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LETTER TO THE EDITOR

Simple renormalisation group method for calculating thermal equations of states

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Abstract. Renormalisation group (RG) techniques are currently used to derive relevant quantities in the vicinity of the critical point. We present here a real space RG procedure which directly yields the order parameter for all values of the external parameters (e.g. temperature). It is as simple as a mean-field calculation, although it provides non-trivial results, which can be systematically improved. The method is successfully illustrated on the square lattice Potts ferromagnet. The whole approach suggests that the order parameter on a hierarchical lattice is, on every site, proportional to its coordination number.

The renormalisation group (RG) techniques have been initially devised for calculating critical exponents; the real space versions also enable the calculation of critical points (phase diagrams in general). However these techniques are commonly used only in the vicinity of the critical point, although in general there is no fundamental reason for such a strong restriction if *approximate* answers are needed. As a matter of fact, RG frameworks are already available [1,2], which enable the calculation of the free energy for arbitrary values of the external parameters (temperature T, applied field H, etc). Through appropriate derivatives of the free energy, the equation of state (as well as the specific heat, susceptibility, etc) can be obtained. However, these procedures tend to be rather complex, operationally speaking. In the present letter, we develop a simple real space RG formalism which enables the direct calculation (without going through the calculation of the free energy) of the order parameter as a function of temperature for arbitrary values of it. The procedure goes, as we shall see, through the inspection of the microscopic configurations of the system, thus developing a good intuition for it. Although we will be referring to the $H=0$ case, the method trivially extends to the calculation of the complete equation of state (in principle, even as a function of the relevant concentrations whenever we are facing disordered systems).

We consider a d-dimensional hypercubic lattice of linear size L, and assume that first-neighbouring sites ferromagnetically interact, $K \equiv J/k_B T$ being the dimensionless coupling constant (we are concerned about models such as the Ising, XY, Heisenberg, Potts or similar models). In the $L \to \infty$ limit, the order parameter M can be defined as $M = N_L(K)/L^d$, where $N_L(K)$ is the thermal canonical average number of sites whose spin is pointing in the easy magnetisation direction (say, the $\sigma_i = 0$ axis for the q-state Potts ferromagnet) minus those whose spin is pointing in any other direction (i.e. $\sigma_i = 1, 2, \ldots, q-1$); if the spins can be inclined with respect to the z axis (as is the case of the Heisenberg model, for instance), the z projections have to be considered. Furthermore, we associate an elementary dimensionless magneton μ with each site of

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the lattice; we could in principle choose $\mu = 1$, but will rather leave it as a variable since it will change under renormalisation. Following Kadanoff in order to understand the scaling, we divide the system of L^d sites into a system of L'^d cells of linear size $B \equiv L/L' > 1$. We then associate with each cell the renormalised variables K' and μ' which will depend on K and μ. The analytic dependencies will differ from one RG to the other, but they all have to satisfy that the total magnetic momentum (extensive quantity) of the system be preserved through renormalisation, i.e.

$$N_{L'}(K')\mu' = N_L(K)\mu. \tag{1}$$

Dividing both terms by L^d we obtain

$$M(K')\mu' = M(K)\mu B^d \tag{2}$$

with $M(K') = N_{L'}(K')/L'^d$. If we start with K and $\mu^{(0)}$ and perform n iterations in (2) we obtain

$$M(K^{(n)})\mu^{(n)} = B^{nd}M(K)\mu^{(0)}. \tag{3}$$

Hence

$$M(K) = \lim_{n\to\infty} \frac{M(K^{(\infty)})\mu^{(n)}}{B^{nd}\mu^{(0)}}. \tag{4}$$

By arbitrarily choosing $\mu^{(0)} = 1$ we obtain

$$M(K) = \lim_{n\to\infty} M(K^{(\infty)})\mu^{(n)}/B^{nd}. \tag{5}$$

This formula has to be used together with the (standard) RG recurrence for the coupling constant, namely

$$K' = f(K) \tag{6}$$

which normally admits three fixed points: $K = 0$ (stable under renormalisation, paramagnetic phase), $K = \infty$ (stable, ferromagnetic phase) and $K = K_c$ (unstable, critical point). Two typical situations occur when using (5): (i) $K < K_c$, hence $K^{(\infty)} = 0$ and hence $M(K^{(\infty)}) = 0$, which yields (through (5)) $M(K) = 0$, as desired; (ii) $K > K_c$, hence $K^{(\infty)} = \infty$ and hence $M(K^{(\infty)}) = 1$ (conventional value for $T = 0$), which yields (through (5))

$$M(K) = \lim_{n\to\infty} \mu^{(n)}/B^{nd}. \tag{7}$$

This is the final formula which provides the thermal dependence of the order parameter in the non-trivial region, namely for $T < T_c$.

