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Optimal Truncation Procedures in Renormalization-Group Calculations

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Renormalization or rescaling transformations generally produce more complicated interactions than are present in the initial Hamiltonian. After each rescaling it is necessary to truncate the Hamiltonian to make the next rescaling mathematically tractable. One is faced with the problem of choosing the coupling constants of the truncated Hamiltonian to obtain the best approximation. Following ideas of McMillan, we consider truncation procedures which give lower and upper bounds to the free energy. Conditions for optimal lower- and upper-bound truncations are derived. These optimal truncations are seen to yield exact results for the free energy in both the high- and low-temperature limits. Some of the problems inherent in all renormalization transformations that incorporate an optimal lower- or upper-bound truncation are discussed. Calculations for the two-dimensional Ising model based on renormalization transformations which combine decimation and an optimal truncation are described. Even in the simplest approximation in which only nearest-neighbor interactions are retained the free energy is obtained to an accuracy of better than 1% for all temperatures if an optimal truncation rather than an ordinary truncation with no readjustment of the coupling constants is made. However, the simplest calculations involving optimal truncations are less successful in predicting derivatives of the free energy and critical exponents than the free energy itself.

KEY WORDS: Renormalization transformations; optimal bounds; Ising model.

1. INTRODUCTION

The application of variational principles in renormalization-group calculations was pioneered by Kadanoff.[1–3] He introduced the approximation of

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translating bonds to facilitate the rescaling operation and showed that renormalization transformations only involving this approximation give lower bounds to the exact free energy. Kadanoff constructed an ingenious lower-bound variational transformation[1,2] which in the meantime has been applied to many models.[3] He showed[3] how Migdal's renormalization transformation[5] can be understood using bond-translation ideas. Kadanoff[1-3] also pointed out that renormalization transformations based on the first-order cumulant expansion give upper bounds to the free energy. A number of authors[6-8] have used this fact to construct optimal first-order cumulant approximations.

In this paper we consider variational approximations of a different kind. Renormalization or rescaling transformations generally produce more complicated interactions than are present in the initial Hamiltonian of interest. To carry out the renormalization transformation repeatedly, it is necessary to truncate the Hamiltonian after each rescaling to make the next rescaling mathematically tractable. In this paper we are concerned with optimal truncation procedures. How should one choose the coupling constants of the truncated Hamiltonian to obtain the best approximation?

McMillan[9] has used lower- and upper-bound variational principles for the free energy in devising truncation procedures in calculations for the X–Y model in two dimensions. In Section 2 we review these variational principles and use them to derive conditions defining optimal lower- and upper-bound truncations. Renormalization transformations consisting of a rescaling transformation which leaves the ground-state energy invariant followed by an optimal truncation are shown to yield exact results for the free energy in both the low- and high-temperature limits. Some of the problems inherent in all renormalization transformations that incorporate lower- and upper-bound optimal truncations are discussed. In Section 3 we present some simple calculations for the two-dimensional Ising model based on renormalization transformations which combine decimation[10] and an optimal truncation. Even in the crudest approximation in which only nearest-neighbor interactions are retained the free energy is reproduced to an accuracy of better than 1% for all temperatures if an optimal lower- or upper-bound truncation rather than an ordinary truncation with no readjustment of the nearest-neighbor coupling is used. However, the simplest calculations we carried out using optimal truncations are less successful in describing the derivatives of the free energy and critical exponents than the free energy itself. Section 4 contains a discussion of the usefulness of optimal truncations as a calculational tool and other concluding remarks.

[3] See Ref. 4 for a list of other applications.

2. OPTIMAL UPPER- AND LOWER-BOUND TRUNCATIONS

Assume that a rescaling transformation has been carried out replacing the Hamiltonian $H(\sigma)$ for the set of spin variables σ with the Hamiltonian $\tilde{H}(\sigma')$ for a smaller number of new spin variables σ'. The Hamiltonian $\tilde{H}$ contains more complicated interactions than H, and one wishes to replace $\tilde{H}$ with a truncated Hamiltonian H' which contains a restricted subset of interactions and has optimally adjusted coupling constants.

