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Use of linear weight factor in real-space renormalization group

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Abstract. An important problem in all real space renormalization group calculations is the choice of appropriate weight factor for different configurations. In this context, the use of linear weight factor has been restricted due to lack of suitable criterion for selecting the parameter q. An elegant matching procedure has recently been developed to fix q. First we undertake a systematic investigation of the variation of critical constants with cell size. A comparison is also made with the results obtained using an earlier criterion proposed by Subbarao. Secondly, we extend the applicability of the theory to the realm of dynamic problems by studying the exponent of energylike perturbation in 2D Glauber-Ising model. The value of the exponent obtained for square and triangular lattices are 2·147 and 1·918 respectively which are in good agreement with the general consensus ($\sim 2 \cdot 0$).

Keywords. Real space renormalization group; linear weight factor; Glauber–Ising model.

1. Introduction

Thermodynamic quantities and correlation functions describing a second order phase transition follow power laws and scaling behaviour near the critical point with an universal character. The pioneering studies of Kadanoff (1966) and Wilson (1971) established the renormalisation group (RG) analysis which provide physical understanding of such behaviour. The central idea behind the RG technique is a step-by-step decimation of the number of degrees of freedom of the system with incorporation of the effect of decimation in one step into the new Hamiltonian of the next step. For detailed calculations, there are basically two approaches namely the lattice method and the field-theoretic technique. Apart from its inherent conceptual simplicity the lattice method has the advantage of being valid for integer dimensions, including $d=2$ where it can be compared with some exact results. Further, some nonuniversal quantities like the critical temperature (T_c) can easily be calculated in this method.

In the real space renormalization group (RSRG) (Niemeijer and van Leeuwen 1976; van Leeuwen 1978; Wallace and Zia 1978) the reduction in the density of degrees of freedom is accomplished by introducing a new set of spins $\{s'\}$ with larger lattice spacing than the initial set $\{s\}$ and defining a new effective Hamiltonian $H'(s')$. The relation between the initial and the renormalized Hamiltonian is given by

$$\exp\,[H'(s')] = \sum_{\{s\}} W(s', s) \exp\, H(s), \tag{1}$$

where $W(s', s)$ is the weight factor having the following properties

(i) $W(s', s) \geqslant 0$ for all s', s,

(ii) $\sum_{\{s'\}} W(s', s) = 1$, which effectively mean that the partition function Z remains invariant under the transformation,

(iii) the symmetries of the Hamiltonian are retained.

The above mentioned restrictions on W still allow an enormous variety in choice for W each leading to a different renormalization transformation. Typically, one chooses a factorisable form for W. A widely used choice of the weight factor was introduced by Niemeijer and van Leeuwen (1976) (hereafter NVL) based on the "majority rule" which associates a new spin s'_i with suitable group of lattice sites ("cell")

$$s'_i = \text{sgn}\ (\Sigma s_i), \tag{2}$$

where the sum runs over all site-spins in the cell. For triangular lattice where cell-spins have been placed in the centre of three sites, the weight factor has the explicit form

$$W(s', s) = \prod_i \tfrac{1}{2}\,[1 + s'_i\,(s_i^1 + s_i^2 + s_i^3 - s_i^1\, s_i^2\, s_i^3)/2], \tag{3}$$

with s_i^α ($\alpha = 1,2,3$) denoting the sites in ith cell. This is an example of a nonlinear transformation.

If we now consider the transformation of the interaction parameter (coupling constant) K, the renormalized interaction parameter K' would be a function of K. The nontrivial fixed point that characterizes the critical point requires

$$K'(K_c) = K_c. \tag{4}$$

There are a number of approximation schemes for getting reliable estimates of $K'(K)$, namely (a) finite lattice, (b) cumulant expansion, and (c) cluster approximation. In this paper, we concentrate on the cumulant expansion scheme.

2. RSRG with linear weight factor

In spite of considerable successes, the RSRG method runs into difficulties in specific applications (Brower *et al* 1977; Kinzel and Fisher 1978). It seems that the nature of errors incurred in the various approximation schemes (Hsu and Gunton 1977) is not clearly understood. This led to suggestions regarding modifications of the original NVL method (Kadanoff 1975). Kadanoff and Houghton (1975) improved the original equal weight scheme of NVL by choosing a nonlinear weight factor optimized by a variational technique. Even then inconsistency remained in fixing the variational parameter (Knops 1977; van Saarloos *et al* 1978).