To finish the procedure we have to specify how the RG recursive relations for K (i.e. (6)) and μ are determined. In particular, let us anticipate that the RG equation for μ will typically be of the form

$$\mu' = g(K)\mu \tag{8}$$

with $g(\infty) = B^d > g(K_c) > g(0) > 0$. From (6)-(8), it is straightforward to establish, in the $T \to T_c$ limit, for the correlation length $\xi \propto |T - T_c|^{-\nu}$ and for $M \sim A(1 - T/T_c)^{\beta}$ that

$$\nu = \ln B/\ln[\mathrm{d}f(K)/\mathrm{d}K]_{K_c} \tag{9}$$

and

$$\beta = \ln[B^d/g(K_c)]/\ln[\mathrm{d}f(K)/\mathrm{d}K]_{K_c}. \tag{10}$$

The critical amplitude A cannot be analytically determined (because (8) is invariant through the scale change $\mu \to \lambda\mu$ and $\mu' \to \lambda\mu'$ for arbitrary λ) but only numerically determined (by iterating).

Several procedures are available in the literature for determining $f(K)$: here we shall adopt that already used in [3,4] (for the q-state Potts and spin-$\frac{1}{2}$ Heisenberg models, respectively). We normalise a two-rooted graph G (with chemical distance b between the roots, and which might generate a hierarchical lattice with intrinsic fractal dimensionality [5,6] $d_b = \ln N_b / \ln b$, where N_b is the number of bonds of the graph) into a smaller one G' (with chemical distance b' between the roots, and which might generate a hierarchical lattice with dimensionality $d_{b'} = \ln N_{b'} / \ln b'$, $N_{b'}$ being the number of bonds). It follows that $B = b/b'$ and $B^{d_{bb'}} = N_b / N_{b'}$. (See figure 1($a$) for an example ($b' = 1$, $b = 2$, $N_b = 5$, $N_{b'} = 1$, $d_{bb'} = d_b = \ln 5/\ln 2$).) We then preserve the correlation function between the two roots (denoted by 1 and 2) by imposing

$$\operatorname{Tr}_{3,4,\ldots,N'_s} \exp(-\mathcal{H}'_{12\ldots N'_s} + K'_0) = \operatorname{Tr}_{3,4,\ldots,N_s} \exp(-\mathcal{H}_{12\ldots N_s}) \tag{11}$$

where $\mathcal{H}_{12\ldots N'_s}$ and $\mathcal{H}_{12\ldots N_s}$ are the dimensionless Hamiltonians corresponding, respectively, to the small (N'_s sites) and large (N_s sites) clusters and K'_0 is an additive constant to be determined. Equation (11) completely determines $f(K)$; we shall note $\mathrm{RG}_{b'b}$, the associated RG. For the example illustrated in figure 1(a) and assuming Potts interactions ($\mathcal{H}/k_B T = -qK \sum_{i,j} \delta_{\sigma_i,\sigma_j}$; $\sigma_i = 1, 2, \ldots, q, \forall i$) we obtain [3] (through (11))

$$t' = \frac{2t^2 + 2t^3 + 5(q-2)t^4 + (q-2)(q-3)t^5}{1 + 2(q-1)t^3 + (q-1)t^4 + (q-1)(q-2)t^5} \tag{12}$$

with the thermal transmissitivity t [3] defined through

$$t \equiv [1 - \exp(-qK)]/[1 + (q-1)\exp(-qK)]$$

(and analogously for t').

