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A variational real-space renormalisation-group transformation based on the cumulant expansion

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Abstract. The first order cumulant expansion of Niemeijer and van Leeuwen is combined with a variational method to find the 'best' value of a fixed point Hamiltonian depending upon a parameter, p. A new method for calculating eigenvalues near this fixed point is proposed, based upon the neglect of terms proportional to the error neglected at the fixed point. This approach determines $\partial p/\partial K$ unambiguously. Calculations are carried out for a few simple models. The results are more accurate than those of most other comparably simple approaches.

1. Introduction

Among the wide variety of real-space renormalisation-group (RSRG) approximations which are now available, there are two approaches which can be applied to a broad variety of problems: the cumulant expansion method (Niemeijer and van Leeuwen 1974, 1976) and the variational method (Kadanoff *et al* 1976). In this paper, we describe how these two methods may be combined. (See the parallel work of van Saarloos *et al* (1978) for a similar—but not identical—combination.)

The new method has three attractive features. It is a very simple method, comparable in complexity to the regular comulant and Migdal approximations (Midgal 1975a, 1975b, Kadanoff 1976). The results from this method seem roughly as accurate as those derived from most other RSRG approximations. Also, this variational cumulant method provides us with insight into other variational methods. In particular, it permits the evaluation of $\partial p/\partial K$. Previous authors (see van Leeuwen 1978 for a review) have stressed that the ambiguity in $\partial p/\partial K$ substantially weakens the viability of the variational method. In the simple approximation outlined here, this viability is restored.

2. Definition of method

Since the variational cumulant method is a slightly modified form of the regular cumulant method, we will first review the regular cumulant and then present the modifications. In this paper we deal with a lattice with statistical variables σ_i at each

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lattice site i. The Hamiltonian H of the system is some function of the σ's. If $\{S_a\}$ is a complete set of functions of the σ's, then

$$H\{\sigma\} = \sum_a K_a S_a\{\sigma\} \tag{1}$$

for some set of coupling constants K_a.

The first step is to divide the lattice into blocks or cells, and assign to each cell α a new statistical variable μ_α. The cells are chosen so that the μ variables form a lattice identical in structure (although different in lattice spacing) to the original σ lattice. By defining a weighting function $W(\{\mu\},\{\sigma\})$ we can define a new Hamiltonian $H'\{\mu\}$ of the μ variables via the recursion relation:

$$H'\{\mu\} = \ln \sum_{\{\sigma\}} W(\{\mu\},\{\sigma\}) \exp(H\{\sigma\}). \tag{2}$$

For most Hamiltonians, the sum involved must be approximated. In the cumulant expansion, one approximates this sum by first splitting H into two parts, $H = H_0 + V$, where H_0 contains all the intracell interactions in H, and V contains all the intercell interactions. We can then expand H' (for the general form of such an expansion, see Kendall 1952);

$$H'\{\mu\} = \ln \sum_{\{\sigma\}} W(\{\mu\},\{\sigma\}) \exp(H_0\{\sigma\}) + \langle V\rangle_{H_0} + \tfrac{1}{2}\langle E^2\rangle_{H_0} + \ldots \tag{3}$$

where we have defined $E = V - \langle V\rangle_{H_0}$ with the average being defined by

$$\langle X\rangle_{H_0} = \frac{\Sigma_{\{\sigma\}} W(\{\mu\},\{\sigma\}) \exp(H_0\{\sigma\}) X(\{\sigma\})}{\Sigma_{\{\sigma\}} W(\{\mu\},\{\sigma\}) \exp(H_0\{\sigma\})}. \tag{4}$$

One finds a first order cumulant approximation by neglecting all but the first two terms on the right-hand side of equation (3); the error incurred depends on $\langle E^2\rangle_{H_0}$ and higher order terms in E. We then have an approximate recursion relation

$$H'\{\mu\} = \ln \sum_{\{\sigma\}} W(\{\mu\},\{\sigma\}) \exp(H_0\{\sigma\}) + \langle V\rangle_{H_0}. \tag{5}$$

Our description of critical phenomena then involves two logically independent steps: first the determination of a fixed point and then the study of small deviations from the fixed point. In this paper, both steps are slightly different from those in the original cumulant expansion papers.