Following McMillan,[9] we now derive sufficient conditions that the truncation approximation give an upper or lower bound to the free energy. From the inequality $e^x \geqslant 1 + x$ it follows that the partition functions Z computed from $\tilde{H}$ and H' satisfy the inequality

$$Z[H'] = \sum_{\{\sigma'\}} e^{H'(\sigma')} \geqslant Z[\tilde{H}](1 + \langle H' - \tilde{H}\rangle_{\tilde{H}}) \tag{1}$$

Defining the free energy f as $-\ln Z/$(number of spins) in the thermodynamic limit, one finds the following sufficient condition for a truncation which gives a lower bound to the free energy:

$$f[H'] \leqslant f[\tilde{H}] \qquad \text{if} \quad \langle H' - \tilde{H}\rangle_{\tilde{H}} = 0 \tag{2}$$

Interchanging $\tilde{H}$ and H' gives an analogous condition for an upper-bound truncation:

$$f[H'] \geqslant f[\tilde{H}] \qquad \text{if} \quad \langle H' - \tilde{H}\rangle_{H'} = 0 \tag{3}$$

$H'(\sigma')$ can be expanded in the form

$$H'(\sigma') = \mathrm{Ng} + \sum_{\alpha} K_\alpha' S_\alpha(\sigma') \tag{4}$$

where N is the number of σ spins, g is a constant, the K_α' are coupling constants, and α runs over the subset of interactions $S_\alpha(\sigma')$ retained in the truncation. Maximizing $f[H']$ with respect to K_α' and with g chosen so that (2) is satisfied, one finds the following sufficient conditions for an optimal lower-bound truncation:

$$\langle H' - \tilde{H}\rangle_{\tilde{H}} = 0 \tag{5}$$

$$\langle S_\alpha\rangle_{H'} - \langle S_\alpha\rangle_{\tilde{H}} = 0 \tag{6}$$

Similarly, one has an optimal upper-bound truncation if the equations

$$\langle H' - \tilde{H}\rangle_{H'} = 0 \tag{7}$$

$$\langle S_\alpha(H' - \tilde{H})\rangle_{H'} = 0 \tag{8}$$

are fulfilled.

When (5)–(6) or (7)–(8) are combined with the rescaling transformation relating $\tilde{H}$ to H, a full renormalization step consisting of a rescaling followed by an optimal truncation is determined. Almost all renormalization transformations give exact results for the free energy in the high-temperature

limit, in which the spins are effectively noninteracting. Exact results for the free energy are obtained in the low-temperature limit as well if the rescaling transformation which precedes the optimal truncation leaves the ground-state energy invariant (decimation transformations and decimations combined with bond translation have this property). In the low-temperature limit the free energy equals the ground-state energy. Equations (5) and (7) imply the invariance of the ground-state energy under an optimal truncation in the low-temperature limit. An ordinary truncation without readjustment of the coupling constants does not leave the ground-state energy invariant, in general.

There are a number of inherent problems in all renormalization transformations that include an optimal truncation. In general, it is impossible to write an explicit formula in terms of coupling constants for the transformation, since evaluating the expectation values in (5)–(8) is comparable in complexity with exactly evaluating the partition function of the original Hamiltonian. An additional difficulty with the full transformation is that it is necessarily nonanalytic in the coupling constants, since the expectation values in (5)–(8) are singular on the critical surfaces of phase transitions. A large class of variational renormalization transformations suffers from this same defect[7,11] if the variational parameters are allowed to change with each renormalization step as in our derivation of (5)–(8). In practice one can avoid these problems by evaluating the expectation values for a large but finite cluster, although it is then no longer clear that the procedure really bounds the free energy. Also, the finite-cluster approach is not completely self-consistent, since the finite-cluster expectation values in (5)–(8) differ from the expectation values obtained by taking derivatives of the free energy calculated using the renormalization transformation.

3. RESULTS FOR THE TWO-DIMENSIONAL ISING MODEL

In the case of the two-dimensional Ising model on the square lattice with nearest-neighbor interactions K a decimation transformation[10] eliminating every second spin can be carried out exactly. The transformation yields a constant contribution to the Hamiltonian K_0 for each of the surviving spins, a new next-nearest-neighbor coupling $\tilde{K}$, a second-neighbor coupling $\tilde{K}/2$, and a four-spin coupling $\tilde{K}_4$ given by

$$\tilde{K}_0(K) = \tfrac{1}{8} \ln \cosh 4K + \tfrac{1}{2} \ln \cosh 2K + \ln 2 \tag{9}$$

$$\tilde{K}(K) = \tfrac{1}{4} \ln \cosh 4K \tag{10}$$

$$\tilde{K}_4(K) = \tfrac{1}{8} \ln \cosh 4K - \tfrac{1}{2} \ln \cosh 2K \tag{11}$$

Because of the second-neighbor and four-spin interactions, additional exact decimation transformations cannot be performed. In the first calculation to be described, optimal truncations eliminating all but the nearest-neighbor interaction are made after each decimation so that a subsequent decimation can be carried out.