Let us now present the new procedure we have devised to determine $g(K)$. In order to break the symmetry (needed for establishing the equation for the order

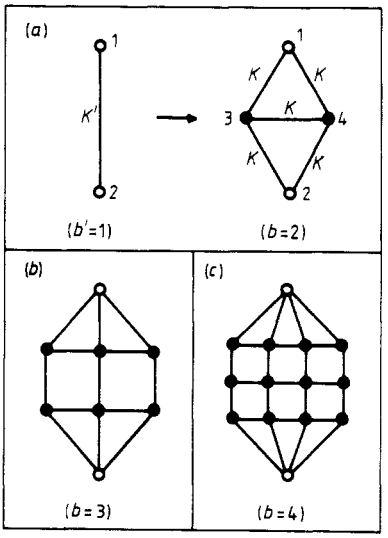


Figure 1. Clusters used to construct $\mathrm{RG}_{b'b}$ for the square lattice. ●, ○ denote, respectively, internal and terminal (root) sites. (a) RG_{12} transformation, (b) $b = 3$ graph, (c) $b = 4$ graph.

parameter) we *impose* the spin of, say, terminal 1 (of both small and large graphs) to be along the easy magnetisation direction (say, the $\sigma_i = 0$ axis), the rest of the spins (terminal 2 included) being free to take all possible orientations (q configurations for each spin). Each cluster configuration will be weighed with the corresponding Boltzmann factor and will be associated with a value for the cluster magnetic momentum m where each spin contributes proportionally to its coordination number (later on we shall come back into this point). We then impose

$$\langle m \rangle_{G'} = \langle m \rangle_G \tag{13}$$

where $\langle \ldots \rangle$ denotes the thermal canonical average; (13) dertermines $g(K)$. The whole procedure is illustrated for the spin-$\frac{1}{2}$ Ising ferromagnet ($\mathcal{H}/k_B T = -K \sum_{i,j} \sigma_i \sigma_j$; $\sigma_i = \pm 1$) in table 1. This result generalises into that for the Potts ferromagnet as follows:

$$\frac{2\exp(qK')+(q-2)}{\exp(qK')+(q-1)}\mu' = \frac{10\exp(5qK)+10(q-2)\exp(3qK)+8(3q-5)\exp(2qK)}{\exp(5qK)+2(q-1)\exp(3qK)+4(q-1)\exp(2qK)}$$
$$+\frac{2(8q^2-39q+45)\exp(qK)+(2q^3-16q^2+44q-40)}{(q-1)(5q-9)\exp(qK)+(q-1)(q-2)^2}\mu \tag{14}$$

where to construct the last column of a table such as table 1 we have used the fact that the Potts order parameter is proportional to $(q\langle\delta_{\sigma_i,0}\rangle - 1)/(q-1)$.

The results obtained by using (12) and (14) together with (7) ($B^d = 5$ in this case), as well as those corresponding to higher values of b, are presented in figures 2 and 3 and table 2. The exact critical point ($t_c = (\sqrt{q}+1)^{-1}$) is recovered for all $R_{b'b}$ (this is a consequence of the self-duality of the chosen clusters). The general trends are very satisfactory and the numerical values quite reliable (they can be further improved by performing extrapolations for increasing b and b' [7]). Note, however, that the present RG fail in reproducing, for $q > 4$, the first-order phase transition expected for $d = 2$ Bravais lattices. To overcome this difficulty (shared by all available phenomenological and hierarchical-lattice-like RG for the pure model) the RG parameter space should be expanded [8].

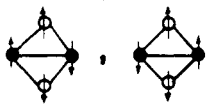
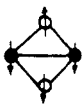
Let us now go back to the point that every spin contributes to the cluster magnetisation, proportionally to its coordination number. This hypothesis follows from our belief that the order parameter on a hierarchical lattice is not uniform (the same on all sites) as in Bravais lattices, but rather is directly related to the number of neighbouring sites with which a given site is interacting. The well known uniform spontaneous magnetisation of Bravais lattices should be a consequence of their translational invariance (lost in hierarchical lattices). The hypothesis we are discussing is equivalent to assuming that the relevant magnetic field (a parameter thermodynamically conjugated to the order parameter) is also proportional to the coordination number: this is precisely what several authors [2,5,10] have assumed in similar contexts. On different but related grounds, the analysis of the Blume-Emery-Griffiths (BEG) model points towards the same direction. The BEG model in a Bravais lattice contains the $q = 3$ Potts model as a particular case if convenient relations are assumed between the BEG coupling constants. The same occurs in a hierarchical lattice if and only if the single-site term of the BEG Hamiltonian is assumed proportional to the coordination number. Last, but not least, if we assume in the present RG framework a uniform order parameter, the successive approximations (increasing b and b') for β run away from the exact answer! Naturally, the full calculation of the Gibbs energy of a specific hierarchical lattice as a function of T and H would unambiguously clarify the situation. Such a

