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Thermodynamic functions and critical properties from a cluster-decimation approximation

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Abstract. A simple hybrid of real space renormalisation group theory and finite-lattice calculations is described. The method is based on a lattice-restructuring transformation, with the criterion that the free energies of the original and restructured lattices be equal. We approximate the free energy per spin of the infinite lattice by an exact evaluation of the partition function for a small cluster. As a result of this transformation, the coupling constant of the restructured lattice is found to be temperature dependent. Our method is illustrated by studying the Ising model in two and three dimensions, and two-dimensional Potts models. The calculations involve little more than is required for a Migdal-Kadanoff transformation, yet the critical properties are found to be significantly improved in comparison. Detailed comparisons are also made with the *global* thermodynamic properties calculated within this approximation (free energy, internal energy, specific heat, spontaneous magnetisation) and exact or best known results for the models. The simplicity of the method allows for the study of more complex lattice models, and several possible applications are discussed.

1. Introduction

The determination of global and critical-point properties of lattice models in statistical mechanics is a central problem. In the absence of exact solutions or mappings, any of a number of approximation methods may be useful; mean-field theory (Domb 1960), series expansions (Stanley 1971), and the now widely used real space renormalisation group (RG) techniques (Burkhardt and van Leeuwen 1982). Of the real space methods, the Migdal-Kadanoff (MK) approximation (Migdal 1975, Kadanoff 1976) is among the most widely used, and has been applied to a variety of problems, including random systems (Kirkpatrick 1977, Jayaprakash *et al* 1978, Kinzel and Domany 1981), surface effects (Lipowsky and Wagner 1981), order-disorder transitions (Berker *et al* 1978) and many others. The great virtue of this method is its simplicity, but its numerical accuracy, in terms of critical temperatures and exponents, and thermodynamic functions, is generally poor, especially in higher dimensions. Of course, under certain implementations, such as the limit of infinitesimal rescaling (Kadanoff 1975), the results improve somewhat. Recently, it has been shown (Walker 1982) that a lattice-restructuring transformation, in which one attempts to preserve the *free energy* of the system, rather than simply preserving the *energy* (i.e. the number of bonds) as in MKRG, can lead to significantly more accurate critical parameters, while at the same time introducing control into what is otherwise an uncontrolled approximation at finite temperatures.

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In this paper, we introduce a hybrid transformation, combining both real space RG techniques (decimation) and finite-lattice (cluster) calculations, which we term a *cluster-decimation approximation* (CDA). Whereas previous work (Walker 1982, Andelman and Walker 1983) involved expressing the free energies of the original and restructured lattices as power series expansions in the coupling constant, the present method approximates the free energy *per spin* of the infinite lattice by that of a finite cluster, for which the partition function is exactly soluble. Since the free energy, and indeed the internal energy, of the infinite systems have only weak non-analyticities, we may expect the finite-lattice results to be quite representative of the infinite system. We emphasise that the singularities in the calculation come from the renormalisation group transformation, and the thrust of our approach is to 'calibrate' the lattice restructuring. This approach leads to the same asymptotic relations between restructured and original couplings as in the earlier works, and in addition provides an accurate interpolating function for intermediate temperatures. Furthermore, since the series expansions for complicated, multiple-parameter Hamiltonians are difficult to construct, the present approach should be easier to implement for such models.

In § 2 we review briefly the Migdal-Kananoff approximation, and motivate the transformation to be studied in § 3, where we present the calculations and results for critical and thermodynamic properties of Ising and Potts models. We conclude in § 4 with a brief recapitulation of the approximation, and examples of other problems for which the method may prove useful.

2. Background

The difficulty in determining thermodynamic properties of lattice models is the topology of site-site interactions, that is, the intricate connectivity of the lattice. The Migdal-Kadanoff approximation consists of reducing the connectivity of a lattice so that a fraction of the sites is coupled one-dimensionally to nearest neighbours. With this new, restructured lattice an exact decimation can be performed on these sites, generating renormalised couplings between the remaining sites, and thereby iterating a map in a finite-dimensional Hamiltonian parameter space. While the advantages of remaining within such a finite space are great, the error introduced in the bond-moving step is substantial and uncontrolled at finite temperature.

