parameters in the renormalization transformation can be chosen such as to optimize the bounds. Thus, an impressively accurate bound to the free energy results and also the reported critical exponents are very close to what is known exactly or may be expected from other sources.

It has been noted by Knops[5]), however, that the variational principle has not been applied fully around the fixed point and that a more consequent application changes the value of α from $\alpha = 0.001756$ to a value around

$\alpha = -0.1$ (for the $d = 2$ quadratic Ising model where $\alpha = 0$). The source of this change is the dependence of the variational parameters on the interaction constants near a fixed point.

This paper is a refinement and perfection of the criticism of Knops by an analysis of the influence of the singularities in the free energy on the behavior of variational parameters.

In section 1 we formulate the variational principle in the renormalization theory and in section 2 the solution is given near a fixed point under the assumption that the variational parameter is a regular function of the interaction. A few examples are given in section 3 to illustrate the type of situations which may occur. In section 4 we present a (simplified) analysis which yields the relation to singularities in the free energy and in the variational parameter. The general case is studied in section 5 and the paper closes with a discussion.

1. The variation principle in renormalization theory

Consider a system of N degrees of freedom s_i interacting through a hamiltonian $\mathcal{H}(s)$. Then, introduce into the system N' new degrees of freedom s'_i, coupling them to the s_i by a hamiltonian $\mathcal{H}_p(s', s)$ fulfilling

$$\mathrm{Tr}'\, \mathrm{e}^{\mathcal{H}_p(s',s)} = 1, \tag{1.1}$$

where Tr′ stands for the sum (integral) over the new variables s'_i. The index p on $\mathcal{H}_p$ symbolizes the fact that the coupling may contain a number of variational parameters denoted collectively by p. The condition (1.1) ensures that the free energy F of the original system

$$F = \log \mathrm{Tr}\, \mathrm{e}^{\mathcal{H}(s)}, \tag{1.2}$$

and that of the combined system, are equal. (The factor $-1/k_B T$ is included in both the energy and free energy.)

$\mathcal{H}_p(s', s)$ induces a renormalization transformation according to

$$\exp[G_p + \mathcal{H}'_p(s')] = \mathrm{Tr} \exp[\mathcal{H}_p(s', s) + \mathcal{H}(s)], \tag{1.3}$$

where the Tr sums through the old variables only. The constant G_p is made explicit because in spin problems it is customary to define hamiltonians such that

$$\mathrm{Tr}\, \mathcal{H}(s) = \mathrm{Tr}'\, \mathcal{H}'_p(s') = 0. \tag{1.4}$$

Relation (1.3) should be seen as a map from $\mathcal{H}(s)$ to $\mathcal{H}(s')$ which has lesser degrees of freedom, namely N', compared to the N original. We put the dilution ratio equal to $N'/N = b^{-d}$, where b is the linear scale reduction of the system and d the dimension of the system.

Because of (1.1) the free energies F of $\mathcal{H}$ and F'_p of $\mathcal{H}'_p$ are related by

$$G_p + F'_p = F. \tag{1.5}$$

We will represent the hamiltonians $\mathcal{H}(s)$ and $\mathcal{H}'(s')$ by their interaction parameters symbolized by K and K'. The K' as well as G_p are functions of the K and of the variational parameters p. We therefore write (1.3) alternatively as

$$G_p = Ng(K;p); \qquad K' = K'(K;p). \tag{1.6}$$

Then (1.5) obtains the form for the free energy $f(K)$ per degree of freedom $(=F/N)$

$$f(K) = g(K;p) + b^{-d} f(K'(K;p)). \tag{1.7}$$

Note that both terms on the right-hand side of (1.7) may depend on p while f does not. Given the expression for G and K, (1.7) yields a free energy $f(K)$ as it may be obtained by iteration of (1.7).

KHY showed that it is possible to define an approximation to (1.6):

$$g = g_a(K;p); \qquad K' = K'_a(K;p), \tag{1.8}$$

which yields an approximate free energy through

$$f_a(K) = g_a(K;\, p(K)) + b^{-d} f_a(K'_a(K;p(K))) \tag{1.9}$$

for any $p(K)$ obeying either of the two inequalities

$$f(K) \lesseqgtr f_a(K) \tag{1.10}$$

depending on whether one has constructed an upper or lower bound approximation. (Note that through inclusion of $-1/k_BT$ the notion of upper and lower are reversed with respect to the usual free energy.)

Now $f_a(K)$ will depend on the choice of $p(K)$ for a given approximation g_a and K'_a and one has the problem of finding the $p(K)$ which gives the best bound. We will assume, as is the case for all applications so far made, that $g_a(K,p)$ and $K'_a(K,p)$ are regular functions of K and p.

As we will be only concerned with the approximate transformation from now on we drop the index a.

2. Fixed point properties of $p(K)$

In this section we will make a preliminary analysis of $p(K)$ in the neighborhood of a fixed point K^*. To simplify the discussion we assume that K and p are single parameters. One may think of K as a nearest neighbor interaction and of p as a coupling constant between new and old degrees of freedom.

The function $p(K)$ should obey the condition that $f(K)$ is stationary with respect to variations of $p(K)$. Thus, if we take (1.9)

$$f(K) = g(K;p(K)) + b^{-d} f(K'(K;p(K))) \tag{2.1}$$

and differentiate with respect to p we obtain

$$0 = g_p(K; p(K)) + b^{-d} f_K(K') K'_p(K; p(K)), \tag{2.2}$$

where the indices p and K denote differentiation with respect to p and K.

The two equations (2.1) and (2.2) contain the two unknown functions $f(K)$ and $p(K)$ and should be solved simultaneously. With regard to the solution one may distinguish three cases.

(1) The equations do not have a solution, which means that no $p(K)$ makes $f(K)$ stationary. Then the best $p(K)$ assumes a boundary value, e.g. $p(K) = \infty$ (see next section for an example).

(2) A special case is when the equations decouple. This happens when, for each K, a p exists such that

$$g_p(K; p) = K'_p(K; p) = 0. \tag{2.3}$$

The solution $p = p(K)$ of (2.3) satisfies (2.2) regardless of the shape of $f(K)$ and using this $p(K)$ in (2.1) $f(K)$ can be determined. This fortuitous case happens in an example of the following section. Eq. (2.3) leads to a $p(K)$ which is a regular function of K.

(3) The general case is that (2.1) and (2.2) have one or more solutions from which the best has to be chosen. As we shall see it may happen that different regions of K have different branches of the optimal solution $p(K)$.

The interesting situation is the behavior near a fixed point. For arbitrary p we may have a $K^*(p)$ satisfying

$$K^*(p) = K'(K^*(p); p). \tag{2.4}$$

Such a point is a fixed point as it is invariant under the renormalization transformation. A qualitative sketch of $K^*(p)$ is drawn in fig. 1. Now an optimal fixed point is a point K^*, p^* where the optimal $p = p(K)$ intersects the line of fixed points $K = K^*(p)$.

