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Upper bounds to free energies by renormalization group methods

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Abstract. The use of variational approximations in the study and application of renormalization groups is discussed. In particular, a simple approximation is derived which yields an upper bound to the free energy of Ising models on d-dimensional lattices. The optimal transformation, which yields the least upper bound, is determined analytically. The criterion proposed by Kadanoff to determine the 'best' approximation to the fixed point is found to fail in this case. The reasons for this failure and several of the basic problems posed by variational approximations are discussed.

1. Introduction

Recently, Kadanoff (1975) reported a remarkably accurate determination of the critical exponents of d-dimensional Ising spin systems ($d = 2, 3, 4$) using a variational approximation to a renormalization group transformation with an arbitrary parameter. The specific approximation—the so called one-hypercube approximation—discussed by Kadanoff (1975), and in more detall by Kadanoff *et al* (1976), yields a lower bound to the exact free energy. An optimum bound then follows by adjusting the parameter of the transformation variationally. The results obtained in this manner (Kadanoff 1975, Kadanoff *et al* 1976) constitute one of the most accurate approximate renormalization group calculations yet performed. As such, they suggest that variational approximations may have considerable potential in the study and application of renormalization groups.

In this paper, we discuss an alternative approximation which leads to an *upper* bound on the free energy. Whilst this approximation is not as accurate as Kadanoff's, it is still rather instructive. In particular, the optimal transformation can be determined analytically. In addition, the approximation is sufficiently simple to exhibit the interplay of renormalization group and variational techniques rather clearly. Consequently, several of the basic questions and problems raised by variational methods become apparent. Some of the special problems of the Kadanoff approximation have been discussed recently by Burkhardt (1976).

Our detailed arguments are arranged as follows. The basic approximation is derived in § 2 for Ising systems on d-dimensional lattices. Section 3 specializes this discussion to the square lattice. However the basic conclusions are easily extended; this being done in § 4. Section 5 contains a concluding discussion in which we compare and contrast this

upper bound approximation with the lower bound approximation of Kadanoff (1975) and, in particular, discuss some of the basic problems posed by these types of approximations.

2. An upper bound transformation

Let $H\{\sigma\}$ be the Hamiltonian of N Ising spins ($\sigma_i = \pm 1, i = 1, \ldots, N$) on a d-dimensional lattice Ω with lattice spacing a. To define a renormalization group transformation we form cells of $n = b^d$ lattice sites, such that the centres of the cells form a lattice Ω' which is isomorphic to Ω but has an increased lattice spacing, $a' = ba$. With each cell is associated a new spin variable $\mu_\alpha = \pm 1$, $\alpha = 1, \ldots, N' = N/b^d$. The Hamiltonian $H'\{\mu\}$ of this 'cell-spin' system is given by

$$\exp(-Ng + H'\{\mu\}) = \sum_{\{\sigma\}} \mathcal{T}\{\mu, \sigma\} \exp(H\{\sigma\}), \tag{2.1}$$

where we explicitly indicate the constant or 'spin-independent' term, $-Ng$, generated in H' by the sum over configurations. (Without loss of generality, we assume that the total energy is shifted so that corresponding term in the initial Hamiltonian H vanishes.)

The transformation (2.1) is an example of a real-space renormalization group transformation with spatial rescaling factor equal to b. (A recent review of such transformations has been given by Niemeijer and van Leeuwen 1976.) The transformation matrix $\mathcal{T}\{\mu, \sigma\}$ is taken to be

$$\mathcal{T}\{\mu, \sigma\} = \prod_\alpha T(\mu_\alpha, \boldsymbol{\sigma}_\alpha), \qquad T(\mu_\alpha, \boldsymbol{\sigma}_\alpha) = \tfrac{1}{2}(1 + \mu_\alpha t(\boldsymbol{\sigma}_\alpha)), \tag{2.2}$$

where $\boldsymbol{\sigma}_\alpha$ denotes the set of spins σ_i in a cell α and the product is over all cells. Different transformations (with the same spatial rescaling factor) correspond to different choices of the function $t(\boldsymbol{\sigma}_\alpha)$. We shall refer to t as the transformation generator. To ensure that (2.1) preserves spin-reversal symmetry, we require $t(\boldsymbol{\sigma}_\alpha)$ to be odd under spin reversal, i.e. $t \to -t$, if $\sigma_i \to -\sigma_i$, for all $i \in \alpha$.