At the fixed point, H_0 and V are chosen variationally. We define a variational parameter p and let H_0 and V be functions of p, where H_0 now contains some but not necessarily all intracell interactions in H. Since the first order approximation is an upper bound variational approximation for the free energy, we can essentially minimise the error by varying p so as to minimise the resulting approximation to the free energy at the fixed point. This allows us to determine the fixed point, and the value of the parameter at the fixed point.

The second modification involves deviations from the fixed point. In previous work (Kadanoff *et al* 1976, van Saarloos *et al* 1978, Barber 1978) no successful scheme has been found for calculating parameter values away from the fixed point in such a way that accurate eigenvalues are obtained. Our method is sufficiently simple that one can see through the parameter setting problem for this case. We require in our calculation of the eigenvalues that the errors incurred when considering deviations from criticality be

proportional to the terms neglected at the fixed point and minimised at the fixed point; i.e. $\langle E^2\rangle_{H_0}$ and higher order terms in E. This requirement sets the value of $\partial p/\partial K_a$ at the fixed point, at least for models with only one non-trivial fixed point coupling.

3. Evaluation of fixed points

As an example of a first order calculation, we consider the two-dimensional Ising model on a square lattice. Each variable σ_i takes on the values $+1$ and -1, and our Hamiltonian includes the three interactions defined below:

$$S_0 = \sum_i 1 \tag{6a}$$

$$S_1 = \sum_i \sigma_i \tag{6b}$$

$$S_2 = \sum_{\langle nn\rangle} \sigma_i \sigma_j \tag{6c}$$

where $\Sigma_{\langle nn\rangle}$ indicates a sum over nearest-neighbour pairs. The lattice is divided into two-by-two square cells (see figure 1), and each cell α is assigned a new statistical variable μ_α, also taking the values $+1$ and -1. Our weighting function is just a modified majority rule:

$$W(\{\mu\},\{\sigma\}) = \prod_\alpha [\tfrac{1}{2}(1+\mu_\alpha \operatorname{sgn}(\alpha))] \tag{7}$$

where $\operatorname{sgn}(\alpha)$ is the sign of the sum of the four σ's in the α cell and is zero if the sum is zero. Let S_2^{in}, S_2^{out} be defined by

$$S_2^{\text{in}} = \sum_{\substack{\langle nn\rangle \\ \sigma_i,\,\sigma_j \text{ in} \\ \text{same cell}}} \sigma_i\sigma_j, \tag{8a}$$

$$S_2^{\text{out}} = \sum_{\substack{\langle nn\rangle \\ \sigma_i,\,\sigma_j \text{ not} \\ \text{in same cell}}} \sigma_i\sigma_j. \tag{8b}$$

S_0, S_1 and S_2^{in} contain all the intracell interactions in H and S_2^{out} contains all the intercell interactions in H. We define H_0 and V in terms of a variational parameter p:

$$H_0(p) = K_0S_0 + K_1S_1 + K_2(1+p)S_2^{\text{in}} \tag{9a}$$

$$V(p) = K_2S_2^{\text{out}} - pK_2S_2^{\text{in}}. \tag{9b}$$

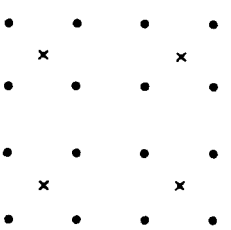

Figure 1. 2×2 cells on the square lattice. Each cell consists of four σ-variables clustered around a μ-variable. ● $=\sigma$, $\times = \mu$.

When $p=0$ these reduce to the definitions of H_0 and V in the regular cumulant expansion. Using the approximate recursion relation in equation (5), we find a new Hamiltonian

$$H'\{\mu\} = K_0' \sum_{\alpha} 1 + K_1' \sum_{\alpha} \mu_\alpha + K_2' \sum_{\langle nn \rangle} \mu_\alpha \mu_\beta \tag{10}$$

where K_0', K_1' and K_2' are functions of K_0, K_1, K_2 and p. For each value of p, there exists a fixed-point Hamiltonian $H^*(p) = K_0^*(p) S_0 + K_2^*(p) S_2$. The variational principle is then used to choose the proper value of p at the fixed point (see the appendix).

The calculation described so far parallels that of van Saarloos *et al* (1978). This method can be easily extended to other lattice types and other models. In table 1, we list the value of the fixed point coupling thus obtained for the Ising model and the s-state Potts model and compare it to exactly known data and results from the regular cumulant method. Notice that the variational cumulant gives improved K_2^* in all cases.