KHY give a prescription to determine this point which reads in our

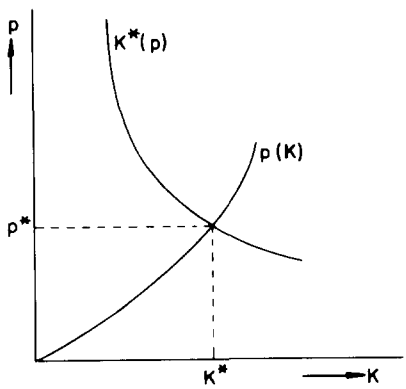

Fig 1 Qualitative sketch of the K–p plane.

simplified version as follows. Differentiate (2.1) with respect to K [using (2.2)]

$$f_K(K) = g_K(K; p(K)) + b^{-d} f_K(K') K'_K(K, p(K)). \tag{2.5}$$

Then, insert $K = K^*$ into both (2.5) and (2.2). As $p(K^*) = p^*$ and $K^*(p^*) = K^*$ and thus with (2.4)

$$K'(K^*; p(K^*)) = K'(K^*(p^*); p^*) = K^*(p^*) = K^*, \tag{2.6}$$

the resulting equations can be written as

$$f^*_K = g^*_K + b^{-d} f^*_K K'^*_K; \qquad 0 = g^*_p + b^{-d} f^*_K K'^*_p, \tag{2.7}$$

where we have used the notation

$$f_K(K^*; p^*) = f^*_K, \qquad g_p(K^*; p^*) = g^*_p, \qquad K'_p(K^*, p^*) = K'^*_p, \quad \text{etc.} \tag{2.8}$$

The two equations (2.7) together with (2.4) [or $K^* = K'(K^*, p^*)$] are three equations for the three unknown K^*, p^* and f^*_K, since all the other quantities like g^*, etc. are known functions of K^* and p^*. We point out that the determination of the *location* of the optimal fixed point goes together with the determination of the *derivative* f^*_K of $f(K)$ at the fixed point K^*. [The value of $f^* = f(K^*)$ then follows from (2.1) by insertion of $K = K^*$.]

Now, once K^* and p^* are determined KHY used K'^*_K to calculate the specific heat exponent α according to

$$b^y = K'^*_K \; (= K'_K(K^*; p^*)), \qquad 2 - \alpha = d/y. \tag{2.9}$$

It was noted by Knops[5]), however, that the variation of $p(K)$ with K contributes also to the derivative of K' with respect to K. Therefore we should equate

$$b^y = K'^*_K + K'^*_p p^*_K, \tag{2.10}$$

where $p^*_K = \partial p(K)/\partial K$ at $K = K^*$.

Thus, the determination of the eigenvalue requires knowledge of the derivative of p and K^*. This quantity can be obtained by differentiating (2.2) and (2.5) once more with respect to K. Then, inserting the fixed point yields the two equations

$$f^*_{KK} = g^*_{KK} + g^*_{Kp} p^*_K + b^{-d}[f^*_{KK}(K'^*_K + K'^*_p p^*_K) K'^*_K + f^*_K(K'^*_{KK} + K'^*_{Kp} p^*_K)]$$

and (2.11)

$$0 = g^*_{Kp} + g^*_{pp} p^*_K + b^{-d}[f^*_{KK}(K'^*_K + K'^*_p p^*_K) K'^*_p + f^*_K(K'^*_{pK} + K'^*_{pp} p^*_K)].$$

The unknowns are f^*_{KK} and p^*_{KK}, all other quantities being known by the previous step.

Now the problem is clear. Whereas in the previous step the determination of f^*_K was required, which generally exists, the calculation of p^*_K involves the second derivative of the free energy f^*_{KK} which will not exist when the specific heat exponent α is positive. Before we embark on the discussion of this point we give some examples to illustrate the procedure given above.

3. Examples

As a first example consider an Ising system with spins $s_i = \pm 1$ interacting through nearest neighbor coupling K on a triangular lattice. We decorate the system with new spins s'_i, in the way indicated in fig. 2. As a coupling hamiltonian for the cell with new spins s' and old spins s_1, s_2, s_3 we take

$$\mathcal{H}_p(s', s_1 s_2 s_3) = ps'(s_1 + s_2 + s_3) - a - b(s_1 s_2 + s_2 s_3 + s_3 s_1), \tag{3.1}$$

which fulfills (1.1) when a and b are defined as

$$a = \tfrac{1}{4}\log[(2\cosh 3p)(2\cosh p)^3]; \qquad b = \tfrac{1}{4}\log[\cosh 3p/\cosh p]. \tag{3.2}$$

For a bound on $f(K)$ the combined hamiltonian is separated into two parts:

$$\mathcal{H}_p(s', s) + \mathcal{H}(s) = \mathcal{H}_0(s', s) + \mathcal{V}(s). \tag{3.3}$$

For a lower bound we may take $\mathcal{H}_0(s', s)$ to be the sum of $\mathcal{H}_p(s', s)$ and the nearest neighbor interactions inside the cells. The remainder, i.e. the interactions between the cells, constitutes $\mathcal{V}(s)$. Then we use the inequality

$$\operatorname{Tr} e^{\mathcal{H}_0(s', s) + \mathcal{V}(s)} = [\operatorname{Tr} e^{\mathcal{H}_0(s', s)}]\langle e^{\mathcal{V}}\rangle \geqslant [\operatorname{Tr} e^{\mathcal{H}_0}]\, e^{\langle \mathcal{V}\rangle_0}, \tag{3.4}$$

where $\langle\ \rangle_0$ is an average involving $\mathcal{H}_0$ as weightfactor.

Thus, the renormalized G and $\mathcal{H}'(s')$ defined as

$$G + \mathcal{H}'(s') = \log[\operatorname{Tr} e^{\mathcal{H}_0}] + \langle \mathcal{V}\rangle_0 \tag{3.5}$$

yield a free energy which is a lower bound to the free energy of a system with $\mathcal{H}(s)$ as hamiltonian. The approximate G and $\mathcal{H}'(s)$ can be readily evaluated[2]). $\mathcal{H}'(s')$ has again only nearest neighbor coupling and one finds

$$g(K; p) = \tfrac{1}{3}\log[e^{3K} + 3e^{-K}],$$

$$K'(K; p) = 2K\left[\frac{(\operatorname{tgh} 3p)\, e^{3K} + (\operatorname{tgh} p)\, e^{-K}}{e^{3K} + 3e^{-K}}\right]^2. \tag{3.6}$$

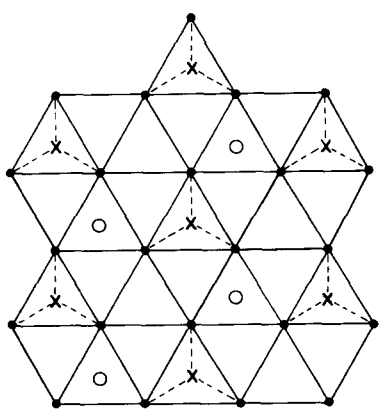

Fig. 2. Decoration of the triangular lattice. ● site-spin; × cell-spin. In the KHY approximation the interactions are shifted in the O-cells.

The free energy $f(K)$ as defined through (3.6) and (2.1) with $b^d = 3$ is a lower bound to the true free energy of a triangular Ising system for any $p(K)$. The search for the optimal $p(K)$ by solving (2.1) and (2.2) leads only to the solution $p = \infty$ for all K. This could have been concluded without calculation by the observation that the best free energy is obtained for given K when K' is as large as possible since g is independent of p and $f(K)$ may be assumed to be increasing with K. Eq. (3.6) shows that the maximum K' for given K is reached for $p = \infty$. For $p = \infty$, (3.6) reduces to the earlier used first cumulant expression[2]) for a renormalization transformation which restricts the possible s for given s' to those configurations where the majority of site spins is in line with the cell spin. Barber[6]) has concluded in a more general context that this type of bound leads to the majority rule transformation.