Combining the exact decimation with a lower-bound optimal truncation retaining only nearest-neighbor couplings, one finds that condition (6) implies a recurrence relation of the form

$$\langle \sigma_1 \sigma_2 \rangle_{K'} = \langle \sigma_1 \sigma_3 \rangle_K \tag{12}$$

for the nearest-neighbor coupling. In (12) spins 1 and 2 are nearest neighbors and spins 1 and 3 next-nearest neighbors. The expectation values are evaluated for infinite Ising systems with nearest-neighbor couplings K' and K, respectively. In obtaining (12) we used the fact that second-neighbor spins become first neighbors if a decimation is carried out, i.e., $\langle \sigma_1 \sigma_2 \rangle_{\tilde{H}} = \langle \sigma_1 \sigma_3 \rangle_H$. The lower-bound approximation to the free energy may be calculated recursively with the formula

$$f_A(K) = -g(K) + \tfrac{1}{2} f_A(K') \tag{13}$$

where $g(K)$, which is determined by (5) and (9), may be put in the form

$$g(K) = \frac{1}{2}\left(\tilde{K}_0 - \tilde{K}_4 \frac{d\tilde{K}_0/dK}{d\tilde{K}_4/dK}\right) + 2\tilde{K}_4 \left(\frac{d\tilde{K}_4}{dK}\right)^{-1} \langle \sigma_1 \sigma_2 \rangle_K$$
$$+ \left(\tilde{K} - \tilde{K}_4 \frac{d\tilde{K}/dK}{d\tilde{K}_4/dK}\right)\left(\langle \sigma_1 \sigma_3 \rangle_K + \frac{1}{2}\langle \sigma_1 \sigma_5 \rangle_K\right) - K' \langle \sigma_1 \sigma_3 \rangle_K \tag{14}$$

In (14), $\langle \sigma_1 \sigma_5 \rangle$ denotes the third-neighbor spin correlation.

Combining the exact decimation with an upper-bound optimal transformation retaining only nearest-neighbor couplings, one finds that (8) implies the recurrence relation

$$K' = \tilde{K} + \frac{\tilde{K}(d/dK')\langle \sigma_1 \sigma_3 \rangle_{K'} + \tilde{K}_4 (d/dK')\langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle_{K'}}{2(d/dK')\langle \sigma_1 \sigma_2 \rangle_{K'}} \tag{15}$$

with

$$g(K) = \tfrac{1}{2}\tilde{K}_0 + (\tilde{K} - K')\langle \sigma_1 \sigma_2 \rangle_{K'} + \tfrac{1}{2}\tilde{K}\langle \sigma_1 \sigma_3 \rangle_{K'} + \tfrac{1}{2}\tilde{K}_4 \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle_{K'} \tag{16}$$

All the two-spin expectation values in (12)–(16) are known exactly from the work of Onsager and others.[12–14] The four-spin expectation value may be related to the first- and third-neighbor spin–spin correlation functions on the dual lattice by using a transformation due to Watson.[15] In obtaining the first set of results to be described, we used exact expectation values

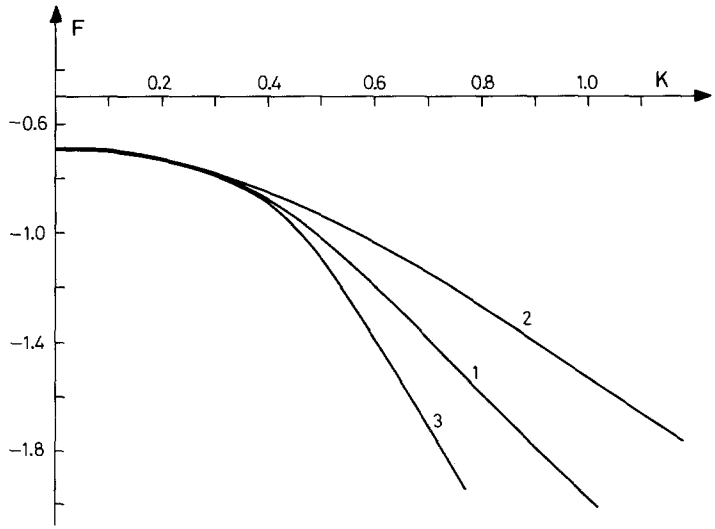

Fig. 1. Curve 1 shows the exact free energy. Curve 2 is obtained by combining the decimation transformation with an ordinary truncation eliminating second-neighbor and four-spin interactions. Curve 3 results when the decimation is used in conjunction with a bond rotation approximation for the second-neighbor interactions and an ordinary truncation to eliminate the four-spin couplings.

in the recurrence formulas, so that the optimal truncation was the only approximation in the calculation.