With $\mathcal{T}\{\mu, \sigma\}$ given by (2.2), the partition function transforms as

$$e^{-Ng} Z_{N'}(H') = Z_N(H) \equiv \sum_{\{\sigma\}} \exp(H\{\sigma\}). \tag{2.3}$$

Hence the free energy per spin

$$f(H) = \lim_{N \to \infty} \left(-\frac{1}{N} \ln Z_N(H) \right), \tag{2.4}$$

satisfies

$$f(H) = g + b^{-d} f(H'). \tag{2.5}$$

This result forms the basis of the calculation of free energies by renormalization group techniques (see e.g. Nauenberg and Nienhuis 1974).

In general, however, the sum over configurations in (2.1) cannot be performed exactly and hence $H'\{\mu\}$ can only be evaluated approximately. Following Kadanoff (1975) we are interested in approximations which ensure a definite bound to $f(H)$. A rather simple approximation, yielding an upper bound, is supplied by Jensen's inequality as follows.

Decompose $H\{\sigma\}$ as

$$H\{\sigma\} = H_0 + V, \qquad H_0 = \sum_\alpha H_{0,\alpha}, \tag{2.6}$$

where $H_{0,\alpha}$ contains all the interactions between spins in cell α and V all the intercell couplings. Substitution of (2.2) and (2.6) allows (2.1) to be written as

$$\sum_{\{\sigma\}} \mathcal{T}\{\mu, \sigma\} \exp(H\{\sigma\}) = \left(\prod_\alpha z_{0,\alpha}\right) \langle e^V \rangle_0, \tag{2.7}$$

where

$$z_{0,\alpha} = \sum_{\{\boldsymbol{\sigma}_\alpha\}} \tfrac{1}{2}(1 + \mu_\alpha t(\boldsymbol{\sigma}_\alpha)) \exp(H_{0,\alpha}), \tag{2.8}$$

and

$$\langle A \rangle_0 = \sum_{\{\sigma\}} A\{\sigma\} P\{\mu, \sigma\}, \tag{2.9}$$

with

$$P\{\mu, \sigma\} = \frac{\mathcal{T}\{\mu, \sigma\} \exp(H_0\{\sigma\})}{\Sigma_{\{\sigma\}} \mathcal{T}\{\mu, \sigma\} \exp(H_0\{\sigma\})}. \tag{2.10}$$

Provided $\mathcal{T}\{\mu, \sigma\}$ is non-negative, $P\{\mu, \sigma\}$ may be regarded as a probability measure and hence by Jensen's inequality (see e.g. Beckenbach and Bellman 1961)

$$\langle e^V \rangle_0 \geqslant \exp(\langle V \rangle_0). \tag{2.11}$$

Combining this result with (2.7) and summing over the configurations of the set $\{\mu\}$ gives

$$Z_N(H) \geqslant e^{-Ng_A} Z_{N'}(H'_A), \tag{2.12}$$

where

$$-Ng_A + H'_A\{\mu\} \equiv \sum_\alpha \ln z_{0,\alpha} + \langle V \rangle_0, \tag{2.13}$$

with $g_A(H)$ the spin-independent part. The required bound on $f(H)$ follows immediately, namely

$$f(H) \leqslant g_A + b^{-d} f(H'_A). \tag{2.14}$$

The approximation (2.13) for the renormalized Hamiltonian $H'\{\mu\}$ will be recognized as equivalent to a first-order cumulant expansion in terms of the intercell interactions (see e.g. Niemeijer and van Leeuwen 1974, 1976).

In general both g_A and H'_A will depend upon the specific transformation chosen, i.e. on the function $t(\boldsymbol{\sigma}_\alpha)$. Hence the optimum bound is

$$f(H) \leqslant f_A(H) = \min_t (g_A(H; t) + b^{-d} f(H'_A(t))), \tag{2.15}$$

where the restriction that $\mathcal{T}\{\mu, \sigma\}$ be non-negative implies that the minimization is to be performed over all functions $t(\boldsymbol{\sigma}_\alpha)$ subject to the constraint that $|t| \leqslant 1$. We shall refer to this approximation as the Jensen (upper) bound approximation.

Since the expression (2.15) still contains the exact (and unknown) free energy, one cannot expect to be able to directly evaluate $f_A(H)$ for most approximations. In the present case, it is however possible to determine the optimal choice of t to ensure that $f_A(H)$ is the optimum bound. To see how this comes about, it is convenient to consider a specific example on the square lattice. The basic conclusions are however easily extended and we shall do so in § 4.