An upper bound is obtained by the method of KHY. When $\mathcal{V}(s)$ is such that it shifts the interactions to the triangles marked with an 0 we have again as $\mathcal{H}_0(s', s)$ a hamiltonian which is the sum of independent triangles. The calculation of

$$G + \mathcal{H}'(s') = \log[\mathrm{Tr}\, \mathrm{e}^{\mathcal{H}_0(s',s)}] \tag{3.7}$$

is straightforward[7]) and leads to a transformation

$$\begin{aligned} g(K;p) &= \tfrac{1}{12}\log[(\mathrm{e}^{9K} + 3\,\mathrm{e}^{-3K})(\mathrm{e}^{9K-4b} + (2+\mathrm{e}^{4b})\,\mathrm{e}^{-3K})^3], \\ K'(K;p) &= \tfrac{1}{4}\log\left[\frac{\mathrm{e}^{9K} + 3\,\mathrm{e}^{-3K}}{\mathrm{e}^{9K-4b} + (2+\mathrm{e}^{4b})\mathrm{e}^{-3K}}\right], \end{aligned} \tag{3.8}$$

with b as a function of p given by (3.2). The free energy of this transformation is an upper bound since $\langle \mathcal{V}(s) \rangle = 0$ [note that the upper and lower bounds are exchanged with respect to KHY because $-1/k_B T$ is included in $f(K)$]. The variational equation (2.2) for this transformation reads

$$g_p = -K'_p = 4\left[\frac{-\mathrm{e}^{9K-4b} + \mathrm{e}^{4b-3K}}{\mathrm{e}^{9K-4b} + (2+\mathrm{e}^{4b})\mathrm{e}^{-3K}}\right]\frac{\partial b}{\partial p} = 0. \tag{3.9}$$

As $\partial b/\partial p > 0$ the only solution is given by

$$b = 3K/2, \tag{3.10}$$

or for p as function of K

$$p(K) = \pm\tfrac{1}{2}\log\tfrac{1}{2}\{1 + \mathrm{e}^{6K} + [(1+\mathrm{e}^{6K})^2 - 4]^{1/2}\}. \tag{3.11}$$

(The sign of p is immaterial as it can be undone by a sign flip in the cell spins.) The solution (3.11) behaves qualitatively as indicated in fig. 1. Inserting (3.10) into (3.8) yields the optimal transformation

$$\begin{aligned} g(K) &= \tfrac{1}{12}\log[(\mathrm{e}^{9K} + 3\,\mathrm{e}^{-3K})(2\,\mathrm{e}^{3K} + 2\,\mathrm{e}^{-3K})^3], \\ K'(K) &= \tfrac{1}{4}\log\left[\frac{\mathrm{e}^{9K} + 3\,\mathrm{e}^{-3K}}{2\,\mathrm{e}^{3K} + 2\,\mathrm{e}^{-3K}}\right]. \end{aligned} \tag{3.12}$$

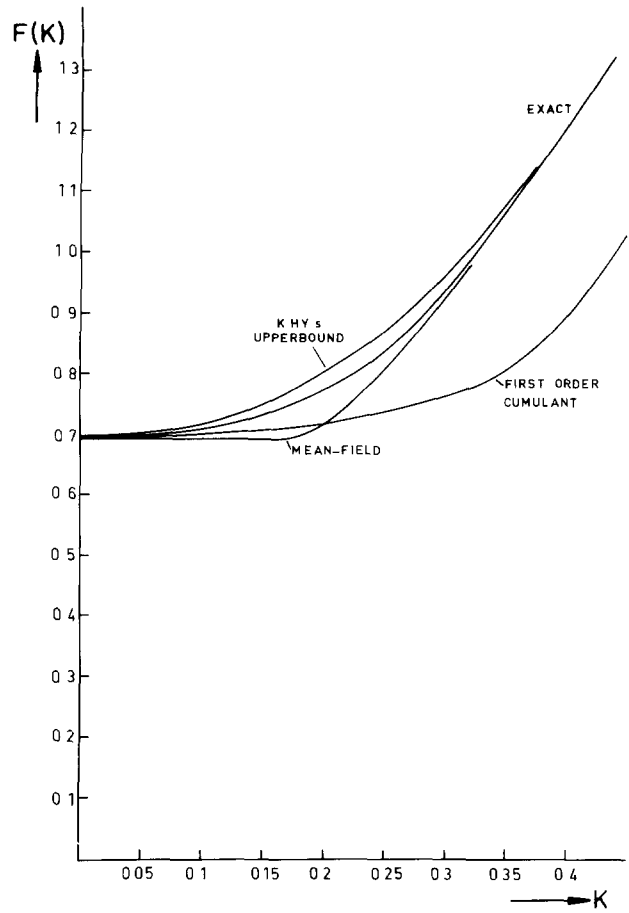

Fig. 3. Comparison of the KHY approximation, the mean-field theory and the first-order cumulant approximation with the exact free energy for the triangular lattice.

The $f(K)$ following from (3.6) (with $p = \infty$) and from (3.12) have been plotted in fig. 3 together with the exact expression. The upper bound is surprisingly good as compared to the lower bound. Both the upper and lower bound free energy have a critical point with a singularity of the type $|K - K^*|^{2-\alpha}$. One finds

	Lower bound	Upper bound	Exact
K	0.3356	0.3798	0.2747
α	−0.2671	−0.5148	0.0

Note that both α values are negative although for these examples no compelling reason exists. In both cases the variational $p(K)$ is not coupled to the free energy it generates.

As a third example we consider the Ising system on a square lattice as

treated by KHY. Their transformation may be written as[3])

$$g = \tfrac{1}{32}\log(Z_1 Z_2^4 Z_3^3/xy^3);$$
$$x' = (Z_1/Z_3)^4; \qquad y' = (Z_2/Z_3)^4, \tag{3.13}$$

with

$$Z_1 = x + 4y + 3, \qquad x = e^{16K},$$
$$Z_2 = \frac{w}{2w^2-1} + 2\frac{w^2+1}{w}y + 3w, \qquad y = e^{4K-8Q}, \tag{3.14}$$
$$Z_3 = \frac{x}{2w^2-1} + 4y + 2w^2 + 1, \qquad w = \cosh 2p.$$

K is the nearest neighbor interaction ($= 2V_2$ of KHY), Q is the four-spin interaction ($= V_4$ of KHY) and p is the coupling between the new spin and a block of four site spins as in (3.1).