Curve 1 in Fig. 1 shows the exact Ising free energy calculated by Onsager. Curve 2 shows the free energy obtained with a renormalization transformation consisting of a decimation transformation given by (9)–(11) followed by an ordinary truncation $K' = \tilde{K}(K)$, $g(K) = \tilde{K}_0(K)/2$ in which the second-neighbor and four-spin couplings are simply discarded without adjustment of the nearest-neighbor coupling or the constant term. The free energy calculated in this approximation deviates from the exact free energy for large K (low temperature) since the ordinary truncation changes the ground-state energy. The recurrence relation for the nearest-neighbor coupling has no critical fixed point at a finite, nonzero value K^*. Any finite initial value of K is mapped toward the attractive fixed point $K^* = 0$.

Using optimal lower- and upper-bound truncations rather than the ordinary truncation produces a striking improvement in the calculated free energy. The deviations of the lower- and upper-bound results from the exact free energy are shown in Fig. 2. The two bounds differ from the exact result by less than 1% for all K. The deviations go to zero in the small- and large-K limits. The maximum deviation of the lower and upper bound

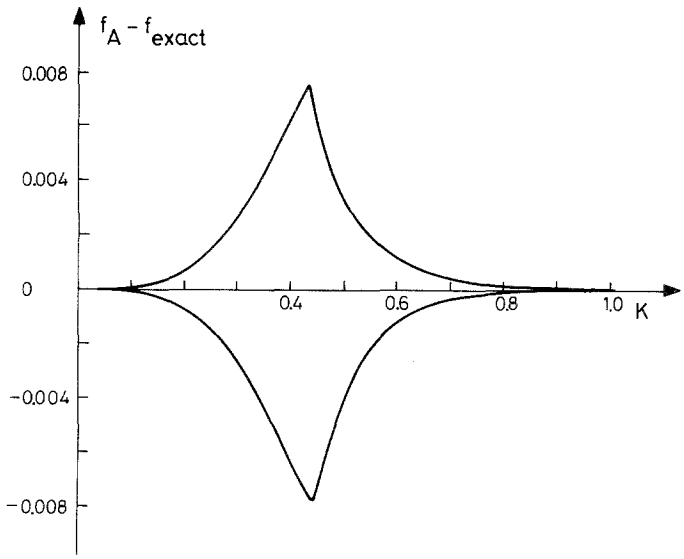

Fig. 2. The upper and lower curves show the deviation of the upper- and lower-bound free energies from the exact result. The approximate free energies were calculated using optimal truncations to eliminate all but the nearest neighbor couplings. Exact results for the correlation functions were used in (12), (14) and (15), (16).

curves occurs at and near the Onsager critical coupling $K_c^0 = \frac{1}{2}\ln(1 + \sqrt{2}) = 0.441$, respectively.

Neither (12) nor (15) has the usual fixed-point topology one expects for a ferromagnetically coupled Ising system with attractive fixed points at $K = 0$ and $K = \infty$ and a repulsive fixed point at an intermediate critical value of K. Since the nearest-neighbor correlation function exceeds the second-neighbor correlation function at the same value of K, it is clear that the lower-bound recurrence relation (12) maps any finite K toward a fixed point at $K = 0$. In addition to attractive fixed points at $K = 0$ and $K = \infty$, the upper bound recurrence relation (15) has weakly repulsive fixed points at $K = 0.439$ and 0.490 and a weakly attractive fixed point at $K = 0.443$.

Due to the unusual fixed-point topology and the singular dependence of the recurrence relation on the coupling constants, both approximations yield grossly inaccurate descriptions of the singularity structure of the free energy. For example, since the derivative of the exact first- and second-neighbor correlation functions with respect to the first-neighbor coupling diverge logarithmically at K_c^0, (12)–(14) imply that in the lower-bound approximation $df_A(K)/dK$ diverges logarithmically at K_c^0 and that $d^2f_A(K)/dK^2$ diverges logarithmically at an infinite number of values of $K > K_c^0$ which are mapped onto K_c^0 by one or more applications of the recurrence relation (12).