Table 1. Fixed point couplings for the Ising model and s-state Potts model†. Only the values of K_2^* are listed.

Model	Fixed point coupling		
	Variational cumulant	Regular cumulant	Exact data
	Ising model		
Triangular lattice	0·2596	0·3356	0·2747
Square lattice	0·3869	0·5186	0·4407
Cubic lattice	0·2582	0·2978	0·2217
	s-state Potts model on a square lattice		
$s=3$	0·3173	0·4239	0·3350
$s=4$	0·2713	0·3634	0·2747
$s=5$	0·2382	0·3201	0·2349

† The Hamiltonian for the s-state Potts model is given by

$$H\{\sigma\} = K_0 \sum_{i} 1 + K_2 \sum_{\langle nn \rangle} (s\delta_{\sigma_i \sigma_j} - 1)$$

where the σ variables take on the integral values 1 through s.

4. Deviations from fixed point

In the fixed point calculation, we took care to neglect systematically all terms of order $\langle E^2 \rangle_{H_0^*}$ in our approximation. We will follow this same rule when considering deviations from the fixed point. Add an infinitesimal perturbation δH to the fixed point Hamiltonian H_0^*. Neglecting all terms second order or higher in E, the resulting change in the new Hamiltonian is given by

$$\delta H' = \langle \delta H \rangle_{H_0^*} + \langle (\delta H - \langle \delta H \rangle_{H_0^*})(V - \langle V \rangle_{H_0^*}) \rangle_{H_0^*}. \tag{11}$$

It is convenient at this stage to split the perturbation into two terms, $\delta H = \delta H_0 + \delta V$, where

$$\delta H_0 = \delta K_0 S_0 + \delta K_1 S_1 + \delta K_2 (1+p) S_2^{\text{in}} + \left(\frac{\partial p}{\partial K_0} \delta K_0 + \frac{\partial p}{\partial K_1} \delta K_1 + \frac{\partial p}{\partial K_2} \delta K_2 \right) K_2 S_2^{\text{in}} \tag{12a}$$

$$\delta V = \frac{V}{K_2}\delta K_2 - K_2 S_2^{\text{in}}\left(\frac{\partial p}{\partial K_0}\delta K_0 + \frac{\partial p}{\partial K_1}\delta K_1 + \frac{\partial p}{\partial K_2}\delta K_2\right). \tag{12b}$$

We can then rewrite $\delta H'$ as

$$\delta H' = \langle \delta H\rangle_{H_0^*} + \langle(\delta H_0 - \langle \delta H_0\rangle_{H_0^*})(V - \langle V\rangle_{H_0^*})\rangle_{H_0^*} + \frac{\delta K_2}{K_2}\langle E^2\rangle_{H_0^*}$$

$$-K_2\left[\frac{\partial p}{\partial K_0}\delta K_0 + \frac{\partial p}{\partial K_1}\delta K_1 + \frac{\partial p}{\partial K_2}\delta K_2\right]\langle(S_2^{\text{in}} - \langle S_2^{\text{in}}\rangle_{H_0^*})(V - \langle V\rangle_{H_0^*})\rangle_{H_0^*}. \tag{13}$$

The first two terms are easily calculated. The third term is not easily calculated, but can be neglected since it is proportional to our error at the fixed point. The last term is hard to calculate, and cannot be neglected since it is first order in E. However, we can make this term vanish by setting $\partial p/\partial K_a = 0$. This removes the ambiguity in the value of $\partial p/\partial K_a$. We have used our freedom in setting $\partial p/\partial K_a$ to avoid computing a second order cumulant in a first order approximation. However, the important point is that we required that all errors introduced in the approximation be systematically limited to second order or higher terms in E, our fixed point error. By setting the value of $\partial p/\partial K_a$, we can fulfil this requirement without introducing unwieldy calculations.

As stated, this method only works with models with one non-trivial coupling in V, since it is absolutely crucial that δV should be proportional to V once we set the value of $\partial p/\partial K_a$. This is what allows us to neglect the third term in equation (13).

Once $\partial p/\partial K_a$ has been set, the eigenvalues are easily obtained. Tables 2(a) and 2(b) list the eigenvalues for the Ising model and s-state Potts model obtained via the variational cumulant†. Also listed are the exact data and results from the regular cumulant. The thermal eigenvalues found in the two cumulant methods are identical.