Table 1. Establishment of (13) associated with RG_{12} for the Ising ferromagnet ($q=2$). (*a*) $\langle m\rangle_{G'}=2e^{K'}\mu'/(e^{K'}+e^{-K'})$. (*b*) $\langle m\rangle_G=(10e^{5K}+8e^{-K}-2e^{-3K})\mu/(e^{5K}+2e^{K}+4e^{-K}+e^{-3K})$. These expressions can be recovered as the particular $q=2$ case of (14).

(*a*)

G' configuration	Weight	m
	$e^{K'}$	$2\mu'$
	$e^{-K'}$	0

(*b*)

G configuration	Weight	m
	e^{5K}	10μ
	e^{K}	6μ
	e^{-K}	4μ
	e^{-3K}	-2μ
	e^{-K}	0
	e^{K}	-6μ

treatment would also tell us to what extent the present RG procedure provides the exact $M(T)$ for that hierarchical lattice. In any case we can already note that the $q=2$ RG_{12} result for β is

$$\ln\left(\frac{5(17+12\sqrt{2})}{2(38+27\sqrt{2})}\right)\left[\ln\left(\frac{18+13\sqrt{2}}{10+7\sqrt{2}}\right)\right]^{-1}=0.18$$

which coincides with the value presented by Melrose [5] as being the exact one for the associated (Wheatstone bridge) hierarchical lattice. For this lattice and arbitrary values of q we obtain

$$\beta=\frac{\ln\{5(2+\sqrt{q})[8(1+q)+(15+q)\sqrt{q}]/2(1+\sqrt{q})[40+18q+(52+q)\sqrt{q}]\}}{\ln[(8+5q+13\sqrt{q})/(8+q+7\sqrt{q})]}. \tag{15}$$

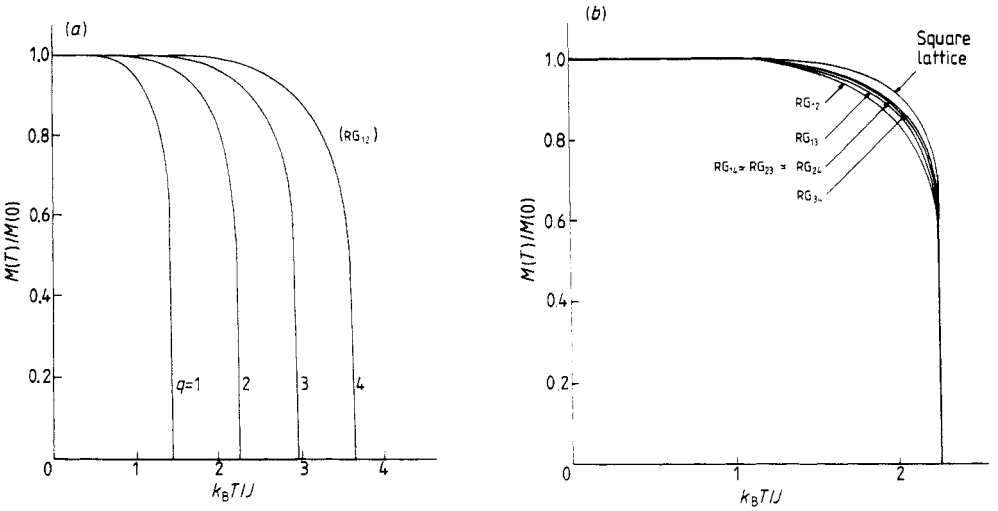


Figure 2. Thermal behaviour of the order parameter for the q-state Potts model. (a) RG_{12} for typical values of q, (b) successive RG approximations for $q = 2$ (Ising).