In this case the space of interaction parameters K, Q is two-dimensional. The optimal fixed point has the values[3])

$$p^* = 0.765983; \qquad K^* = 0.279433; \qquad Q^* = -0.006865. \tag{3.15}$$

The method described in the previous section may be used to determine the optimal slope of $p(K, Q)$ at the fixed point. The only difference is that we have to compute simultaneously the two derivatives p^*_K and p^*_Q and the three second derivatives f^*_{KK}, f^*_{KQ} and f^*_{QQ}. The equivalent to (2.11) has a solution

$$p^*_K = 3.890460; \qquad f^*_{KK} = 74.779,$$
$$p^*_Q = 0.937846; \qquad f^*_{KQ} = 24.353, \tag{3.16}$$
$$f^*_{QQ} = 9.361.$$

We point out that $f(K, Q)$ has the correct positive curvature at K^*, Q^*. With the values (3.16) for p^*_K and p^*_Q the linearized renormalization transformation can be computed with the matrix

$$\begin{pmatrix} K'^*_K + K'^*_p p^*_K & K'^*_Q + K'^*_p p^*_Q \\ Q'^*_K + Q'^*_p p^*_K & Q'^*_Q + Q'^*_p p^*_Q \end{pmatrix} \tag{3.17}$$

It has the eigenvalues

$$\lambda_T = 1.921030; \qquad \lambda_2 = 0.456844, \tag{3.18}$$

which implies a specific heat exponent $\alpha = -0.123413$. Setting $p^*_K = p^*_Q = 0$ the value of KHY follows which equals $\alpha = 0.001756$. Now it is important to observe that α is negative, the reason of which will become clear in the next sections.

4. The singularities in $p(K)$

After the previous intermezzo of some examples we return to the main problem of how the unknown functions of the problem, the free energy $f(K)$ and the variational function $p(K)$ mutually influence each other, and in particular what the impact is of singularities in $f(K)$ on $p(K)$. It will turn out that, if we assume the existence of a singularity in the free energy, then eqs. (2.1) and (2.2) can only be fulfilled around the fixed point, when the variational $p(K)$ will have also a singularity.

We split $f(K)$ and $p(K)$ into a regular and singular part:

$$\begin{aligned} f(k) &= f^{\mathrm{r}}(K) + f^{\mathrm{s}}(K), \\ p(K) &= p^{\mathrm{r}}(K) + p^{\mathrm{s}}(K). \end{aligned} \tag{4.1}$$

The discussion is kept simple in this section by considering K and p as one-dimensional variables (the general situation will be treated in the section 5). The $f^{\mathrm{s}}(K)$ near K^* behaves as

$$f^{\mathrm{s}}(K) = A|K - K^*|^{2-\alpha}. \tag{4.2}$$

Similarly, $p^{\mathrm{s}}(K)$ will be proportional to some power of $K - K^*$, the determination of which is the subject of this section.

We have to go back to eqs. (2.1) and (2.2) and investigate the impact of the separation (4.1). Using that $g(K; p(K))$ and $K'(K; p(K))$ are by assumption regular in K and $p(K)$ and that $p^{\mathrm{s}}(K)$ is small near K^*, we may expand around the regular parts:

$$\begin{aligned} g(K; p(K)) &= g(K; p^{\mathrm{r}}(K)) + g_p^* p^{\mathrm{s}}(K) + \frac{1}{2!} g_{pp}^* [p^{\mathrm{s}}(K)]^2 + \cdots, \\ K'(K; p(K)) &= K'(K; p^{\mathrm{r}}(K)) + K_p'^* p^{\mathrm{s}}(K) + \frac{1}{2!} K_{pp}'^* [p^{\mathrm{s}}(K)]^2 + \cdots. \end{aligned} \tag{4.3}$$

The expansion of $f(K')$ and $f_K(K')$ is rather more subtle; on the basis of (4.1) and (4.3) we find

$$\begin{aligned} f(K') &= f^{\mathrm{r}}(K') + A|K' - K^*|^{2-\alpha} \\ &= f^{\mathrm{r}}(K'^{\mathrm{r}}) + f_K^{\mathrm{r}*} K_p'^* p^{\mathrm{s}}(K) + \frac{1}{2!} f_{KK}^{\mathrm{r}*} [K_p'^* \cdot p^{\mathrm{s}}(K)]^2 \\ &\quad + \frac{1}{2!} f_K^{\mathrm{r}*} K_{pp}'^* [p^{\mathrm{s}}(K)]^2 + A|K' - K^*|^{2-\alpha}, \end{aligned} \tag{4.4}$$

where $K'^{\mathrm{r}} = K'(K; p^{\mathrm{r}}(K))$. Using (4.3) again, we find for small $K - K^*$

$$K' - K^* = \lambda(K - K^*) + K_p'^* p^{\mathrm{s}}(K), \tag{4.5}$$

with

$$\lambda = K_K'^* + K_p'^* p_K^*. \tag{4.6}$$

Now p^{r}_K is the derivative of the regular part of $p(K)$ (note that $p^{\mathrm{s}}(K)$ has either $p^{\mathrm{s}}_K = 0$ or $p^{\mathrm{s}}_K = \infty$ at the fixed point, depending on the power of the singularity). Thus, (4.4) may be written as

$$f(K') = f^{\mathrm{r}}(K'^{\mathrm{r}}) + f^{\mathrm{r}}_K * K'_p * p^{\mathrm{s}}(K) + \frac{1}{2!} f^{\mathrm{r}}_{KK} * [K'_p * p^{\mathrm{s}}(K)]^2$$

$$+ \frac{1}{2!} f^{\mathrm{r}}_K * K'_{pp} * [p^{\mathrm{s}}(K)]^2 + A|\lambda(K - K^*) + K'_p * p^{\mathrm{s}}(K)|^{2-\alpha}. \tag{4.7}$$

Similarly we can expand $f_K(K')$ which leads to

$$f_K(K') = f^{\mathrm{r}}_K(K'^{\mathrm{r}}) + f^{\mathrm{r}}_{KK} K'_p * p^{\mathrm{s}}(K) + \cdots. \tag{4.8}$$

Now we can collect the various contributions and arrange them according to the singularities appearing. In the lowest order one has

$$\begin{aligned} f^{\mathrm{r}}(K) &= g(K; p^{\mathrm{r}}(K\cdot)) + b^{-d} f^{\mathrm{r}}(K'^{\mathrm{r}}), \\ 0 &= g_p(K; p^{\mathrm{r}}(K)) + b^{-d} f^{\mathrm{r}}_K(K'^{\mathrm{r}}) K'^{\mathrm{r}}_p. \end{aligned} \tag{4.9}$$

Comparison with (2.1) and (2.2) shows that (4.9) is exactly the same as these previously obtained equations for the location of the optimal fixed point.

To first order in the singularities we have

$$\begin{aligned} A|K - K^*|^{2-\alpha} &= \tfrac{1}{2} B[p^{\mathrm{s}}(K)]^2 + b^{-d} A|\lambda(K - K^*) + K'_p * p^{\mathrm{s}}(K)|^{2-\alpha}, \\ 0 &= B p^{\mathrm{s}}(K) + b^{-d} A(2-\alpha) K'_p * |\lambda(K - K^*) + K'_p * p^{\mathrm{s}}(K)|^{1-\alpha}, \end{aligned} \tag{4.10}$$

owing to the fact that in the first equation the term linear in $p^{\mathrm{s}}(K)$ has dropped because of the second equation of (4.9). B stands for

$$B = g^*_{pp} + b^{-d}[f^{\mathrm{r}}_{KK}(K'^*_p)^2 + f^{\mathrm{r}}_K * K'^*_{pp}]. \tag{4.11}$$

Then, in both eqs. (4.10) one has to decide whether $p^{\mathrm{s}}(K)$ or $K - K^*$ is dominant. We treat them separately.