The possibility of using linear weight factors was first explored by Subbarao (1975). The explicit form of the linear weight factor is given by

$$W_q(\{s'\}, \{s\}) = \prod_a \tfrac{1}{2}\,[1+q^{(l)} s'_a \sum_{i\in a} s_i], \tag{5}$$

where $q^{(l)}$ is the adjustable parameter for this transformation with rescaling factor l. Every value of $q^{(l)}$ would yield a fixed point of its own. One is then faced with the problem as to which fixed point to accept. A number of possibilities exists for setting up a proper criterion to fix $q^{(l)}$ (Bell and Wilson 1975).

First, we note that the linear weight factor has the interesting property that its nth power, $(W_q)^n$ $(n=1,2,3.....)$, associated with a rescaling factor l^n, is also linear with the new parameter

$$q^{(l^n)} = \left[q^{(l)}\right]^n. \tag{6}$$

The group structure of block-spin transformation requires that $K_c - q^{(l)}$ plots should be identical for cells with rescaling factors l^n. In actual computations the curves are never coincident. Stella *et al* (1979) have shown in a variety of cases that the intersections of $K_c - q^{(l)}$ curves for l and l^2 usually provide a reliable estimate not only for K_c but also for the thermal (Y_T) and magnetic (Y_H) exponents. This method would be referred to as intersection method from now on.

On the other hand, Subbarao (1975) showed from a study of the limit of the spin-spin correlation function that the existence of a local non-trivial fixed point requires $q^{(l)}$ to be given by

$$q^{(l)} = 3^{-1+(\eta/4)}, \tag{7}$$

where η is the corresponding critical exponent. The magnetic eigenvalue $\lambda_H^{(l)}$ is also related to η through

$$\lambda_H^{(l)} = 3^{1-(\eta/4)}. \tag{8}$$

Hence for an infinite lattice

$$\lambda_H^{(l)} = 1/q^{(l)}. \tag{9}$$

Although for a finite lattice this condition is not exactly satisfied, we may use it as a criterion for the choice of $q^{(l)}$.

Equation (9) can also be utilized to establish the relationship between $q(l_1)$ and $q(l_2)$:

$$q^{(l_2)} = \left[q^{(l_1)}\right]^{(\log l_2)/(\log l_1)}. \tag{10}$$

That (6) follows as a special case of (10) for $l_2 = (l_1)^n$ is obvious. The added advantage of this method is that one need not consider more than one type of cell to arrive at an optimal selection of $q^{(l)}$.

Table 1. Result of intersection method for planar triangular Ising lattice.

l'	$\ln l' / \ln l^*$	K_c	$q^{(l)}$	$Y_T^{(l)}$	$Y_T^{(l')}$	Y_H
2	1.262	0.101	0.579	0.602	0.366	1.227
$\sqrt{7}$	1.771	0.194	0.487	0.959	0.993	1.477
3	2.000	0.257	0.437	1.114	1.057	1.443
$2\sqrt{3}$	2.262	0.221	0.464	1.034	1.049	1.521
Exact		0.275		1.000	1.000	1.875

$^*l = \sqrt{3}$

Table 2. Result of "$1/\lambda_H$ method" for planar triangular Ising lattice.

l	K_c	q	Y_T	Y_H
$\sqrt{3}$	0.212	0.471	1.010	1.369
2	0.218	0.424	0.699	1.238
$\sqrt{7}$	0.232	0.238	1.100	1.475
3	0.240	0.205	1.024	1.443
$2\sqrt{3}$	0.246	0.152	1.112	1.518
Exact	0.275		1.000	1.875

We now undertake a numerical investigation of the comparative merit of these two techniques.

The approximation used in all the cases is the simple first-order cumulant expansion technique. The calculations are performed for a planar triangular lattice with progressively larger rescaling factors. In the intersection method the comparison is always made with the smallest cell type ($l = \sqrt{3}$). The results for the intersection method and the $1/\lambda_H$ method are summarized in tables 1 and 2 respectively.

In the intersection method, the value of K_c shows the closest approach to the exact value for $l^1 = l^2$. Even for a cell with larger rescaling factor ($l' = 2\sqrt{3}$) the value of K_c falls off, thereby establishing the viability of the intersection method though it lacks a firm theoretical basis. The thermal exponent shows reasonable agreement with the exact result for intersections corresponding to cells with large rescaling factors. The values of magnetic exponent are poor in all cases.