Figure 1 illustrates the MK approximation as applied to the square lattice ($d = 2$). First, the lattice is divided into $b \times b$ supersquares (b is the length rescaling factor in

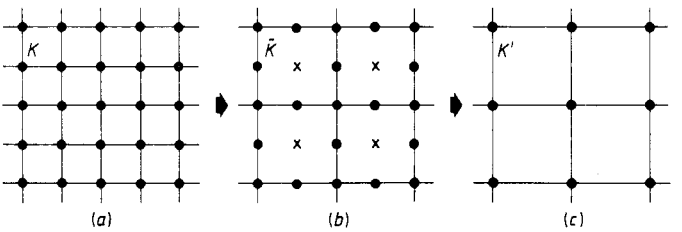

Figure 1. Standard Migdal-Kadanoff transformation illustrated for the two-dimensional square lattice, and rescaling factor $b = 2$. The bond-moving transformation maps the original lattice (a), with coupling constant K, to the restructured lattice (b), with couplings $\tilde{K}$ and disconnected spins indicated by ×'s. An exact decimation then maps the system to the lattice shown in (c), with renormalised couplings K'.

units of the lattice constant; $b=2$ in the figure) and all interior bonds are moved to the supersquare edges. (Note that we consider the symmetric version of bond moving.) The initial coupling is denoted by K (e.g. an Ising model interaction Ks_is_j; $s_i=\pm 1$) and the strengthened remaining couplings by $\tilde{K}$. MKRG determines $\tilde{K}$ in terms of K by requiring that the total number of bonds is preserved in the bond-moving step. For a d-dimensional lattice the relationship is (Kadanoff 1976)

$$\tilde{K}/K = b^{d-1}. \tag{1}$$

Note that the ratio is temperature independent. Kadanoff has shown that this prescription will generate a free energy which is a lower bound to the true free energy. For most statistical models, it will be exact at zero temperature, since the free energy is entirely energetic in that limit, and preserving the number of bonds guarantees matching the free energy. Exceptions to this occur in systems with finite ground state entropy per spin, such as antiferromagnetic q-state Potts (Potts 1952) models with $q>2$ (Wu 1982), and other frustrated systems. Following the approximate bond-moving step, an exact one-dimensional decimation is performed on the supersquare edge sites, generating a renormalised coupling, K', where, for an Ising model with $b=2$,

$$K' = \tfrac{1}{2}\ln[\cosh(2\tilde{K})]. \tag{2}$$

When applying MK to multiple-parameter Hamiltonians, the usual approximation is to choose the ratio of bond-moved to original couplings to be b^{d-1} for all interaction terms. Attempts have been made to improve on standard MK by altering the bond-moving pattern (Swendsen and Zia 1979), for example, or by introducing variational parameters into the transformation (Caracciolo 1981, Lipowsky 1982).

In this work, we construct a more general restructuring transformation, one that does not involve bond moving at all, but rather is based on preserving the free energy. In so doing, we find that the ratio of couplings, $\tilde{K}/K$, takes on a temperature dependence, and that the ratios for different interaction terms assume different functional forms. Though not often thought of in these terms, it is worth noting that other theoretical techniques also rely on preserving the free energy. Examples include the Niemeijer-van Leeuwen cluster approximation (Niemeijer and van Leeuwen 1973, 1974), dedecoration transformations (Fisher 1959, Syozi 1972, Wheeler 1977), and methods for tracing out non-ordering degrees of freedom (Vause and Walker 1982, Goldstein and Walker 1983). These latter methods generally involve taking only a single bond as the finite cluster on which to evaluate the approximate free energy, yet, in spite of the calculational simplicity, the results are found to be quite accurate.

Another approach based on studying finite systems is the phenomenological renormalisation group (Nightingale 1982, and references therein), in which renormalised couplings are computed by matching correlation lengths or other diverging quantities for systems of varying sizes. These methods, coupled with a scaling ansatz, lead to extremely precise critical properties, although the numerical implementation can be quite demanding. Finally, recent work (Kaufman and Mon 1984) has applied the idea of finite-size scaling to models defined on hierarchical lattices.

3. Calculations

In this section we describe the general procedures involved in the cluster-decimation approximations. For the various properties of interest we illustrate the method in some detail for a particular system, and simply present the results for others.

3.1. Critical properties

3.1.1. Ising model. We consider first the smallest non-trivial cluster for the CDA; the 2×2 cluster with periodic boundary conditions shown in figure 2(a). These boundary conditions ensure proper bond counting, which is especially important in the strong-coupling limit. The reduced Hamiltonian for this system is ($\beta = 1/k_B T$)

$$-\beta\mathcal{H}_{2\times2}(K) = 2K(s_1s_2 + s_2s_3 + s_3s_4 + s_4s_1), \tag{3}$$

where $s_i = \pm1$, and the factor of 2 comes from the periodic boundary conditions. The reduced free energy per site, f, is

$$\begin{aligned} f_{2\times2}(K) &= \tfrac{1}{4}\ln\sum_{\{s\}}\exp[-\beta\mathcal{H}_{2\times2}(K;\{s\})] \\ &= \tfrac{1}{4}\ln[2\exp(8K) + 12 + 2\exp(-8K)]. \end{aligned} \tag{4}$$