(i) $p^{\mathrm{s}}(K) \ll |K - K^*|$. In this case the two equations reduce to

$$\begin{aligned} 1 &= b^{-d} \lambda^{2-\alpha} \\ \text{and} \qquad & \\ p^{\mathrm{s}}(K) &= -AB^{-1} b^{-d} (2-\alpha) \lambda^{1-\alpha} K'^*_p |K - K^*|^{1-\alpha}. \end{aligned} \tag{4.12}$$

The first equation is the normal connection between the specific heat exponent α and the eigenvalue λ [see (4.6), (2.11) and (2.10)]. The second equation shows that $p^{\mathrm{s}}(K)$ is singular with power $|K - K^*|^{1-\alpha}$, provided that $K'^*_p \neq 0$. This is only consistent with the ansatz if $\alpha < 0$, because otherwise $p^{\mathrm{s}}(K) \gg |K - K^*|$.

(ii) $p^{\mathrm{s}}(K) \gg |K - K^*|$. Now (4.10) becomes

$$\begin{aligned} A|K - K^*|^{2-\alpha} &= \tfrac{1}{2} B[p^{\mathrm{s}}(K)]^2 + A b^{-d} |K'^*_p p^{\mathrm{s}}(K)|^{2-\alpha}, \\ 0 &= B p^{\mathrm{s}}(K) + A b^{-d} (2-\alpha) K'^*_p |K'^*_p p^{\mathrm{s}}(K)|^{1-\alpha}. \end{aligned} \tag{4.13}$$

It is impossible to satisfy these equations. The first equation implies that

$p^s(K)$ should be of order $|K - K^*|$, contrary to the ansatz. Also, the second equation is not possible to fulfill when $K_p^* \neq 0$, as it requires $p^s(K)$ to be of the same order as $|p^s(K)|^{1-\alpha}$. (For $\alpha = 0$ one should include a log term with the same conclusion.) So, we conclude that this case does not occur. When $K_p'^* = 0$ the singular contribution to $p(K)$ of order $|K - K^*|^{1-\alpha}$ disappears. Then $p^s(K)$ is generated by terms of order $|K - K^*|^{2-\alpha}$ and one is in the case (i) as long as $\alpha < 1$.

So far we have discussed the question of whether a singular behavior of the free energy is compatible with fulfilling the variational equations (2.1) and (2.2), and found that this is only possible of $\alpha < 0$. We will now take up the question of whether it is always possible to solve eqs. (2.11) at the fixed point, which is necessary to calculate the eigenvalue λ.

In eqs. (2.11) the two unknowns are f_{kK}^* and p_k^*; however, we can equally well consider λ as unknown since λ and p_k^* are related by (4.6). It turns out that one can eliminate one of the unknowns of (2.11), for instance f_{kK}^*, and one gets the quadratic equation in λ

$$\lambda^2 C_1 + D\lambda + b^d C_1 = 0, \tag{4.14}$$

with

$$\begin{aligned} C_1 &= g_{pK}^* K_p'^* - g_{pp}^* K_K'^* + b^{-d} f_k^* (K_{pK}'^* K_p'^* - K_{pp}'^* K_K'^*), \\ C_2 &= g_{kK}^* K_p'^* - g_{pK}^* K_K'^* + b^{-d} f_k^* (K_{KK}'^* K_p'^* - K_{pK}'^* K_K'^*), \\ D &= b^d g_{pp}^* + K_{pp}'^* f_k^* - K_K'^* C_1 + K_p'^* C_2. \end{aligned} \tag{4.15}$$

[Note that f_k^* is given by (2.7).] Eq. (4.14) has two roots λ_1 and λ_2, fulfilling $\lambda_1 \lambda_2 = b^d$ and one can easily check that we have to consider three possibilities:

(i) the equation has no real solutions;

(ii) the equation has one solution, namely $\lambda = b^{d/2}$, so that $\alpha = 0$; and

(iii) the equation has two real solutions, λ_1 and λ_2.

In the last case one has $\alpha_1 < 0$ and $\alpha_2 > 0$ due to (2.9), (2.10) and (4.6). Although we see that one can find an eigenvalue leading to a positive value of α, we must disregard this solution because the foregoing as a local solution (near K^*) cannot be part of a possible variational function $p(K)$ for which the approximation to the free energy is optimal for all K. In order to see what is likely to happen if (4.14) has no real solutions, we studied a somewhat more sophisticated lower bound to the free energy of the triangular lattice. If we take as $\mathcal{H}_0(s, s')$ in (3.3) the hamiltonian

$$\mathcal{H}_0(s, s') = \sum_i p s_i' s_i \tag{4.16}$$

[so that $\mathcal{V}(s)$ now becomes the sum of $\mathcal{H}_p(s', s)$ and the hamiltonian $\mathcal{H}(s)$ minus $\mathcal{H}_0(s, s')$], where s_i' is the cell spin to which the site i belongs, we have

in first order cumulant the renormalization transformation

$$g(K;p) = \tfrac{2}{3}\log 2 - \tfrac{1}{12}(1+3x)\log(1+3x) - \tfrac{1}{4}(1-x)\log(1-x) + Kx,$$
$$K'(K;p) = 2Kx, \tag{4.17}$$

with $x = \mathrm{tgh}^2 p$. The variation equations for $f(K)$ and $p(K)$ cannot be solved explicitly but for $K \to 0$ and $K \to \infty$ one finds for the optimal $x(K)$

$$K \to 0, \qquad x(K) = K + K^2 + K^3 + \tfrac{7}{3}K^4 + \cdots,$$
$$K \to \infty, \qquad x(K) = 1 - 4\,\mathrm{e}^{-12K}. \tag{4.18}$$

The renormalization transformation (4.17) has a line of fixed points for $x = \frac{1}{2}$, and the eqs. (2.7) yield for the optimal fixed point

$$K^* = \tfrac{1}{6}\log 5 = 0.2684; \qquad f_K^* = \tfrac{3}{4}. \tag{4.19}$$

However, eq. (4.14) has only complex solutions.

In order to see what happens, one can somewhat artificially force the equation to get real solutions by varying b^d, since one can consider b^d as a parameter by which one can change the solution of (2.7) and so of (4.14). When one increases b^d, the optimal fixed point is driven to the fixed point where $g_p^* = 0$ [as can be seen from the second equation (2.7)], and (4.14) will always get real solutions provided that $g_{pp}^* \neq 0$. For this example, the solutions become real beyond

$$b^d = 9.0709; \qquad K^* = 0.3580. \tag{4.20}$$

The following picture shown in fig. 4 is borne out by a numerical calculation for $b^d = 3$. The curve $x(K)$ has two branches, one coming from the region with small K and one from the region with large K, each terminating at a point where $\mathrm{d}x/\mathrm{d}K = \infty$. In the region where a double solution exists is a point

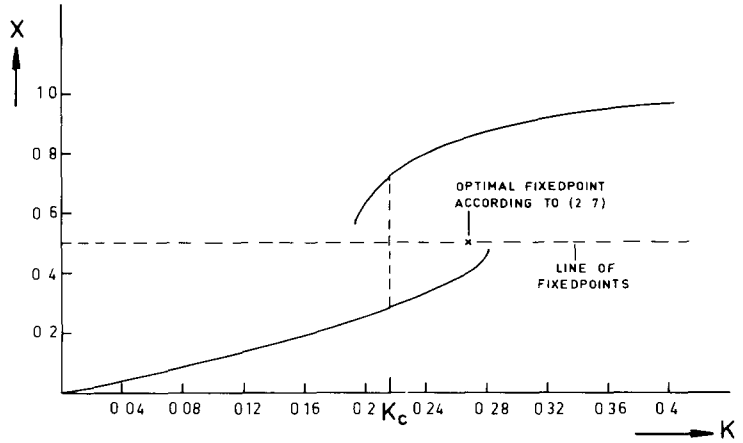

Fig 4 The variational function $x(K)$ for the renormalization transformation (4.17).