3. Square lattice

We consider the site–cell transformation indicated in figure 1; the spins $\{\mu_\alpha\}$ being associated with the shaded cells. Since $t(\boldsymbol{\sigma}_\alpha)$ is required to be odd under spin reversal, we parametrize it as

$$t(\boldsymbol{\sigma}_\alpha) = \tfrac{1}{4}(p + q\sigma_1^\alpha\sigma_2^\alpha\sigma_3^\alpha\sigma_4^\alpha)(\sigma_1^\alpha + \sigma_2^\alpha + \sigma_3^\alpha + \sigma_4^\alpha), \tag{3.1}$$

where σ_i^α, $i = 1, \ldots, 4$, are the four spins at the vertices of the cell α (see figure 1). This transformation is, in fact, the most general transformation which preserves the point-group symmetry of a square of four spins. To avoid the problems associated with a linear weight factor (Subbarao 1975, Bell and Wilson 1975, Niemeijer and van Leeuwen 1976) we require q to be non-zero, while the condition $|t| \leqslant 1$ implies that

$$|p+q| \leqslant 1, \qquad |p-q| \leqslant 2. \tag{3.2}$$

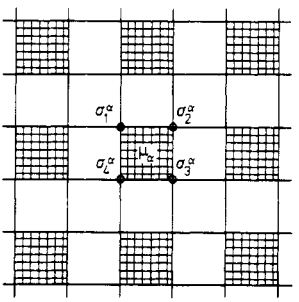

Figure 1. Square lattice illustrating the cell transformation used in the variational calculation. The renormalized spins are associated with the shaded cells.

In passing we note that the transformation treated by Kadanoff (1975) is given by (with ρ replacing his p)

$$p = \tfrac{1}{2}(\tanh 4\rho + 2\tanh 2\rho), \qquad q = \tfrac{1}{2}(\tanh 4\rho - 2\tanh 2\rho). \tag{3.3}$$

3.1. Determination of the optimal transformation

For our immediate purposes it suffices to take $H\{\sigma\}$ to be the sum over nearest-neighbour pairs, namely,

$$H\{\sigma\} = K_2 \sum_{\langle i,j \rangle} \sigma_i\sigma_j. \tag{3.4}$$

The determination of $z_{0,\alpha}$ and $\langle V\rangle_0$ now follows that of an ordinary cumulant expansion (see e.g. Niemeijer and van Leeuwen 1974, 1976). Explicitly we find

$$g_A = -\tfrac{1}{4}\ln z_{0,\alpha} = -\tfrac{1}{4}\ln(6+2\cosh 4K_2) \tag{3.5}$$

and

$$\langle V\rangle_0 = K_2' \sum_{\langle\alpha\beta\rangle} \mu_\alpha\mu_\beta, \tag{3.6}$$

where the sum is over all nearest-neighbour pairs of cell spins. The renormalized pair interaction K_2' is given by

$$K_2' = R(K_2; p, q) \equiv 2K_2 h^2(e^{-4K_2}; p, q), \tag{3.7}$$

where

$$h(x; p, q) = \frac{p+q+(p-q)x}{1+6x+x^2}. \tag{3.8}$$

Equation (3.7) constitutes the basic recursion relation. Given K_2, we now require p and q to minimize (2.15) which becomes, since $b = 2$,

$$f(K_2) \leqslant f_A(K_2) = \min_{p,q} (g_A(K_2) + \tfrac{1}{4} f(R(K_2; p, q))) \tag{3.9}$$

subject to the constraints (3.2). Since g_A is independent of p and q, we immediately have

$$f_A(K_2) = g_A(K_2) + \tfrac{1}{4} \min_{p,q} (f(R(K_2; p, q))). \tag{3.10}$$

If we now invoke the GKS inequality (Griffiths 1967, Kelly and Sherman 1968), which is valid for Ising systems with positive coupling constants, it is straightforward to show that $\partial f/\partial K$ is negative for all K and hence $f(K)$ is a *monotonic decreasing function of its argument.* This implies that to achieve the minimum in (3.10), we must choose p and q such that

$$(R(K_2; p, q) - K_2) \qquad \text{is a maximum if } R > K_2$$

and

$$(K_2 - R(K_2; p, q)) \qquad \text{is a minimum if } R \leqslant K_2.$$

Both these conditions are equivalent to the criterion that $h(x; p, q)$ be a maximum subject to (3.2) for fixed $x = e^{-4K_2}$. This is a simple linear programming problem and yields

$$p^\dagger = \tfrac{3}{2} \qquad q^\dagger = -\tfrac{1}{2} \tag{3.11}$$

for all K_2.