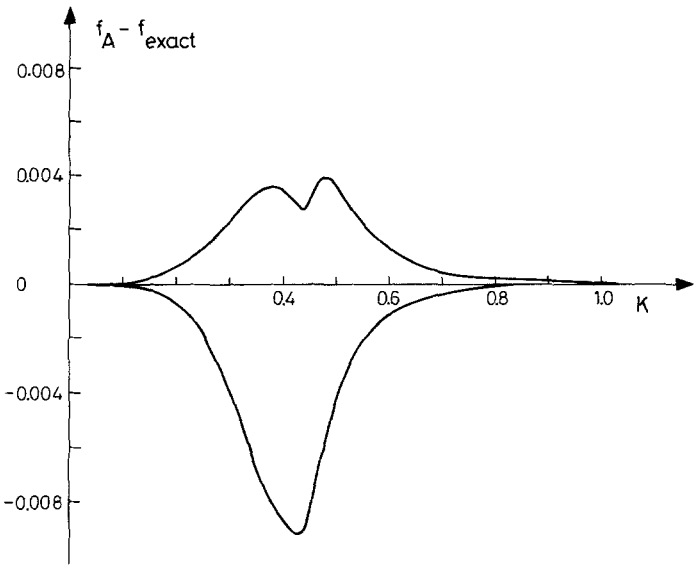

Fig. 3. Same as Fig. 2 except that the correlation functions in (12), (14) and (15), (16) were evaluated for finite clusters with periodic boundary conditions. Clusters of 32 and 16 spins were used for (12), (14) and (15), (16), respectively.

Normally, exact correlation functions are not available for setting up optimal truncation schemes. Figure 3 shows the deviations of the lower- and upper-bound free energies from the exact free energy with the expectation values in (12), (14) and (15), (16) evaluated for 32- and 16-spin clusters[4] with periodic boundaries, respectively. Again less than 1% deviation is found.[5] In the finite-cluster approximation the expectation values in (12)–(16) are nonsingular functions of the coupling constants. The lower-bound recursion relation (12) maps all finite K toward a fixed point at $K = 0$. Thus the lower-bound free energy is a nonsingular function of K. Instead of the three fixed points at finite, nonzero values of K mentioned above, the upper-bound recursion formula has a single repulsive fixed point at $K = 0.511$ in the finite-cluster approximation.

To obtain a satisfactory description of the leading singular behavior of the free energy it is probably important to retain other couplings besides the nearest-neighbor coupling in the truncated Hamiltonian. One should begin

[4] To simplify the numerical computations, the 32-spin cluster was reduced to a 16-spin cluster using an exact decimation transformation.

[5] In the finite-cluster approximation the derivatives of the different correlation functions in (15) have finite peaks at different values of K instead of logarithmic divergences at the same critical value. This is presumably the source of the structure in the upper curve between $K = 0.4$ and 0.5 in Fig. 3.

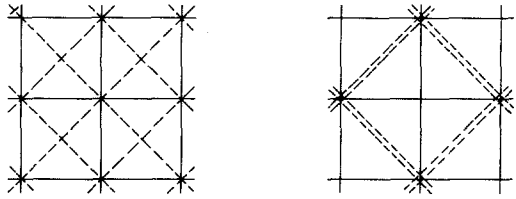

Fig. 4. When half of the second-neighbor bonds (dashed lines) in (a) are rotated as in (b), the central spin can be eliminated with a decimation transformation.

with a rescaling transformation which when combined with an ordinary truncation already has the expected three fixed points before trying to improve matters with an optimal truncation. Following McMillan,[9] we now consider a rescaling transformation which with the help of a bond-shifting approximation can be applied to truncated Hamiltonians with both nearest- and next-nearest-neighbor interactions.

Figure 4 shows a square lattice with bonds between first and second neighbors. If half of the second-neighbor bonds are rotated as in Fig. 4b, the spins at the centers of the squares of doubled second-neighbor bonds can be decimated. The decimation yields new first- and second-neighbor bonds and a four-spin interaction. Once the four-spin interaction is eliminated by truncating the Hamiltonian, the process of bond rotation followed by decimation can be repeated.