K_c located such that beyond K_c the upper branch before K_c the lower branch is the best approximation to the free energy. For K_c we found $K_c \simeq 0.216$ which is much smaller than the value of K at the optimal fixed point [see (4.19)].

The free energy approximation of this renormalization transformation is shown in fig. 5. One can read of the value of K_c from the intersection of the lower- and upper-branch approximations. The free energy at the line of fixed points can easily be calculated by setting $x = \frac{1}{2}$ in (4.17); one sees how bad the approximation of the free energy would be at any fixed point.

This situation is very reminiscent of mean field theory [(4.16) may be seen as the mean field approximation]. It may generally happen that the variational equations have more than one solution in a given region. Then the best solution has to be taken and if the best solution switches from one branch to

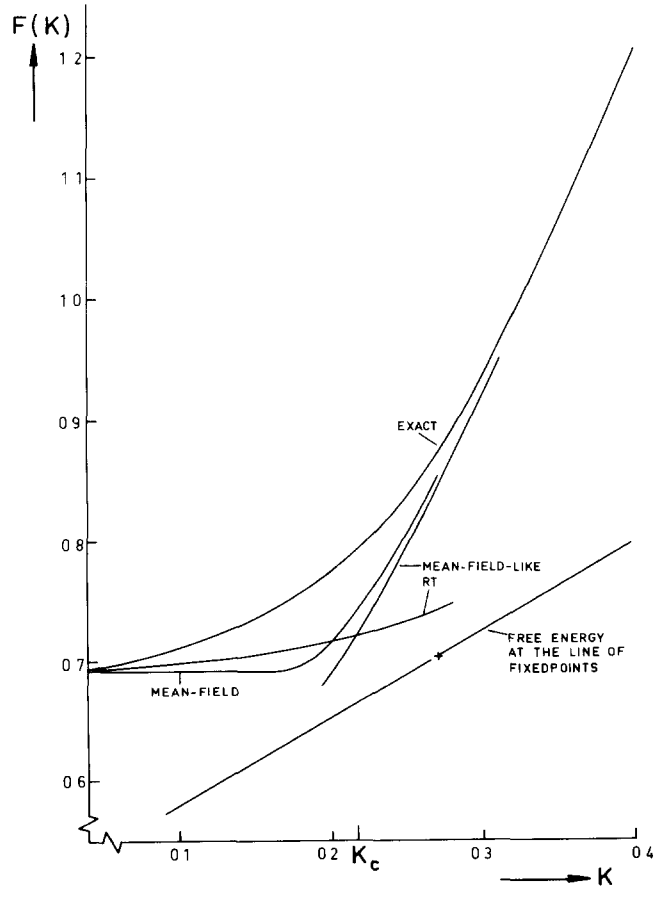

Fig. 5. The free energy given by the renormalization transformation (4 17) and the variational function $x(K)$, compared with the mean-field value and the exact solution

the other as in the previous example a phase transition occurs in the free energy which is in general of first order having $\alpha = 1$. In such a case the fixed point plays no role as in the example where the solution jumps over the line of fixed points.

5. The general situation

For simplicity we have so far concerned ourselves with a situation where the hamiltonian could be represented by a single parameter K. In general, we have a set of n parameters K_α and a set of m parameters p_ι. The main difference when more parameters K_α are present, is that a simple form for the singularity in the free energy cannot be used. Such a singularity is associated with a relevant eigenvalue λ (>1) of the derivative matrix. We assume that we deal with one relevant eigenvalue (e.g. the non-magnetic Ising model). Then we have near the fixed point for the singular part of the free energy (we now use K and p to represent the whole set of parameters K_α and p_ι)

$$f^{\mathrm{s}}(K) = A\left|\sum_\alpha \varphi_\alpha (K_\alpha - K_\alpha^*)\right|^{d/y_{\mathrm{T}}}. \tag{5.1}$$

where φ_α is the left eigenvector of the eigenvalue problem

$$\sum_\alpha \varphi_\alpha \left[\frac{\partial K'_\alpha}{\partial K_\beta} + \sum_\iota \frac{\partial K_\alpha}{\partial p_\iota}\frac{\partial p_\iota}{\partial K_\beta}\right]_{K_\alpha = K_\alpha^*} = \lambda \varphi_\beta, \tag{5.2}$$

and with y_{T} in (5.1) given by $\lambda = b^{y_{\mathrm{T}}}$.

To shorten the notation, we write for the fixed point values again

$$\begin{aligned}\left[\frac{\partial K'_\alpha(K; p(K))}{\partial K_\beta}\right]_{K=K^*} &= K'^*_{\alpha,\beta},\\ \left[\frac{\partial K'_\alpha(K; p(K))}{\partial p_\iota}\right]_{K=K^*} &= K'^*_{\alpha,\iota}, \text{ etc.}\end{aligned} \tag{5.3}$$

and we will abbreviate the matrix (5.2) to $T^*_{\alpha\beta}$

$$T^*_{\alpha\beta} = K'^*_{\alpha,\beta} + \sum_\iota K'^*_{\alpha,\iota} p^*_{\iota,\beta}. \tag{5.4}$$

Finally, using Wegner's scaling fields, defined by

$$u^{\mathrm{T}} = \sum_\alpha \varphi_\alpha (K_\alpha - K_\alpha^*) + \cdots. \tag{5.5}$$

one can write for the singular part of the free energy

$$f^{\mathrm{s}}(K) = A|u^{\mathrm{T}}|^{d/y_{\mathrm{T}}}. \tag{5.6}$$

The variational equations are obtained by the condition that $f(K)$ is stationary with respect to all variations of the $p_\iota(K)$ of the set $p(K)$. Thus, the variation

problem is now given by

$$f(K) = g(K; p(K)) + b^{-d} f(K'),$$
$$0 = g_\iota(K; p(K) + b^{-d} \sum_\alpha f_\alpha(K') K'_{\alpha,\iota}, \tag{5.7}$$

while the location of the optimal fixed point can be determined by

$$f^*_\alpha = g^*_\alpha + b^{-d} \sum_\beta f^*_\beta K'^*_{\beta,\alpha},$$
$$0 = g^*_\iota + b^{-d} \sum_\beta f^*_\beta K'^*_{\beta,\iota}. \tag{5.8}$$

Provided the second order derivatives of $f(K)$ exist, one may determine the derivatives $p^*_{\iota,\alpha}$ and $f^*_{\alpha\beta}$ from

$$f_{\alpha\beta} = h_{\alpha\beta} + b^{-d} \sum_{\gamma\delta} f^*_{\gamma\delta} K'^*_{\gamma,\alpha} T^*_{\delta\beta},$$
$$0 = k_{\alpha\iota} + b^{-d} \sum_{\beta\gamma} f^*_{\beta\gamma} K'^*_{\beta,\iota} T^*_{\gamma\alpha}, \tag{5.9}$$

where

$$h_{\alpha\beta} = g^*_{\alpha\beta} + \sum_\iota g^*_{\alpha\iota} p^*_{\iota,\beta} + b^{-d} \sum_\gamma f^*_\gamma \Big(K'^*_{\gamma,\alpha\beta} + \sum_\iota K'^*_{\gamma,\alpha\iota} p^*_{\iota,\beta} \Big),$$
$$k_{\alpha\iota} = g^*_{\alpha\iota} + \sum_j g^*_{ij} p^*_{j,\alpha} + b^{-d} \sum_\gamma f^*_\gamma \Big(K'^*_{\gamma,\iota\alpha} + \sum_j K'^*_{\gamma,ij} p^*_{j,\alpha} \Big). \tag{5.10}$$

To determine the eigenvalues of the matrix $T^*_{\alpha\beta}$, one has to solve these $\frac{1}{2}n(n+1) + m \cdot n$ equations.