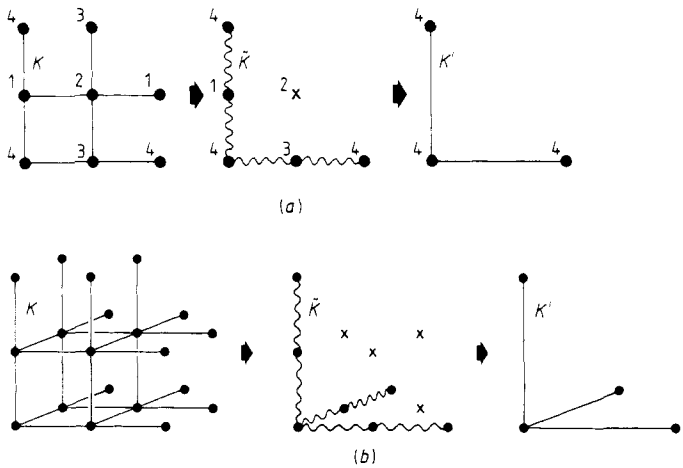

Figure 2. Cluster-decimation approximation (CDA) illustrated for the 2×2 cluster (a), and for the $2\times2\times2$ cluster (b). The coupling constants have the same role in the transformation as those in figure 1. Site numbering in (a) indicates the periodic boundary conditions.

In anticipation of a decimation transformation, we choose the restructured lattice shown in the centre of figure 2(a). Note that there is one decoupled site, and that the remaining lattice, if repeated via the periodic boundary conditions, generates the MK-restructured lattice of figure 1(b). The free energy per site of this cluster, denoted by $\tilde{f}(\tilde{K})$, is determined from the modified Hamiltonian

$$-\beta\tilde{\mathcal{H}}_{2\times2}(\tilde{K}) = 2\tilde{K}(s_1s_4 + s_3s_4). \tag{5}$$

The statistical summation gives

$$\tilde{f}_{2\times2}(\tilde{K}) = \tfrac{1}{4}\ln[4\exp(4\tilde{K}) + 8 + 4\exp(-4\tilde{K})]. \tag{6}$$

Preserving the free energy means choosing $\tilde{K}(K)$ so that $\tilde{f}_{2\times2}(\tilde{K}) = f_{2\times2}(K)$. We find that

$$\tilde{K}(K) = \tfrac{1}{4}\ln[y + (y^2-1)^{1/2}], \tag{7}$$

where

$$y = \tfrac{1}{2}[1 + \cosh(8K)]. \tag{8}$$

In the strong-coupling limit, $T \to 0$ ($K \to +\infty$), the strengthening factor becomes

$$\lim \tilde{K}/K = 2 = b^{d-1}, \qquad (b = d = 2) \tag{9}$$

which is just the MK prescription.

However, as $T \to \infty$ ($K \to 0$), we find

$$\lim_{K \to 0} \tilde{K}/K = \sqrt{2} = b^{(d-1)/2}, \tag{10}$$

the square root of the MK rule. These results are in agreement with those from series expansion results for infinite systems (Walker 1982, Andelman and Walker 1983). The full function $\tilde{K}/K$ against K is shown in figure 3, from which it is clear that the MK factor always overstrengthens the bonds, therefore overestimating the transition temperature.

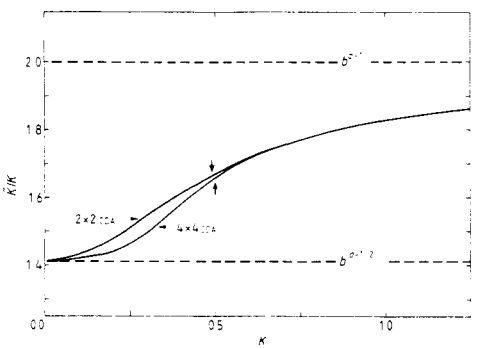

Figure 3. Bond-strengthening factor, $\tilde{K}/K$, for the two-dimensional Ising model using the 2×2 and 4×4 CDAs. Arrows indicate the critical couplings for the two cases. Notice that the MK result ($b^{d-1} = 2$) always overstrengthens the bonds.