It is instructive to note that this optimal transformation is equivalent to the specification of the transformation matrix (2.2) in the form

$$T(\mu_\alpha, \sigma_\alpha) = \begin{cases} 1 & \text{if } \mu_\alpha = \operatorname{sgn}(S_1^\alpha),\ S_1^\alpha \neq 0 \\ \tfrac{1}{2} & \text{if } S_1^\alpha = 0 \\ 0 & \text{if } \mu_\alpha = -\operatorname{sgn}(S_1^\alpha),\ S_1^\alpha \neq 0, \end{cases} \tag{3.12}$$

where $S_1^\alpha = \Sigma_{i\in\alpha}\sigma_i$. In this form the transformation is very similar to the original site–cell transformations of Niemeijer and van Leeuwen (1973, 1974), except for the possibility that S_1^α is zero since we have an even number of sites in a cell. This suggests that the Niemeijer–van Leeuwen transformations may in general be optimal with respect to the Jensen bound. In § 4, we shall confirm this expectation. Before doing so, we briefly describe the critical behaviour which follows from (3.7) with $p = p^\dagger$ and $q = q^\dagger$. This transformation has also been considered in a different context by Hsu and Gunton (1977).

3.2. Fixed point and thermal eigenvalue

The determination of the fixed point and critical eigenvalues from (3.7) is standard (see e.g. Niemeijer and van Leeuwen 1976). We find

$$K_2^* = 0{\cdot}5187, \tag{3.13}$$

with a single relevant eigenvalue

$$\Lambda_T = (\partial K_2'/\partial K_2)^* = 2{\cdot}0082 \tag{3.14}$$

which implies that

$$2-\alpha = 2\nu = \frac{2\ln b}{\ln \Lambda_T} = 1{\cdot}9881. \tag{3.15}$$

Considering the crudity of the basic approximation this result agrees remarkably well with the exact value of $2-\alpha = 2\nu = 2$. Even the fixed-point value (3.13) agrees reasonably well with the exact critical temperature $K_c = 0{\cdot}4407$.

3.3. Free energy and specific heat

Since the optimal choice of p and q is independent of K_2, the determination of the approximate free energy $f_A(K_2)$ from (3.7) and (3.9) follows precisely the same procedure as utilized by Nauenberg and Nienhuis (1974). Iterating (3.9) we have

$$f(K_2) \leqslant f_A(K_2) = \sum_{l=0}^{n-1} 4^{-l} g_A(K_2^{(l)}) + 4^{-n} f(K_2^{(n)}), \tag{3.16}$$

where

$$K_2^{(l+1)} = R^\dagger(K_2^{(l)}) = R(K_2^{(l)}; p^\dagger, q^\dagger); \qquad K_2^{(0)} \equiv K_2.$$

The sequence terminates when $K_2^{(n)}$ is such that $f(K_2^{(n)})$ can be directly evaluated from the partition function.

The resulting free energy is illustrated in figure 2, where we also plot the exact free energy (Onsager 1944) and

$$\hat{g}_A(K_2) = g_A(K_2) - \tfrac{1}{4}\ln 2. \tag{3.17}$$

That $\hat{g}_A(K_2)$ is itself an upper bound to the exact free energy can be seen explicitly by observing that $R(K_2; 0, 0) \equiv 0$ and hence from (3.9)

$$f(K) \leqslant g_A(K) + \tfrac{1}{4}f(0) = g_A(K) - \tfrac{1}{4}\ln 2. \tag{3.18}$$

This bound is asymptotically exact for small K (i.e. at high temperatures) but is a very poor bound for large K (i.e. low temperatures). On the other hand, we observe that the

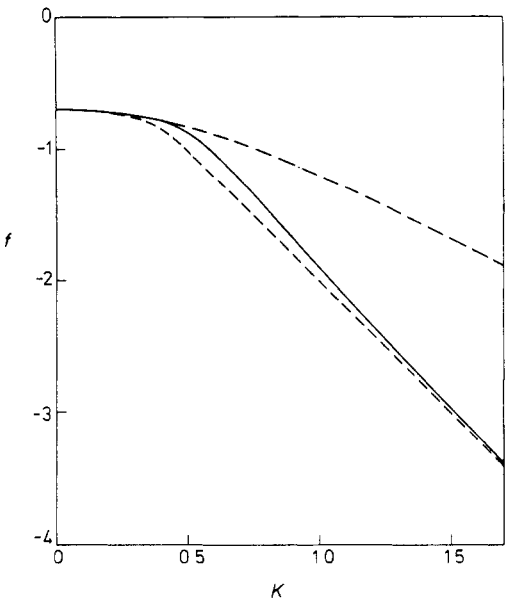

Figure 2. Comparison of the optimal bound (full curve) given by equation (3.16) with exact free energy (broken curve) and the trivial bound (chain curve) of equation (3.17).