The procedure to investigate the impact of a singularity in the free energy on the $p_\iota(K)$ is completely analogous to the one in the previous section. We split $f(K)$ and $p_\iota(K)$ in regular and singular parts

$$f(K) = f^{\mathrm{r}}(K) + f^{\mathrm{s}}(K),$$
$$p_\iota(K) = p_\iota^{\mathrm{r}}(K) + p_\iota^{\mathrm{s}}(K), \tag{5.11}$$

and assume that $p^{\mathrm{s}}(K)$ is small near K^*; then one can expand $g(K; p(K))$, $K'(K; p(K))$ and $f^{\mathrm{r}}(K)$ around the regular parts. Since this can be done analogously to the expansion in section 4, we only give the result for $f(K')$:

$$\begin{aligned} f(K') &= f^{\mathrm{r}}(K) + f^{\mathrm{s}}(K) \\ &= f^{\mathrm{r}}(K'') + \sum_{\alpha,\iota} f^{\mathrm{r}}_\alpha {}^* K'^*_{\alpha,\iota} p^{\mathrm{s}}_\iota(K) + \frac{1}{2!} \sum_{\alpha,\beta} f^{\mathrm{r}}_{\alpha\beta}{}^* K'^*_{\alpha,\iota} K'^*_{\beta,\jmath} p^{\mathrm{s}}_\iota(K) p^{\mathrm{s}}_\jmath(K) \\ &\quad + \frac{1}{2!} \sum_{\substack{\alpha \\ \iota\jmath}} f^{\mathrm{r}}_\alpha {}^* K'^*_{\alpha,\iota\jmath} p^{\mathrm{s}}_\iota(K) p^{\mathrm{s}}_\jmath(K) + A \Big| \lambda u^{\mathrm{T}} + \sum_{\alpha,\iota} \varphi_\alpha K'^*_{\alpha,\iota} p^{\mathrm{s}}_\iota(K) \Big|^{d/y_{\mathrm{T}}}. \end{aligned} \tag{5.12}$$

In the lowest order we get only regular parts in equations which are the same

as (5.7)

$$f^{r}(K) = g(K; p_i^{r}(K)) + b^{-d} f^{r}(K'(K; p_i^{r}(K))),$$
$$0 = g_i(K; p_i^{r}(K)) + b^{-d} \sum_{\alpha} f_{\alpha}^{r}(K'(K; p_i^{r}(K))) K'^{r}_{\alpha,i}. \tag{5.13}$$

We define B_{ij}

$$B_{ij} = g_{ij}^{*} + b^{-d}\left[\sum_{\alpha,\beta} f_{\alpha\beta}^{r*} K'^{*}_{\alpha,i} K'^{*}_{\beta,j} + \sum_{\substack{\alpha \\ i,j}} f_{\alpha}^{r*} K'^{*}_{\alpha,ij} p_i^{s}(K) p_j^{s}(K)\right] \tag{5.14}$$

and, to first order in the singularities, one obtains

$$A|u^{T}|^{d/y_T} = \tfrac{1}{2}\sum_{i,j} B_{ij} p_i^{s}(K) p_j^{s}(K) + b^{-d} A\left|\lambda u^{T} + \sum_{\alpha,i} \varphi_{\alpha} K'^{*}_{\alpha,i} p_i^{s}(K)\right|^{d/y_T},$$
$$0 = \sum_{j} B_{ij} p_j^{s}(K) + b^{-d} A \frac{d}{y_T} \sum_{\alpha} \varphi_{\alpha} K'^{*}_{\alpha,i}\left|\lambda u^{T} + \sum_{\beta,j} \varphi_{\beta} K'^{*}_{\beta,j} p_j^{s}(K)\right|^{d/y_T - 1}. \tag{5.15}$$

As in the simple case, we have to distinguish two cases, depending on whether $p_i^{s}(K)$ or u^{T} is the dominant term.

(i) All $p_i^{s}(K) \ll |u^{T}|$. Then the equations reduce to

$$b^{-d}\lambda^{d/y_T} = 1,$$
$$\sum_{j} B_{ij} p_j^{s}(K) = -b^{-d} A \frac{d}{y_T} \sum_{\alpha} \varphi_{\alpha} K'^{*}_{\alpha,i} |u^{T}|^{d/y_T - 1}. \tag{5.16}$$

Using that $d/y_T = 2 - \alpha$, the first equation gives the normal connection between the largest eigenvalue and the specific heat component α. The set of m equations for the $p_i^{s}(K)$ show that in general all $p_i^{s}(K)$ will be singular with power $|u^{T}|^{1-\alpha}$, provided that at least one term $\Sigma_{\alpha} \varphi_{\alpha} K'^{*}_{\alpha,i} \neq 0$. However, this is only consistent with the ansatz if $\alpha < 0$ because otherwise at least for one of the $p_i^{s}(K)$ would hold $p_i^{s}(K) \gg |u^{T}|$. If all terms $\Sigma_{\alpha} \varphi_{\alpha} K'^{*}_{\alpha,i} = 0$ the $p_i^{s}(K)$ become of order $|u^{T}|^{2-\alpha}$ by terms omitted in (5.11).

(ii) At least for some terms $p_i^{s}(K)$ holds $p_i^{s}(K) \gg |u^{T}|$. Then the equations read

$$A|u^{T}|^{d/y_T} = \tfrac{1}{2}{\sum_{i,j}}' B_{ij} p_i^{s}(K) p_j^{s}(K) + b^{-d} A\left|{\sum_{i}}' \sum_{\alpha} \varphi_{\alpha} K'^{*}_{\alpha,i} p_i^{s}(K)\right|^{d/y_T},$$
$$0 = {\sum_{j}}' B_{ij} p_j^{s}(K) + b^{-d} A \frac{d}{y_T} \sum_{\alpha} \varphi_{\alpha} K'^{*}_{\alpha,i}\left|{\sum_{j}}' \sum_{\beta} \varphi_{\beta} K'^{*}_{\beta,j} p_j^{s}(K)\right|^{d/y_T - 1}, \tag{5.17}$$

where Σ' stands for a summation over all terms for which $p_i^{s}(K) \gg |u^{T}|$. Since neither of the equations can be fulfilled in consistency with the ansatz, we conclude that this case does not occur. When all $\Sigma_{\alpha} \varphi_{\alpha} K'^{*}_{\alpha,i} = 0$ then the $p_i^{s}(K)$ become of order $|u^{T}|^{2-\alpha}$ and one is back to case (i).