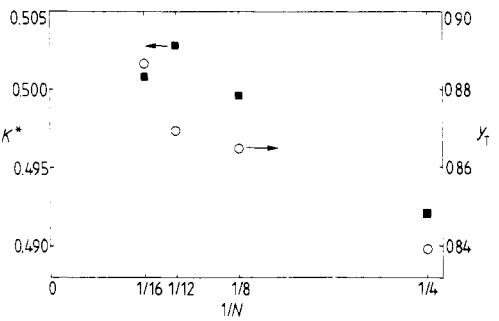

Figure 4. Critical coupling, K^*, and thermal exponent, y_T, for the two-dimensional Ising model using cluster-decimation approximations of various sizes (N = number of sites in the CDA).

Once the function $\tilde{K}(K)$ is known, the exact decimation step of the RG transformation proceeds as usual, with the result given by

$$K' = \tfrac{1}{2} \ln[\cosh\{2\tilde{K}(K)\}]. \tag{11}$$

The non-trivial fixed point occurs for $K^* = 0.492\ldots$, to be compared with the exact result (Onsager 1944) of $\frac{1}{2}\ln(1+\sqrt{2}) = 0.440\,68\ldots$ and the MK result of 0.305.

The thermal exponent $y_T = 1/\nu$ is defined through the relation

$$\partial K'/\partial K|_{K^*} = b^{y_T}, \tag{12}$$

where $b = 2$ in this calculation. From equation (11)

$$\partial K'/\partial K = \tanh\{2\tilde{K}(K)\}(\partial \tilde{K}/\partial K). \tag{13}$$

The quantity $\partial \tilde{K}/\partial K$ is obtained from implicit differentiation of the relation defining $\tilde{K}(K)$, that is $\tilde{f}_{2\times 2}(\tilde{K}) = f_{2\times 2}(K)$. We find $y_T = 0.839\ldots$, an improvement over the MK approximation, which gives $y_T = 0.747$. The exact result is unity.

Of course, it is of interest to study how the size of the cluster used in the calculation affects the estimates of the critical properties. To illustrate this, we have, by straightforward enumeration, generated the partition functions for the 2×4, 2×6 and 4×4 clusters, again using periodic boundary conditions. Although an analytic solution of the form $\tilde{K}(K)$ is not generally possible, it is straightforward to solve numerically for the relation. As with the 2×2 calculation described above, the high- and low-temperature limits of $\tilde{K}/K$ are $b^{(d-1)/2}$ and b^{d-1}, respectively. The results for K^* and y_T are collected in table 1 and plotted in figure 4 as a function of $1/N$, where N is the number of sites in the cluster. The apparently non-monotonic convergence of the results is a consequence of the fact that clusters of different shapes have different free energies, even when they have the same number of sites. While the results tend toward well defined and fairly accurate limits, these values differ from the exact results. We can trace this to the one-dimensional nature of our Hamiltonian parameter space (Walker 1982).

Table 1. Critical properties of the two-dimensional Ising model, as calculated with several cluster-decimation approximations (CDA), compared with those obtained from the Migdal-Kadanoff (MK) transformation, and the exact results (Onsager 1944, Yang 1952).

	CDA (2×2	2×4	2×6	4×4)	MK ($b=2$)	Exact
K^*	0.492	0.500	0.503	0.501	0.305	0.441
y_T	0.839	0.865	0.870	0.887	0.747	1
y_H	1.909	1.940	1.967	1.953	1.879	1.875

The three-dimensional Ising model can be studied similarly (see figure 2(b) for the restructured cluster) with the results collected in table 2. The critical coupling is within 4% of the accepted value, whereas the MK value is more than a factor of 3 too small.

In all the above examples we have determined the relation between the restructured coupling, $\tilde{K}$, and the original coupling, K, by matching cluster free energies. We have explored matching other thermodynamic functions in the same way, such as the reduced internal energy per site $e = K\partial f/\partial K$. The thermal exponent in this case is found to be within 5% of the exact result. A possible explanation for the improvement obtained by matching the internal energy is seen if one considers graphical expansions of the free energy and internal energy: whereas only closed graphs contribute to the partition function series, both closed and open graphs contribute to the energy series (Stanley 1971). As a result, the finite clusters may be more representative of the infinite system in terms of calculating the internal energy.

Table 2. As in table 1, but for the three-dimensional Ising model. The column labelled 'estimates' collects results from Blöte and Swendsen (1979).