renormalization group bound $f_A(K)$ is apparently also asymptotically exact for large K. That this is in fact the case can be easily checked analytically. For sufficiently large K, the recursion relation (3.7) approximates to

$$K_2' \simeq 2K_2 \qquad \text{or} \qquad K_2^{(l)} \simeq 2^l K_2, \tag{3.19}$$

while

$$g_A(K_2) \simeq -K_2. \tag{3.20}$$

Substituting these results in (3.16) and letting n tend to infinity yields

$$f_A(K_2) \simeq -2K_2 \qquad \text{as } K_2 \to \infty, \tag{3.21}$$

which matches the exact limiting behaviour of the exact free energy $f(K_2)$. Since the basic approximation (2.11) is, by itself, at best valid for high temperatures (i.e. K small), where higher-order cumulants can be neglected, this result illustrates the inherent power obtained by incorporating a renormalization group transformation into the variational procedure. If nothing else, this allows a substantial improvement in the *numerical* accuracy of the bound. Indeed, most of the discrepancy between $f_A(K_2)$ and $f(K_2)$ in figure 2, is due to the relatively large error in K_2^* as compared to K_c. If one re-scales the temperature variables so that K_2^* and K_c are both unity much of the error disappears. For example

$$f_A(K_2^*) = 0{\cdot}8818 \tag{3.22}$$

while

$$f(K_c) = 0{\cdot}9297.$$

The internal energy and specific heat can also be calculated from (3.16) (see e.g. Nauenberg and Nienhuis 1974). These results are qualitatively in accord with the exact results but not as accurate as those obtained by Kadanoff *et al* (1976). On the other hand, it should be noted that there are no grounds on which to expect that the derivatives of f_A should approximate those of f at all well, even if f_A ia a *very* good approximation to f. Nevertheless in this case, as in the lower bound approximation of Kadanoff *et al* (1976), the use of a renormalization group transformation somehow appears to ensure that the derivatives of $f_A(K_2)$ *are* reasonable approximations to those of $f(K_2)$.

4. Extension to other lattices

In this section we show that the optimal transformations with respect to the Jensen bound are identical to the original site–cell transformations of Niemeijer and van Leeuwen (1973, 1974) for cells with an odd number of sites. We first show that if H_0 is spin-reversal symmetric then $z_{0,\alpha}$ is independent of the transform generator $t(\boldsymbol{\sigma}_\alpha)$. To do so we write the sum over the configurations of the set $\boldsymbol{\sigma}_\alpha$ in (2.8) as

$$\sum_{\{\boldsymbol{\sigma}_\alpha\}} = \sum_{\{\boldsymbol{\sigma}_\alpha ; S_1^\alpha > 0\}} + \sum_{\{\boldsymbol{\sigma}_\alpha ; S_1^\alpha < 0\}}, \tag{4.1}$$

where $S_1^\alpha = \Sigma_{i\in\alpha}\,\sigma_i$. Reversing all the spin variables σ_i in the second sum and making use of the fact that $H_{0,\alpha}$ is even, while $t(\boldsymbol{\sigma}_\alpha)$ is odd, under spin reversal yields

$$z_{0,\alpha} = \sum_{\{\boldsymbol{\sigma}_\alpha ; S_1^\alpha > 0\}} \exp(H_{0,\alpha}) \equiv z_0, \tag{4.2}$$

which is the desired result.

Turning now to the computation of $\langle V\rangle_0$, it is again sufficient to assume H has the form (3.4). The intercell coupling V then consists of a sum of terms, each of which is a product of two spin variables associated with different cells. The expectation value of this term with respect to H_0 therefore factors and we find that the renormalized pair interaction has the form

$$K_2' = K_2 \sum m_{\alpha_i} m_{\beta_j}, \tag{4.3}$$

where the sum runs over all bonds linking cells α and β, and

$$m_{\alpha_i} = \mu_\alpha \langle \sigma_i^\alpha \rangle = \mu_\alpha z_0^{-1} \sum_{\{\boldsymbol{\sigma}_\alpha\}} \tfrac{1}{2}\sigma_i^\alpha (1 + \mu_\alpha t(\boldsymbol{\sigma}_\alpha)) \exp(H_{0,\alpha})$$

$$= z_0^{-1} \sum_{\{\boldsymbol{\sigma}_\alpha ; S_1^\alpha > 0\}} \sigma_i^\alpha t(\boldsymbol{\sigma}_\alpha) \exp(H_{0,\alpha}). \tag{4.4}$$

The last step of (4.4) follows from the decomposition (4.1).