In contrast, the $1/\lambda_H$ method produces a systematic improvement in the value of K_c with increase in cell-size. We conclude that computation with a cell of large enough size is capable of yielding a K_c close to the exact value. The agreement of Y_T with the exact value is in general good. As in the previous method the value of Y_H is unreliable.

3. Critical relaxation in Glauber-Ising model

A number of recent theoretical investigations (Achiam 1979; Bolton and Johnson 1976; Rácz and Collins 1976; Suzuki 1977; Yalabik and Gunton 1979) have been able to arrive at a general consensus regarding the value of the dynamic exponent for two-dimensional problems within the framework of the Glauber-Ising model (Glauber 1963). The approach to equilibrium is described by a time scale $\tau \sim |T - T_c|^{-\Delta}$ where Δ is the dynamic exponent. The dependence of the relaxation time on the bulk correlation length ξ is characterised by the exponent z. The two dynamic exponents are related by $\Delta = \nu z$ where ν is the static exponent describing the divergence of ξ. The only exact result available is the lower bound of Δ : $\Delta \geqslant 1{\cdot}75$ (Abe 1968).

The extended dynamic scaling hypothesis predicts the equality of the index for critical relaxation of energy like perturbation (Δ_E) and that of magnetic perturbation (Δ_M). The high-temperature expansion gives $\Delta_M = 2{\cdot}125$ (Rácz and Collins 1976) while Monto-Carlo simulations give $\Delta_M = 2{\cdot}30$ (Bolton and Johnson 1976) and $\Delta_E = 2{\cdot}0$ (Stoll *et al* 1973). Recently the real-space renormalization group (RSRG) method has been utilized to study these problems. For triangular lattice, Achiam obtained $\Delta_E = 2{\cdot}09$ (Achiam 1979*a*), $\Delta_M = 2{\cdot}07$ (Achiam 1978), and for the square lattice $\Delta_E = 2{\cdot}131$ (Achiam 1979*b*), $z_M = 2{\cdot}24$ (Achiam 1980). Kadanoff-Migdal like RG transformation leads to a value of $z = 1{\cdot}96$ (Suzuki *et al* 1979). A recent extension of the same method yields $z = 1{\cdot}98$ (Droz and Malaspinas 1980).

In this section we utilize the RSRG analysis to study the decay of energy like perturbation in the first-order cumulant expansion technique with a linear transformation function in contrast to the equal-weight scheme adopted by Achiam.

In the Glauber-Ising model, the relaxation process is constrained by a single spin-flip at a time with a transition probability rate $\omega_i(\{s\})$. The spin probability distribution $P(\{s\}, t)$ satisfies the empirical master equation

$$\tau \frac{dP(\{s\}, t)}{dt} = -\sum_i (1 - p_i)\, \omega_i(s)\, P(\{s\}, t), \tag{11}$$

where p_i is the spin-flip operator. The master equation can also be written in the general form

$$\tau \frac{dP(s, t)}{dt} = -\mathscr{L}\, \phi(s,t), \tag{12}$$

where $\phi(s,t) = P(s,t) / P(s, t \to \infty)$, and $\mathscr{L}$ the Liouville operator, is given by $\mathscr{L} = \sum_i P(s, t \to \infty)\, \omega_i (1 - p_i)$.

Renormalization of the dynamic problem consists of the static RG transformation followed by a time-rescaling that leaves the master equation of the system invariant. We represent ϕ in a perturbation series:

$$\phi = 1 + \sum_a h_a(t) O_a(s), \tag{13}$$

where $O_a(s)$ is the time-independent spin operator even under spin-reversal and $h_a(t)$ are operators containing their time-dependence. In first order, we retain only h_2, the nearest-neighbour term. The scaling factor for τ is given by

$$\lambda/\omega = l^z, \tag{14}$$

where l is the change of length scale by renormalization and ω and λ the scale factors for the time-dependent and time-independent operators respectively.