	CDA ($2\times2\times2$)	MK ($b=2$)	Estimates
K^*	0.215	0.065	0.222
y_T	1.16	0.94	1.6
y_H	2.49	2.56	2.5

An example of an enlarged parameter space is that involving both the bilinear exchange term K and a magnetic field H. Thus, we add to the Hamiltonian the term

$$\frac{H}{2d}\sum_{\langle ij\rangle}(s_i+s_j). \tag{14}$$

Here we have chosen to associate the magnetic field with bonds, hence the factor of $1/2d$. For the restructured cluster we include the term

$$\tilde{H}\sum_i s_i, \tag{15}$$

where the summation is over all 'connected' sites of the lattice. Straightforward enumeration of the configurations gives

$$Z_{2\times 2}=x^8(w^4+w^{-4})+4(w^2+1+w^{-2})+2x^{-8}, \tag{16}$$

and

$$\tilde{Z}_{2\times 2}=2[\tilde{x}^4(\tilde{w}^3+\tilde{w}^{-3})+(\tilde{x}^{-4}+2)(\tilde{w}+\tilde{w}^{-1})], \tag{17}$$

where

$$x=\exp(K), \qquad \tilde{x}=\exp(\tilde{K}) \tag{18}$$

$$w=\exp(H), \qquad \tilde{w}=\exp(\tilde{H}). \tag{19}$$

In the presence of a magnetic field, the recursion relations for the $b=2$ decimation transformation are

$$K'=\tfrac{1}{4}\ln\{R(++)R(--)/R(+-)^2\} \tag{20}$$

$$H'=\tfrac{1}{2}d\,\ln\{R(++)/R(--)\}+\tilde{H} \tag{21}$$

where

$$R(++)=\tilde{x}^2\tilde{w}+\tilde{x}^{-2}\tilde{w}^{-1}, \qquad R(--)=\tilde{x}^2\tilde{w}^{-1}+\tilde{x}^{-2}\tilde{w}$$

$$R(+-)=\tilde{w}+\tilde{w}^{-1}. \tag{22}$$

The spontaneous magnetisation, M, is calculated recursively from the relation,

$$M(K)=b^{-d}\frac{\partial H'}{\partial H}\bigg|_{H=0}M(K'), \tag{23}$$

which becomes

$$M(K)=b^{-d}\{1+d\,\tanh[2\tilde{K}(K)]\}\frac{\partial\tilde{H}}{\partial H}\bigg|_{H=0}M(K'). \tag{24}$$

Migdal-Kadanoff RG sets $\partial\tilde{H}/\partial H=b^{d-1}$. We choose to determine this by matching free energies of the clusters. This can be easily done by expanding the partition functions

$$Z_{2\times 2}(K,H)=Z_{2\times 2}(K,H=0)+16H^2(x^8+1)+\mathrm{O}(H^4), \tag{25}$$

$$\tilde{Z}_{2\times 2}(\tilde{K},\tilde{H})=\tilde{Z}_{2\times 2}(\tilde{K},\tilde{H}=0)+2\tilde{H}^2(9\tilde{x}^4+2+\tilde{x}^{-4})+\mathrm{O}(\tilde{H}^4). \tag{26}$$

Thus, for $H,\tilde{H}\to 0$

$$\frac{\partial\tilde{H}}{\partial H}=\left(\frac{8(x^8+1)}{9\tilde{x}^4+2+\tilde{x}^{-4}}\right)^{1/2}, \tag{27}$$

and $\tilde{K}(K)$ is determined from the zero-field free energy match. Here is an explicit example of different interaction parameters strengthened by different factors, as mentioned in § 2.

The magnetic exponent, y_H, is determined from the relation

$$\left.\frac{\partial H'}{\partial H}\right|_{\substack{H=0 \\ K=K^*}} = b^{y_H}. \tag{28}$$

Results for the 2D and 3D clusters are collected in tables 1 and 2, and compared with MKRG, exact results (2D), and current estimates (3D).

3.1.2. Potts models. The extension of the above techniques to Potts models is straightforward. As in an earlier work (Andelman and Walker 1983), however, we do choose to make a distinction between two versions of the Potts model; the standard version (denoted by subscript s), and the traceless version (subscript t). The significance of this distinction is discussed below. The coupling in the model is $K\delta_{\sigma_i\sigma_j}$, where $\sigma_i = 1, 2, \ldots, q$ and $\delta_{\sigma_i\sigma_j}$ is the Kronecker delta function. Taking into account periodic boundary conditions, the appropriate 2×2 Hamiltonians are

$$-\beta\mathcal{H}_s(K, q) = 2K[\delta_{\sigma_1\sigma_2} + \delta_{\sigma_2\sigma_3} + \delta_{\sigma_3\sigma_4} + \delta_{\sigma_4\sigma_1}], \tag{29}$$

$$-\beta\tilde{\mathcal{H}}_s(\tilde{K}, q) = 2\tilde{K}[\delta_{\sigma_1\sigma_4} + \delta_{\sigma_3\sigma_4}], \tag{30}$$

$$-\beta\mathcal{H}_t(K, q) = -\beta\mathcal{H}_s(K, q) - 8K/q, \tag{31}$$

$$-\beta\tilde{\mathcal{H}}_t(\tilde{K}, q) = -\beta\tilde{\mathcal{H}}_s(\tilde{K}, q) - 4\tilde{K}/q. \tag{32}$$