The optimal choice of t must now be such that

$$g_A(K_2) + b^{-d} f(K_2') = \tfrac{1}{4} \ln z_0 + b^{-d} f(K_2') \tag{4.5}$$

is a minimum. Applying the GKS inequality as before implies that t^+ should maximize $(K_2' - K_2)$ if $K_2' > K_2$ and minimize $(K_2 - K_2')$ if $K_2' \leqslant K_2$, which is equivalent to

maximizing m_{α_i} subject to $|t|<1$. The required choice is clearly

$$t^{\dagger}(\boldsymbol{\sigma}_\alpha)=\begin{cases}1 & \text{if } S_1^\alpha>0\\ -1 & \text{if } S_1^\alpha<0.\end{cases} \tag{4.6}$$

Hence we obtain that

$$T^{\dagger}(\mu_\alpha,\boldsymbol{\sigma}_\alpha)=\begin{cases}1 & \text{if } \mu_\alpha=\operatorname{sgn}(S_1^\alpha),\\ 0 & \text{if } \mu_\alpha=-\operatorname{sgn}(S_1^\alpha),\end{cases} \tag{4.7}$$

which is the transformation of Niemeijer and van Leeuwen (1973, 1974).

The generalization to cells with an even number of sites is straightforward if $t(\boldsymbol{\sigma}_\alpha)$ is such that

$$t(\boldsymbol{\sigma}_\alpha)=0 \qquad \text{if } S_1^\alpha=0. \tag{4.8}$$

The optimal transformation in this case is again (3.12), which was the transformation applied on an *ad hoc* basis by Oitmaa and Barber (1977) to the simple cubic lattice using an eight-site cell. In this case one can check that (4.8) is satisfied for transformations which preserve the point-group symmetry of a cube of eight cells. It is possible to construct transformations which do not satisfy (4.8). Whether such transformations yield a better bound is uncertain since they require a large cell and become more cumbersome to handle.

5. Discussion

In table 1, we list, for reference, the results of various first-order cumulant approximations to Niemeijer–van Leeuwen site–cell transformations, which have been reported in the literature. These transformations are, by the analysis of the preceding section, all optimal with respect to the Jensen bound derived in § 2. The overall agreement with exact or series results is not particularly impressive. Consequently, the accuracy obtained in § 3 is probably somewhat fortuitous. This is borne out if the calculation is

Table 1. Results of first-order cumulant expansions to optimal transformations.

Lattice	Cell size $n=b^d$	K_2^*	K_c (exact)	Λ_T	$2-\alpha$ approximate	$2-\alpha$ exact	Reference
Triangular ($d=2$)	3	0·3356	0·2744	1·642	2·266	2	Niemeijer and van Leeuwen (1973)
	7	0·3303		2·444	2·178		Subdø and Hemmer (1976)
Square ($d=2$)	4	0·5187	0·4407	2·0082	1·988	2	Present work
	9	0·4697		2·769	2·158		Hsu *et al* (1975)
	16	0·4607		3·640	2·146		Hsu and Gunton (1977)
Simple cubic ($d=3$)	8	0·298	0·222[a]	2·371	2·409	1·875[a]	Oitmaa and Barber (1977)
	27	0·259		3·596	2·575		Hsu and Gunton (1977)

[a] Series results.

extended to yield the magnetic eigenvalue Λ_H. One finds $\Lambda_H = 2{\cdot}367$ instead of the exact value of $3{\cdot}668$. On the other hand, there is evidence (Plischke and Austin 1975, Barber to be published) which indicates that the Kadanoff approximation is also less successful when applied to other two-dimensional lattices than the square.

A couple of features of the results in table 1 are worth additional comment. Firstly, an increase in the cell size apparently leads to an increase in the accuracy of the estimate of the critical temperature. There is, however, not always a corresponding improvement in the estimate of $2-\alpha$. It would be interesting to know if the approximate free energy $f_A(H; n)$ obtained using a cell of size n is a monotonic decreasing bound on the exact free energy as n increases. We have not, however, explored this point further.

Secondly, all these calculations have been extended to at least second order in the cumulant expansion of $\langle \exp V \rangle$ (see the references cited in table 1). Whilst the comparison of the estimates of K_c and $2-\alpha$ with the exact values improves in second order, there is no longer an objective criterion to distinguish between different choices of the transformation generator. Since there is no evidence that the cumulant expansion is convergent (see in particular, Hsu and Gunton 1977), this is one of the major disadvantages of these types of approximation; a disadvantage that the variational approach attempts to overcome.