In the one-parameter case, it turned out that if eqs. (2.11) have any real solutions, one will find two solutions for the derivative of the variational parameter at the fixed point, and so two different eigenvalues, one with $\alpha < 0$ and one that would yield $\alpha > 0$.

TABLE I

$p^* = 0.765983$	$K^* = 0\ 279433$	$Q^* = -0.006865$
I $p^*_K = 3.890460$		II $p^*_K = -4.128780$
$p^*_Q = 0\ 937850$		$P^*_Q = -1.584011$
I $\lambda_1 = 1\ 921030$		II $\lambda_1 = 2.082217$
$\lambda_2 = 0\ 456844$		$\lambda_2 = 0.456844$
$\alpha_1 = -0.123413$		$\alpha_2 = 0.109856$
$F^*_{KK} = 74\ 779$		$F^*_{KK} = -255.617$
$F^*_{KQ} = 24.353$		$F^*_{KQ} = -79\ 549$
$F^*_{QQ} = 9.361$		$F^*_{QQ} = -23.313$

To see what can happen in the more general case, we reconsider KHY's[3]) bound to the free energy of the square lattice (see section 3), where we have two interaction parameters and one variational parameter. It turns out that in this example the behavior is strikingly analogous to that of the one-parameter case since again two solutions are found, with $\lambda_1\lambda_2 = b^d$ and so specific heat exponents α of different sign (see table I). Note that the second solution gives a wrong curvature for the free energy, and that the derivatives of $p(K, Q)$ are negative.

As in the case of the mean-field-like lower bound to the free energy, we can vary b^d which changes the solution of eqs. (5.8) and (5.9). When b^d is increased (see fig. 6), starting from $b^d = 4$, p^* approaches the value $p^* = 0.757562$ where $g^*_p = 0$ and the first solution of eq. (5.9) yields an eigenvalue

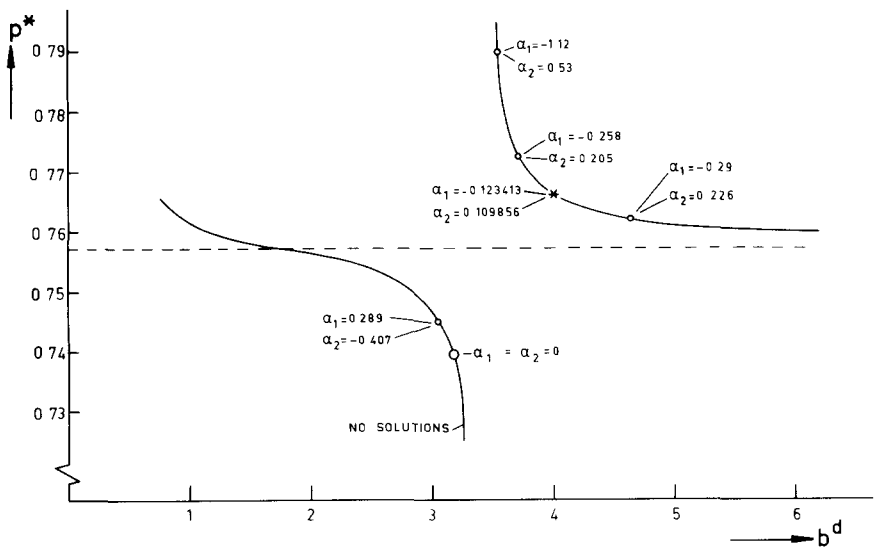

Fig 6 The optimal values of p at the fixed point, for various values of b^d

that approaches a finite value, $\lambda_1 \approx 1.95$, such that $\alpha_1 \to -\infty$; the other solution yields a slowly increasing α_2, since also λ_2 increases with b^d. When b^d is decreased, the specific heat exponents reach optimum values for $b^d = 3.990252$, where $\alpha_1 = -0.123278$ and $\alpha_2 = 0.109748$. When b^d is decreased further, p^* seems to go to infinity, while α_1 decreases more and more whereas α_2 increases. There is another branch of solutions of (5.8). At this branch, eqs. (5.9) have no real solutions for $b^d > 3.162703$. For $b^d = 3.162703$, there is just one solution, $\lambda = b^{d/2}$ such that $\alpha = 0$. For $b^d < 3.162703$ again two solutions are found, with α values of different sign. However, for these solutions the second derivatives of the free energy are negative and therefore lead to an unstable free energy.

6. Discussion

The analysis of the variational equations for the optimal parameter(s) $p(K)$ as a function of interaction constant(s) K leads to three possibilities.

(i) The optimal $p(K)$ is basically not coupled to the singularities of the energy $f(K)$ at the fixed point K^*. This may be due either to the fact that $p(K)$ is optimal at the boundary of its domain (e.g. $p = \infty$) or due to a fortuitous coincidence of two conditions [see (2.3)].

(ii) The optimal $p(K)$ has a singularity at K^* with exponent $1 - \alpha$, which is induced by the free energy singularity with exponent $2 - \alpha$. Only for $\alpha < 0$ a consistent set of $p(K)$ and $f(K)$ can be obtained.

(iii) The optimal $p(K)$ has several branches and a discontinuous phase transition occurs between the branches.

The analysis has been restricted to a temperature-like singularity. For the stronger magnetic-like singularity one would in general expect a similar picture. However, in the ferromagnetic Ising model transition a symmetry in the field causes the basic quantity H'_p (the renormalized field derivative with respect to the variational parameter p) to vanish at the fixed point. This will make the singularity in the variational parameter in the field direction of equal strength as the free energy singularity. A more precise analysis is in progress to study the possible complications of a second singular direction.

The findings of this paper throw a shadow on the variational method because a basic ansatz of the renormalization approach, i.e. that of a regular transformation, is violated. One usually tries to explain the free energy singularities from a regular renormalization transformation. The induced singularities in the variational paramater are mild as long as $\alpha < 0$ in the sense that the leading singularity can still be obtained in the conventional way. Corrections to scaling would however be affected by these singularities in $p(K)$. Although the variational technique leads to accurate free energies it is of limited value for the determination of unknown but presumably strong singularities.

Acknowledgements

The authors are indebted to Dr. H.J.F. Knops and M.P.M. den Nijs for stimulating discussions.

References

1) K.G. Wilson, Rev. Mod. Phys. **47** (1975) 773.
2) Th. Niemeyer and J.M.J. van Leeuwen, Physica **71** (1974) 17.
3) L.P. Kadanoff, A. Houghton and M.C. Yalabik, J. Stat. Phys. **14** (1976) 171.
4) T W Burkhardt, Phys. Rev **B14** (1976) 1196
T W Burkhardt, H.J.F. Knops and M.P M. Den Nijs, J. Phys. **A9** (1976) L 179
M Droz, S.L. Katz and J.D. Gunton, Phys. Rev. **B15** (1977) 237
S.L Katz, M Droz and J D. Gunton, Phys. Rev. **B15** (1977) 1597.
T W Burkhardt and H.J.F Knops, Phys. Rev **B15** (1977) 1602.
S C. Hsu and J.D Gunton, Phys. Rev. **B15** (1977) 2692.
C. Dasgupta, Phys. Rev. **B15** (1977) 3460.
S.L. Katz and J D Gunton, Phys Rev **B16** (1977) 2163.
5) H J F. Knops, Physica **86A** (1977) 448
6) M N. Barber, J Phys. **A10** (1977) 1187.
7) M. Pliske, private communication