The important difference between these two versions of the Potts model is seen by expanding the free energies of the 2×2 cluster for high temperatures

$$f_s = \ln q + 2q^{-1}K + 2q^{-1}(1-q^{-1})K^2 + \ldots \tag{33}$$

$$\tilde{f}_s = \ln q + q^{-1}\tilde{K} + q^{-1}(1-q^{-1})\tilde{K}^2 + \ldots \tag{34}$$

$$f_t = \ln q + 2q^{-1}(1-q^{-1})K^2 + \ldots \tag{35}$$

$$\tilde{f}_t = \ln q + q^{-1}(1-q^{-1})\tilde{K}^2 + \ldots. \tag{36}$$

Thus, in this limit, the standard Potts model strengthening factor, obtained by equating f_s and $\tilde{f}_s$, is $\tilde{K}/K = b^{d-1} = 2$ just as in the MK approximation. Note that this is a direct consequence of the linear term in the weak-coupling expansion. This is in contrast to the traceless models (such as the Ising model) which give $\tilde{K}/K = b^{(d-1)/2} = \sqrt{2}$. Even though the MK result is recovered in both the strong- and weak-coupling limits for standard models, there are deviations for intermediate temperatures, as shown in figure 5(a). Figure 5(b) displays the results for several traceless Potts models, again showing the characteristic sigmoidal shapes.

The critical point and thermal exponent are found from the decimation transformation

$$K' = \tfrac{1}{2}\ln\{[x^4 + (q-1)]/[2x^2 + (q-2)]\}. \tag{37}$$

These results for the traceless version of the model, and those obtained by matching reduced internal energies, are shown in figures 6(a) and (b). As before, substantial improvement over MK results is found, especially when matching the internal energy. For small values of q we find that the standard model approximation for y_T breaks

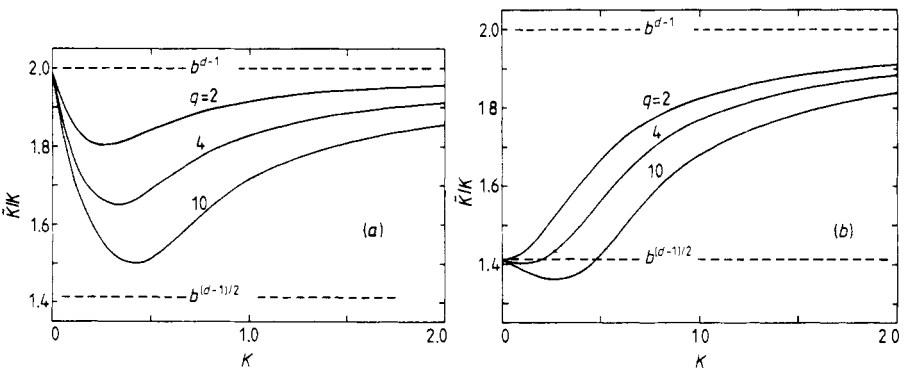

Figure 5. Bond-strengthening factors for two-dimensional Potts models, for various values of q, using a 2×2 CDA: (a) standard, (b) traceless Potts models, as in equations (29) and (31).