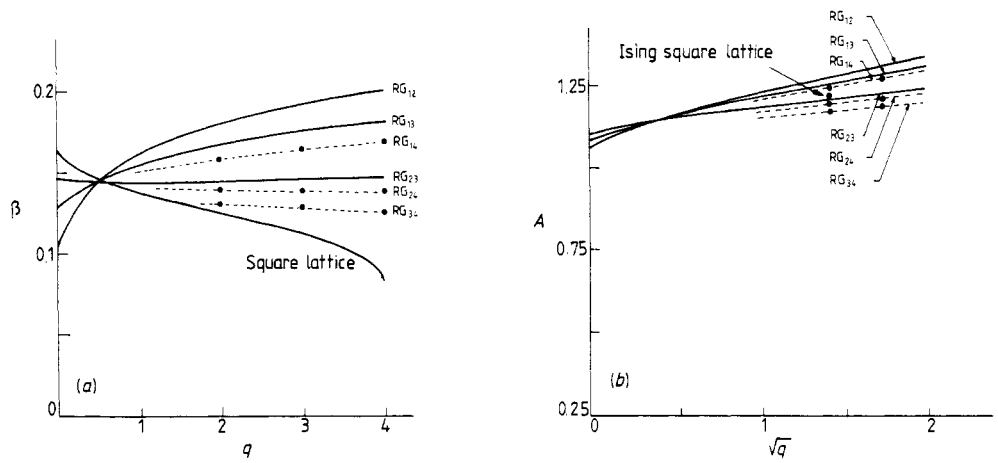


Figure 3. (a) Critical exponent β and (b) amplitude A as functions of q within successive RG approximations (β for a square lattice is taken from [9]). The broken lines are indicative and have been used when the calculation was available only for integer values of q.

Also it is worth mentioning that, for all the self-dual hierarchical lattices considered in this letter, we have verified that, in the $q \to \infty$ limit, $\nu \to 1/d_b$ (see [6]) and $\beta \to 1 - 1/d_b$.

To summarise, let us say that the real space RG procedure we have introduced here enables in principle the calculation, for all temperatures (and similar external parameters), of the order parameter(s) associated with any Hamiltonian system. The calculation is direct (no calculation of thermodynamical energy is needed), helps intuition (in the sense that microscopic configurations have to be visualised), is as simple operationally as a mean-field approach and provides non-trivial results which can be systematically improved. Its degree of efficiency has been satisfactorily tested here with the square lattice Potts ferromagnet, whose exact thermal dependence on

Table 2. Successive RG approximate and exact values for critical exponents and amplitudes. A few numerical values are missing because their calculation would have needed a supplementary non-trivial computational effort.

		RG_{12}	RG_{13}	RG_{14}	RG_{23}	RG_{24}	RG_{34}	Exact
ν	$q=1$	1.428	1.380	1.363	1.305	1.303	1.301	$\frac{4}{3}=1.333\ldots$
	$q=2$	1.149	1.109	1.095	1.048	1.046	1.043	1
	$q=3$	1.024	0.988	0.975	0.933	0.931	0.928	$\frac{5}{6}=0.833\ldots$
	$q=4$	0.948	0.916	0.903	0.864	0.862	0.859	$\frac{2}{3}=0.666\ldots$
β	$q=1$	0.161	0.154	—	0.144	—	—	$\frac{5}{36}=0.139\ldots$
	$q=2$	0.180	0.166	0.159	0.145	0.139	0.131	$\frac{1}{8}=0.125$
	$q=3$	0.193	0.175	0.165	0.147	0.139	0.129	$\frac{1}{9}=0.111\ldots$
	$q=4$	0.204	0.182	0.170	0.148	0.139	0.127	$\frac{1}{12}=0.083\ldots$
A	$q=1$	1.225	1.210	—	1.182	—	—	?
	$q=2$	1.275	1.253	1.235	1.206	1.196	1.171	1.222...
	$q=3$	1.310	1.284	1.271	1.225	1.215	1.177	?
	$q=4$	1.338	1.309	—	1.240	—	—	?

the magnetisation is still unknown for all $q \neq 2$; further applications would be very welcome.

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