Table 2. (a) Thermal (y_T) and magnetic (y_M) eigenvalues for the Ising model. (b) Thermal eigenvalues (y_T) for the s-state Potts model.

		Eigenvalues		
		Variational cumulant	Regular cumulant	Exact data
(a) Lattice type				
Triangular lattice	y_T	0·894	0·894	1·0
	y_M	1·805	2·022	1·875
Square lattice	y_T	1·006	1·006	1·0
	y_M	1·871	2·146	1·875
Cubic lattice	y_T	1·246	1·246	1·587
	y_M	2·622	2·788	2·485
(b) s-value				
3		1·117	1·117	(1·174)[a]
4		1·218	1·218	(1·290)[a]
5		1·305	1·305	—[b]

[a] Series values from Zwanzig and Ramshaw (1977).
[b] Known to be first order transition (Baxter 1973).

† For another variational treatment of the s-state Potts model see den Nijs and Knops (1978).

The direct application of this method does not give the magnetic eigenvalues for the s-state Potts model for $s>2$ since this perturbation leads to multiple-spin coupling terms which we cannot handle easily. However, a potential-moving trick offers some hope of simple answers for this case as well.

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Appendix: Recursion relation and fixed point for the Ising model on a square lattice

The effective weighting function for a single cell is given by a product of $W(\{\mu\},\{\sigma\})$ and $\exp(H_0)$ of the form

$$\exp(h(\sigma,\mu))=\tfrac{1}{2}(1+\mu\ \mathrm{sgn}(S_1))\exp[4K_0+K_1S_1+K_2(1+p)S_2] \tag{A.1}$$

Here, the S's stand for the portion of the previously defined S's (see equation (6)) which lie within the cell. This effective Hamiltonian has a partition function

$$\exp(f(\mu))=\sum_{\{\sigma\}}\exp(h(\sigma,\mu))=\exp(4K_0)$$
$$\times\{\exp[4K_2(1+p)+4K_1\mu]+4\exp(2K_1\mu)+2+\exp[-4K_2(1+p)]\} \tag{A.2}$$

and may then be used to calculate averages

$$\overline{S_1(\mu)}=\partial f/\partial K_1 \qquad \overline{S_2(\mu)}=(1+p)^{-1}\partial f/\partial K_2. \tag{A.3}$$

These can then be split into pieces even and odd in μ according to

$$f(\mu)=f_e+\mu f_0 \qquad \overline{S_1(\mu)}=s_{1,e}+\mu s_{1,o} \qquad \overline{S_2(\mu)}=s_{2,e}+\mu s_{2,o}. \tag{A.4}$$

Then the recursion relation defined by equation (10) becomes

$$\begin{aligned}K_0'&=f_e+\tfrac{1}{8}K_2(s_{1,e})^2+K_1(s_{1,e})-pK_2(s_{2,e})\\ K_1'&=f_o+K_1(s_{1,o})+\tfrac{1}{2}K_2(s_{1,e})(s_{1,o})-pK_2(s_{s,o})\\ K_2'&=\tfrac{1}{8}K_2(s_{1,o})^2.\end{aligned} \tag{A.5}$$

To find the fixed point, set $K_1=0$. Then the last equation in (A.5) determines the value of $(1+p)K^*(p)$, since this requires that at the fixed point,

$$2^{3/2}=s_{1,o}=\frac{4\{\exp[4(1+p)K_2^*(p)]+2\}}{\exp[4(1+p)K_2^*(p)]+6+\exp[-4(1+p)K_2^*(p)]}. \tag{A.6}$$

To find the 'best' value of p, use the variational principle. This requires that one calculate the matrix

$$B_{ij}=\partial K_i'/\partial K_j \tag{A.7a}$$

and the vector

$$w_i=\partial K_i/\partial p. \tag{A.7b}$$

The condition for extremal frec energy is that the left eigenvector of B_{ij} connected with the largest eigenvalue be orthogonal to the vector $\boldsymbol{w}$. The net result of this calculation is the simple formula for p,

$$p = \tfrac{2}{3} \times \frac{\partial/\partial p(\ln s_{1,o})}{\partial/\partial p(\ln s_{2,e})} \tag{A.8}$$

where the derivatives are taken at fixed K_2.

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