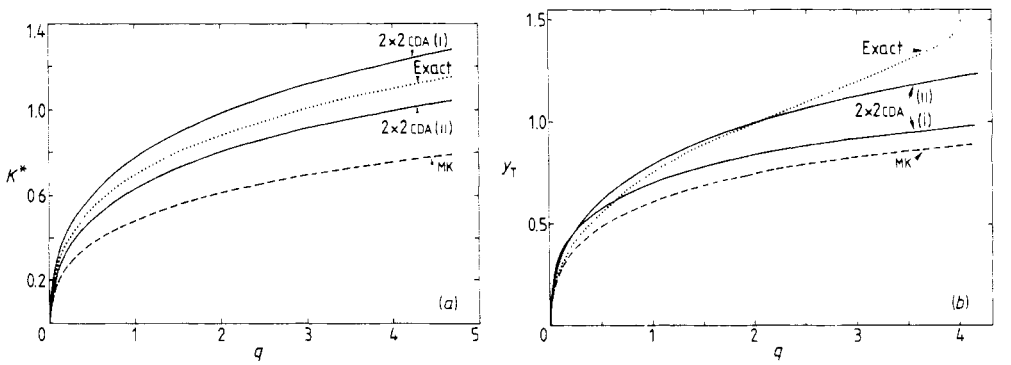

Figure 6. (a) Critical coupling K^* for the Potts model, as a function of q. The results of the 2×2 CDA using the criterion of free energy matching (i), and internal energy matching (ii), show a clear improvement over the MK results. (b) As in (a), but for the thermal exponent y_T.

down, the cause of which is not clear, though the effect has been seen in other approximation schemes (Nienhuis *et al* 1979, Andelman and Berker 1981). Finally, in order to observe the first-order behaviour for $q>4$ it is necessary to employ other methods, such as enlarging the parameter space (Nienhuis *et al* 1979), or mapping to an Ising model (Walker and Vause 1985).

3.2. Thermodynamic properties

The starting point for the calculation of thermodynamic properties within the cluster-decimation approximation is the rescaling relation (Niemeijer and van Leeuwen 1973, 1974) for the free energy f

$$f(K)=a\ln 2+db^{-d}K_0'+b^{-d}f(K'). \tag{38}$$

Here, $a=b^{-d}[b^d-1-d(b-1)]$ is the fraction of decoupled spins in the restructured lattice, each of which contributes only an entropic term of $\ln 2$ to the free energy per

site, and $K_0' = K' + \ln 2$ is a zero-spin coupling generated in the decimation transformation. The reduced internal energy e is

$$e = K\partial f/\partial K, \tag{39}$$

and the specific heat C is

$$C = K^2\partial^2 f/\partial K^2. \tag{40}$$

In practice, we organise the recursion relations in a continued matrix product:

$$\begin{pmatrix} \partial f/\partial K \\ \partial^2 f/\partial K^2 \\ 1 \end{pmatrix} = b^{-d} \begin{pmatrix} \partial K'/\partial K & 0 & d(\partial K_0'/\partial K) \\ \partial^2 K'/\partial K^2 & (\partial K'/\partial K)^2 & d(\partial^2 K_0'/\partial K^2) \\ 0 & 0 & b^d \end{pmatrix} \begin{pmatrix} \partial f/\partial K' \\ \partial^2 f/\partial K'^2 \\ 1 \end{pmatrix}, \tag{41}$$

where

$$\partial K'/\partial K = \partial K_0'/\partial K = \tanh(2\tilde{K})\partial\tilde{K}/\partial K, \tag{42}$$

and

$$\partial^2 K'/\partial K^2 = \tanh(2\tilde{K})\partial^2\tilde{K}/\partial K^2 + 2\,\mathrm{sech}^2(2\tilde{K})(\partial\tilde{K}/\partial K)^2. \tag{43}$$

As before, the partial derivatives of $\tilde{K}$ with respect to K are obtained by implicit differentiation of the free energy matching equation. At each iteration of the RG calculation, we determine $\tilde{K}(K)$ as described in previous sections, and evaluate the continued matrix product until the density vector converges.

In figure 7 we show the free energy calculated from equation (38) in various approximations. The 2D and 3D correlations $\langle s_i s_j \rangle$ are plotted in figures 8(a) and (b) on an absolute temperature scale, in units of the exact or best-estimate transition temperature. The improvement of the internal energy over the MK approximation is reflected in an improved specific heat, as shown for the $d = 2$ case in figure 9. The spontaneous magnetisation in three dimensions, when compared with the MK result, shows a particularly striking example of the cluster-decimation approximation (figure 10).

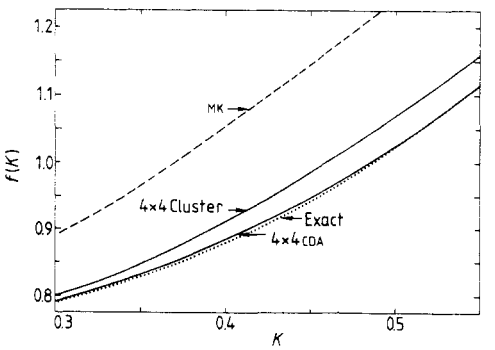

Figure 7. Reduced free energy per spin of the two-dimensional Ising model, for various approximations, compared with the exact result (Onsager 1944).