The actual accuracy of the Jensen bound approximation, however, is not our primary concern in this paper. Rather, as discussed in § 1, our motivation has been in the variational method itself. In this concluding section, we therefore want to use the results of § 3 to illustrate and discuss some of the basic problems which arise in variational approximations to renormalization group transformations.

We begin by indicating how some of the simplifying features of the Jensen bound are probably modified in more sophisticated approximations. Firstly, the minimization in (2.15) cannot be expected to be tractable as it stands, since it involves the unknown exact free energy functional $f(\cdot)$. To eliminate f, (2.15) must be iterated as in (3.16) to yield†

$$f(H) \leqslant f_A(H) = \min_t \left(\sum_{l=0}^{n-1} b^{-ld} g_A(H_A^{(l)}; t) + b^{-nd} f(H_A^{(n)}(t) \right), \tag{5.1}$$

where the minimization is to be performed subject to any necessary constants. The sequence

$$H_A^{(l)} = \mathbb{R}_b^A(t) H_A^{(l-1)}; \qquad H_A^{(0)} \equiv H, \tag{5.2}$$

terminates where $H_A^{(n)}$ is such that $f(H_A^{(n)})$ can be directly evaluated from the partition function. The approximate recursion operator $\mathbb{R}_b^A$ as indicated depends explicitly on the choice of parameters in the generator t.

In writing (5.1) we have tacitly assumed that the optimal mapping of H to H' is independent of H. This was found to be the case in § 3 but is not so for the Kadanoff approximation (see Kadanoff *et al* 1976). Thus, in general, the least upper bound to $f(H)$ is given not by (5.1) but by

$$f(H) \leqslant f_A(H) = \min_{\{t_1, \ldots, t_n\}} \left(\sum_{l=0}^{n-1} b^{-ld} g_A(H_A^{(l)}; t_{l+1}) + b^{-nd} f(H_A^{(n)}(t_n)) \right), \tag{5.3}$$

where t_k denotes the transformation generator at stage k, i.e. $H_A^{(k)} = \mathbb{R}_b^A(t_k) H_A^{(k-1)}$.

† We shall continue to assume that the approximation yields an upper bound to $f(H)$. The extension to lower bound approximations is, however, straightforward, involving only the replacement of minimizations by maximizations.

Clearly the evaluation of $f_A(H)$ for arbitrary H will be rather non-trivial since it involves a multi-dimensional optimization subject to constraints.

On the other hand, we are usually not that interested in $f_A(H)$ itself, but in the fixed point of the recursion relation (5.2) and its critical parameters. Depending on the choice of the transformation generator, the approximate recursion relations (5.2) possess a set of fixed points $\{H_t^*\}$ parametrized by t. The associated critical parameters consequently also depend (in general) upon the choice of t. In contrast, the analysis of Bell and Wilson (1975), based on the Gaussian model, suggests that a non-linear transformation such as (3.1) possesses a single fixed point. All critical Hamiltonians flow to this point provided t is suitably constrained†. Thus we would like to be able to select one of the points in $\{H_t^*\}$ as the best approximation to the exact fixed point. Clearly, it would be advantageous if this could be achieved without directly evaluating (5.3) for $f_A(H)$.

One such criterion has been proposed by Kadanoff (1975). Let us recall the basic result (2.15) and let $t^\dagger$ denote the generator which achieves the minimum, i.e.

$$f_A(H) = g_A(H; t^\dagger) + b^{-d} f(H'_A(t^\dagger)). \tag{5.4}$$

Now provided $t^\dagger$ satisfies any inequality constraints with strict inequality, e.g. if the minimization is subject to $|t| \leqslant 1$ then $t^\dagger$ must be such that $|t^\dagger| < 1$, the minimum can be found by the ordinary methods of calculus. Consequently, if $t^\dagger$ is replaced by $t^\dagger + \delta t$, the change in $f_A(H)$ will be second order in δt. The Kadanoff criterion now asserts that this condition is also satisfied at the 'best' fixed point.

Since each of the points in $\{H_t^*\}$ is by definition invariant under the approximate recursive operator, the evaluation of $f_A(H_t^*)$ by (5.3) involves no optimization. Hence letting n tend to infinity yields

$$f_A(H_t^*) = (1 - b^{-d})^{-1} g_A(H_t^*; t) \equiv G^*(t). \tag{5.5}$$

The 'best' fixed point is now such that $G^*(t)$ is an extremum at $t = t^\dagger$.

Using this criterion and a lower bound approximation to $f(H)$, Kadanoff (1975) located a fixed point which gave $2 - \alpha = 1{\cdot}9983$ and $\delta = 15{\cdot}040$. As remarked earlier, these estimates of the exponents of the two-dimensional Ising model are some of the most accurate yet obtained by renormalization group techniques. In view of this success, it is instructive to apply this criterion to the transformation defined by (3.7).