For the square lattice with four-spin cell ($l=2$) the condition for fixed point is given by

$$\begin{aligned} &2f_1^2 = 1 \\ &\text{where } f_1 = \langle s_i^\alpha \rangle_0 = 4q\,[1+\exp(4K)]\,/\,Z_0, \\ &\text{with } Z_0 = \exp 4K + 6 + \exp(-4K),\ s_i^\alpha\ (i=1,2,3,4), \end{aligned} \tag{15}$$

being the site spins of cell α. λ in equation (14) can be identified with the thermal eigenvalue (λ_T) and can be readily evaluated from the expression

$$\lambda = \frac{d}{dK}(2f_1^2 K)\bigg|_{K=K_c}. \tag{16}$$

Following Achiam, ϕ is now expressed in the exponential form

$$\phi = \exp\left[\tfrac{1}{2}\sum_i s_i \{h_2(t) \sum_j s_j\}\right]. \tag{17}$$

Retaining only the leading term, we get the renormalized $h_2(t)$

$$h'_2 = 2h_2 f_1 Z_1 / Z_0, \tag{18}$$

where Z_1 is the modified partition function when one spin has all its interactions removed. In the present problem, Z_1 is given by

$$Z_1 = 2q\,[\exp(2K) + 2 + \exp(-2K)]. \tag{19}$$

$$\text{Hence } \omega = \frac{dh'_2}{dh_2}\bigg|_{K=K_c} \tag{20}$$

The intersection of the curves (q vs K_c) for cells with $l=2$ and $l=4$ gives $q=0{\cdot}325$ and $K_c=0{\cdot}435$ (Stella *et al* 1979). This yields

$$\Delta_E = 2{\cdot}147$$

This result is not only above the lower bound of Δ set by the well-known inequality, but also in close agreement with Achiam's result ($\Delta_E=2{\cdot}131$), which is obtained using the conventional Niemeijer and van Leeuwen formalism. An exactly similar procedure has been used to study the dynamic problem of planar triangular lattice, giving a value $\Delta_E = 1{\cdot}918$. The agreement with Achiam's second-order result ($\Delta_E=2{\cdot}09$) is gratifying.

4. Conclusions

The first-order linear weight scheme has been successfully applied to a series of static RG problems by Stella *et al* (1979). In this communication we have demonstrated that the same technique is capable of providing reliable results for dynamic problems as well. We have also critically investigated two of the available methods for fixing the parameter q in linear weight factor scheme. The "intersection method" provides reasonable results with limited computational effort whereas "$1/\lambda_H$ method" can give increasingly better result with larger cell size.

References

Abe R 1968 *Prog. Theor. Phys.* **39** 947
Achiam Y 1978 *J. Phys.* **A11** L129
Achiam Y 1979a *Phys. Rev.* **B19** 376
Achiam Y 1979b *Phys. Lett.* **A72** 35
Achiam Y 1980 *J. Phys.* **A13** 1355
Bell T L and Wilson K G 1975 *Phys. Rev.* **B11** 3431
Bolton H C and Johnson C H J 1976 *Phys. Rev.* **B13** 3025
Brower R C, Kuttner F, Neuenberg M and Subbarao K 1977 *Phys. Rev. Lett,* **38** 1231
Droz M and Malaspinas A 1980 *J. Phys.* **C13** 4365
Glauber R J 1963 *J. Math. Phys.* **4** 294
Hsu S and Gunton J D 1977 *Phys. Rev.* **B15** 2688
Kadanoff L P 1966 *Physics* **2** 263
Kadanoff L P 1975 *Phys. Rev. Lett.* **34** 1005
Kadanoff L P and Houghton A 1975 *Phys. Rev.* **B11** 377
Kinzel W and Fisher K H 1978 *J. Phys.* **C11** 2115
Knops H J F 1977 *Physica* **A86** 448
Niemeijer Th and van Leeuwen J M J *Phase transitions and critical Phenomena* Vol. **6** (ed.) C Domb and M S Green (London: Academic Press, 1976) 425
Racz Z and Collins M F 1976 *Phys. Rev.* **B13** 3025
Stella A L, Dekeyser R, Indekeu J and Toigo F 1979 *Phys. Rev.* **B20** 3799
Stoll E, Binder K and Schneider T 1973 *Phys. Rev.* **B8** 3266
Subbarao K 1975 *Phys. Rev.* **B11** 1165
Suzuki M 1977 *Prog. Theor. Phys.* **58** 1142
Suzuki M, Sogo K, Ikuo M, Ikeda H, Chikama T and Takano H 1979 *Prog. Theor. Phys.* **61** 864
van Leeuwen J M J 1978 *Ann. Israel Phys. Soc.* **2** 174
van Saarloos W, van Leeuwen J M J and Pruisken A M M 1978 *Physica* **A92** 323
Wallace D J and Zia R K P 1978 *Rep. Prog. Phys.* **41** 1
Wilson K G 1971 *Phys. Rev.* **B4** 3174 and 3184
Yalabik M C and Gunton J D 1979 *Prog. Theor. Phys.* **62** 1573