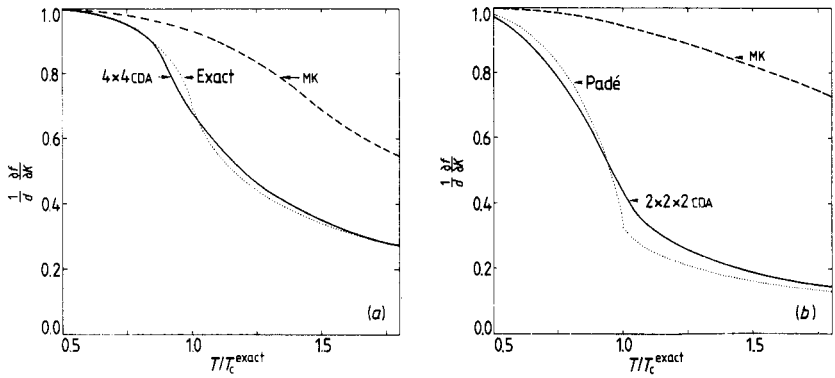

Figure 8. Nearest-neighbour correlation $\langle s_i s_j \rangle$ for (*a*) two- and (*b*) three-dimensional Ising models. Horizontal axis is absolute temperature in units of the exact or best-estimate ($d = 3$) transition temperature. Note the dramatic improvement over the Migdal-Kadanoff approximation.

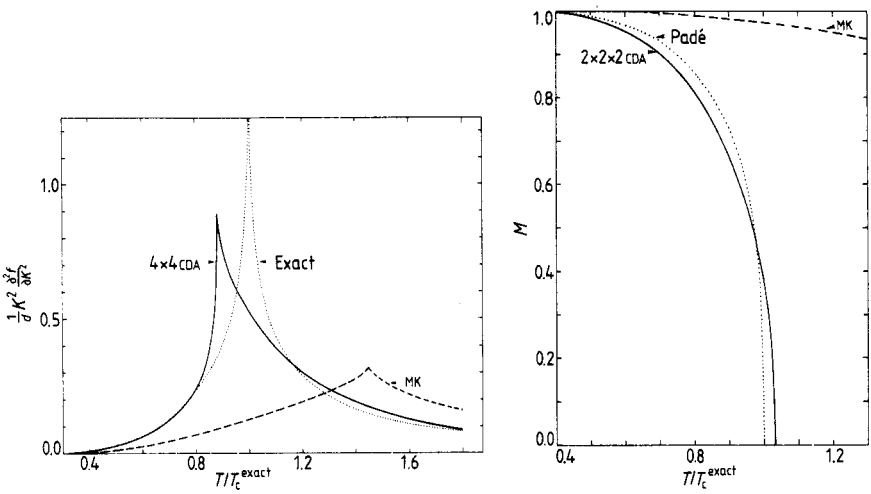

Figure 9. Specific heat of the two-dimensional Ising model. The temperature axis is as in figure 8.

Figure 10. Spontaneous magnetisation of the three-dimensional Ising model. The Padé approximant results are from Scesney (1970).

4. Conclusions

We have described a method for systematically introducing control into real space renormalisation group calculations. The technique involves the same topological restructuring as the Migdal-Kadanoff transformation but determines the couplings on the restructured lattice by the criterion of free energy matching. Approximations to the free energy per spin are obtained from those of finite clusters, whose statistical properties are solved exactly. No adjustable parameters are used in any of the calculations.

As in other finite-system approximations, this approach allows for a systematic extrapolation of results to larger systems, and appears to give convergence to well

defined quantities. Further, the calculations explicitly show how different coupling parameters (such as bilinear and field terms) can be treated differently in the CDA transformations, leading to improved numerical results. Further investigation is needed to extend this analysis to all regions of a multi-parameter Hamiltonian space.

In addition to much-improved critical-point properties, we have shown that the global thermodynamic functions calculated with this method are substantially more accurate than Migdal-Kadanoff approximations.

We have restricted ourselves to small lattice clusters primarily for reasons of calculation simplicity. We envisage that a potentially useful approach for larger clusters, and more complicated models, is the use of Monte Carlo (Binder 1979) methods to determine the relation between the restructured and original couplings, by, for instance, matching internal energies of finite lattices.

A second area of investigation is that of random systems such as bond-dilute magnets. Previous renormalisation group approaches (Jayaprakash *et al* 1978, Kinzel and Domany 1981) have focused on renormalisation of the bond distribution, usually by matching its first few moments. More recent work (Andelman and Berker 1984) has considered the entire distribution. With the approach proposed in the present work, one may explore matching, for instance, the *quenched* free energies of original and restructured clusters, which can be calculated explicitly.

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