For simplicity suppose

$$p = 3\lambda, \qquad q = -\lambda \tag{5.6}$$

and consider a one-parameter variational approximation. By (3.2), the variational parameter λ is restricted to

$$|\lambda| \leqslant \tfrac{1}{2}. \tag{5.7}$$

As a function of λ, the fixed points of (3.7) are given by

$$x^*(\lambda) = \exp(-4K_2^*(\lambda)) = 2\sqrt{2}[|\lambda| + (\lambda^2 + 1 - 5|\lambda|/2\sqrt{2})^{1/2}] - 3. \tag{5.8}$$

By the Kadanoff criterion the optimal value of λ is that which makes

$$G^*(\lambda) = \tfrac{4}{3} g_A(K^*(\lambda); \lambda) = -\tfrac{1}{3} \ln[6 + 2\cosh(4K_2^*(\lambda))] \tag{5.9}$$

† The effect of these types of constraints on a variational calculation is unclear. If they could be determined *a priori*, they can, of course, simply be incorporated in the constraints on the optimization.

extremal. It is straightforward to show that $dG^*/d\lambda$ vanishes at

$$\lambda = 2\sqrt{2}/3 = 0{\cdot}9428. \tag{5.10}$$

The corresponding value of K_2^* by (5.8) is zero! However, this value of λ is unacceptable since it violates the constraint (5.7).

Clearly the Kadanoff criterion has failed completely to determine the 'best' fixed point. The reason for this is not difficult to find. The optimal choice of λ, as determined from (3.11), is $\lambda^+ = \frac{1}{2}$. This value satisfies the constraint (5.7) as an *equality*. Thus the underlying assumption of the Kadanoff criterion that variations in λ from λ^+ yield changes in $f_A(H)$ which are second order in $\lambda - \lambda^+$ need not be valid and is, in this case, invalid.

The attraction of the Kadanoff criterion lies in its simplicity. It does not require detailed knowledge of $f_A(H)$ which involves a complex optimization (recall (5.3)). On the other hand, there is evidence (Bell and Wilson 1975) that the parameters of a non-linear renormalization group are by necessity constrained to some degree. Consequently the occurrence of boundary optima, such as in § 3, cannot be ruled out in more sophisticated approximations. Thus it is of interest to ask if a generalization of the Kadanoff criterion can be found to cover this possibility.

The simplest such generalization is to take the nearest permissible value of the variational parameter (or parameters) to that given by the Kadanoff criterion. That is, since (5.9) is unacceptable we take $\lambda^+ = \frac{1}{2}$ and thereby recover the result derived directly in § 3. Although this criterion has worked in this example and does so in others, e.g. the Kadanoff lower bound approximation on the triangular lattice, where the original criterion fails, it remains rather *ad hoc*.

The Kadanoff criterion, however, suffers from several additional weaknesses and problems. These suggest that its use to determine critical parameters is open to question on fundamental grounds. Firstly, as noted by Kadanoff *et al* (1976), the conclusion that the optimal choice of variational parameters depends on H implies that the determination of critical eigenvalues at *fixed* values of the parameters (equal to those of the optimal fixed point) is internally inconsistent. Numerically, this is probably not very significant since small changes in H hopefully make only small changes in the optimal values of t.

More significant is the problem of determining the fixed point, if there exist two or more values of t at which $G^*(t)$ is extremal. This actually happens in the Kadanoff lower bound approximation (Barber to be published, Burkhardt 1976). To distinguish between these possible fixed points requires further knowledge than can be obtained from the Kadanoff criterion. In particular, one needs to know the critical surfaces associated with both points. It is then possible to determine the fixed point to which the particular critical Hamiltonian of interest flows.

The determination of the flow trajectories of Hamiltonians involves a detailed knowledge of the optimal values of the variational parameters as functions of the coupling constants. This information can only be obtained from (5.3). Thus we are led back to the optimization problem posed by this equation.

If the recursion relation is relatively simple (i.e. computationally rapid) and parametrized by only one parameter a straightforward numerical search to determine the optimum is probably feasible, particularly if the number of iterations is small. This was the procedure adopted by Kadanoff *et al* (1976). For more elaborate approximations and/or transformations, more sophisticated and powerful optimization techniques are necessary. Such techniques have been developed within the context of modern

control theory of sequential processes. The application of these methods to the determination of optimal renormalization group transformations from variational approximations will be discussed in a subsequent paper. In this way, it is hoped to resolve some of the basic questions and problems raised in this discussion.

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