If an ordinary truncation without adjustment of the first- or second-neighbor couplings or the constant term is used to eliminate the four-spin coupling, one finds that the first- and second-neighbor couplings K and L satisfy the recurrence relations

$$K' = \tilde{K}(K) + 2L \tag{17}$$

$$L' = \tilde{K}(K)/2 \tag{18}$$

The constant term contributing to the free energy is given by

$$g(K, L) = \tilde{K}_0(K)/2 \tag{19}$$

Here $\tilde{K}_0$ and $\tilde{K}$ are defined by (9) and (10). Curve 3 in Fig. 1 shows the free energy in this approximation. Since both the bond rotation and the ordinary truncation are lower-bound approximations,[6] curve 3 lies below curve 1. Since the ground-state energy is changed by the ordinary truncation, the

[6] The bond-rotation approximation belongs to the class of lower-bound bond-shifting approximations considered by Kadanoff.[1-3] Since $\tilde{K}_4$ defined by (11) is negative and the expectation value $\langle \sigma_1\sigma_2\sigma_3\sigma_4 \rangle$ is positive for a ferromagnetically coupled system, (1) implies that the ordinary truncation is a lower-bound approximation.

approximate free energy deviates from the exact result in the large-K limit. The discrepancy for large K would disappear if an optimal rather than an ordinary truncation were made.

Equations (17)–(19) describe the singular structure of the free energy more successfully than the other approximations we have considered so far. In addition to attractive fixed points at the origin and at infinity, there is a repulsive critical fixed point at $K^* = 4L^* = 0.305$. The critical nearest-neighbor coupling $K_c = 0.403$ maps onto this fixed point as compared with the exact value 0.441. The scaling index y, which determines the exponent α characterizing the divergence in the specific heat by $2 - \alpha = d/y$, has the value 1.03 as compared with the exact result $y = 1$.

If the four-spin interaction is eliminated with an optimal lower-bound truncation instead of an ordinary truncation, (6) implies that K and L satisfy the recurrence relations

$$\langle \sigma_1 \sigma_2 \rangle_{K',L',0} = \langle \sigma_1 \sigma_2 \rangle_{\tilde{K}(K)+2L, \tilde{K}(K)/2, \tilde{K}_4(K)} \tag{20}$$

$$\langle \sigma_1 \sigma_3 \rangle_{K',L',0} = \langle \sigma_1 \sigma_3 \rangle_{\tilde{K}(K)+2L, \tilde{K}(K)/2, \tilde{K}_4(K)} \tag{21}$$

where the three subscripts of the angular brackets denote the first-neighbor, second-neighbor, and four-spin interactions for which the correlation function is evaluated, and $\tilde{K}$ and $\tilde{K}_4$ are defined by (10) and (11).

We have carried out calculations using a 16-spin cluster with periodic boundary conditions (probably too small a cluster to give very reliable results for the second-neighbor correlation) to evaluate the expectation values in (20) and (21). One finds attractive fixed points at the origin and at infinity and a repulsive critical fixed point at $K^* = 0.312$, $L^* = 0.082$. The critical nearest-neighbor coupling $K_c = 0.423$ maps onto this fixed point. The scaling index y associated with the fixed point has the value $y = 0.919$. Thus, using an optimal lower-bound truncation in a rather crude finite-cluster approximation instead of an ordinary truncation is seen to improve the value of K_c and to worsen the value of y. It is not clear, of course, to what extent the excellent value of y obtained with the ordinary truncation is fortuitous.

4. CONCLUSION

Optimal upper- and lower-bound truncations appear to be highly effective in calculations of the free energy. Even in the simplest approximation, in which only nearest-neighbor couplings are kept, quite accurate results for the free energy of the two-dimensional Ising model are obtained. Because of the variational principle it is clear that retaining more coupling constants decreases the error caused by truncating the Hamiltonian. In general the

expectation values in (5)–(8) must be evaluated for finite clusters, but our results suggest that small clusters are sufficient.

In systems which exhibit a continuous transition one is normally more interested in the derivatives of the free energy and the critical exponents than in the free energy itself. An accurate free energy does not, of course, guarantee accurate derivatives. Renormalization transformations involving an optimal truncation have the same defect as a large class of other variational transformations: the transformations involve functions of the coupling constants which are singular at the critical fixed point. The use of finite-cluster expectation values in (5)–(8) is not a self-consistent approximation, but avoids this difficulty. Our results indicate that in two-dimensional systems it is certainly essential to retain other couplings besides the nearest-neighbor coupling if reliable information about critical behavior is desired. The single calculation we carried out retaining both first- and second-neighbor couplings was somewhat inconclusive. Use of an optimal rather than an ordinary truncation improved one critical quantity and worsened another. Additional work with more refined approximations is necessary before one can judge the usefulness of the optimal truncation procedures in calculations of derivatives of the free energy and critical exponents as opposed to the free energy itself.

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