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SIMPLE RENORMALIZATION-GROUP METHOD FOR CALCULATING THERMAL EQUATIONS OF STATES

by

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ABSTRACT

Renormalization-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 succesfully 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*.

Key-words: Equations of states; Renormalization-group; Potts model; Order parameter; Hierarchical lattice.

The renormalization-group (RG) techniques have been initially deviced for calculating critical exponents; the real-space versions enable also 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 searched. 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 states (as well as the specific heat, susceptibility, etc.) can be obtained. However these procedures tend to be rather heavy, operationally speaking. In the present paper, 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 of it. Although we will be referring to the H=0 case, the method trivially extends to the calculation of the complete equation of states (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-neighboring 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 models or similar ones). 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 magnetization 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 it is the case for the Heisenberg model, for instance), the z-projections have to be considered. Furthermore, we associate an elementary dimensionless magneton μ with each site of the lattice; we could in principle choose $\mu=1$, but we will rather leave it as a variable since it will change under renormalization. Following along the lines of Kadanoff for understanding 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 renormalized variables K' and μ' which will depend on K and μ. The analytic dependences 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 renormalization, 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 $\mu^{(o)}$ and perform n iterations in Eq. (2) we obtain

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

hence

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

By arbitrarily choosing $\mu^{(o)} = 1$ 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 renormalization; paramagnetic phase), K=∞ (stable; ferromagnetic phase), and $K=K_c$ (unstable; critical point). Two typical situations occur when using Eq. (5): (i) $K < K_c$, hence $K^{(\infty)}=0$, hence $M(K^{(\infty)})=0$, which yields (through Eq. (5)), M(K)=0, as desired; (ii) $K > K_c$, hence $K^{(\infty)} = \infty$, hence $M(K^{(\infty)}) = 1$ (conventional value for T=0), which yields (through Eq. (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 close the procedure we have to specify how the RG recursive relations for K(i.e. Eq. (6)) and for 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 Eqs. (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

$$\nu = \ell n\, B / \ell n [df(K)/dK]_{K_c} \tag{9}$$

and

$$\beta = \ell n [B^d/g(K_c)] / \ell n [df(K)/dK]_{K_c} \tag{10}$$

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

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

$$\mathrm{Tr}_{3,4,\ldots,N'_s} e^{-\mathcal{H}'_{12\ldots N'_s}+K'_o} = \mathrm{Tr}_{3,4,\ldots,N_s} e^{-\mathcal{H}_{12\ldots N_s}} \qquad (11)$$

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'_o is an additive constant to be determined. Eq. (11) completely determines f(K); we shall note $RG_{b',b}$ the associated RG. For the example illustrated in Fig. 1(b) and assuming Potts interactions ($\mathcal{H}/k_BT = -qK\sum_{i,j}\delta_{\sigma_i,\sigma_j}$; $\sigma_i=1,2,\ldots,q,\forall i$) we obtain[3] (through Eq. (11))

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

with the *thermal transmissivity*[3] t defined through $t \equiv (1-e^{-qK})/[1+(q-1)e^{-qK}]$ (analogously for t').

Let us now present the new procedure we have deviced to determine g(K). In order to break the symmetry (needed for establishing the equation for the order parameter) we *impose* the spin of say terminal 1 (of both small and large graphs) to be along the easy magnetization 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

$$\langle m\rangle_{G'} = \langle m\rangle_G \qquad (13)$$

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

$$\frac{2e^{qK'}+(q-2)}{e^{qK'}+(q-1)}\,\mu' = \frac{10e^{5qK}+10(q-2)e^{3qK}+8(3q-5)e^{2qK}}{e^{5qK}+2(q-1)e^{3qK}+4(q-1)e^{2qK}}$$

$$\frac{+2(8q^2-39q+45)e^{qK}+(2q^3-16q^2+44q-40)}{+(q-1)(5q-9)e^{qK}+(q-1)(q-2)^2}\,\mu \qquad (14)$$

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 Eqs. (12) and (14) together with formula (7) ($B^d=5$ in this case), as well as those corresponding to higher values of b are presented in Figs. 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's 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's 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 magnetization, proportionally to its coordination number. This hypothesis follows from our belief that the order parameter on a hierarchical lattice is not uniform (same on all sites)

as in Bravais lattices, but rather is directly related to the number of neighboring sites with which a given site is interacting. The well known *uniform* spontaneous magnetization of Bravais lattices should be a consequence of their translational invariance (lost in hierarchical lattices). The hypothesis we are discussing is equivalent to assume that the relevant magnetic field (parameter thermodynamically conjugated to the order parameter) *also* is proportional to the coordination number: this is precisely what several authors[2,5,10] have assumed within 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 fact 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 an *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 function of T and H would unambiguously clarify the situation. Such a treatment would also tell us in 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 $\ell n[\frac{5(17+12\sqrt{2})}{2(38+27\sqrt{2}}]/\ell n[\frac{18+13\sqrt{2}}{10+7\sqrt{2}}] \simeq 0.18$, 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

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

Also it is worthy to mention that, for all the self-dual hierarchical lattices considered in this paper, 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 summarize, 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 visualized), it is as simple operationally as a mean field approach, and it 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 of the magnetization is still unknown for all $q \neq 2$; further applications would be very welcome.

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CAPTION FOR FIGURES AND TABLES

Fig. 1 - Clusters used to construct $RG_{b',b}$ for the square lattice; ● and O respectively denote internal and terminal (root) sites. (a) RG_{12} transformation; (b) b=3 graph; (c) b=4 graph.

Fig. 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).

Fig. 3 - (a) critical exponent β, and (b) amplitude A as functions of q within successive RG approximations ($\beta_{sq.latt.}$ is taken from [9]); dashed lines are indicative and have been used when the calculation was available only for integer values of q.

Table 1 - Establishement of Eq. (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 q=2 particular case of Eq. (14).

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

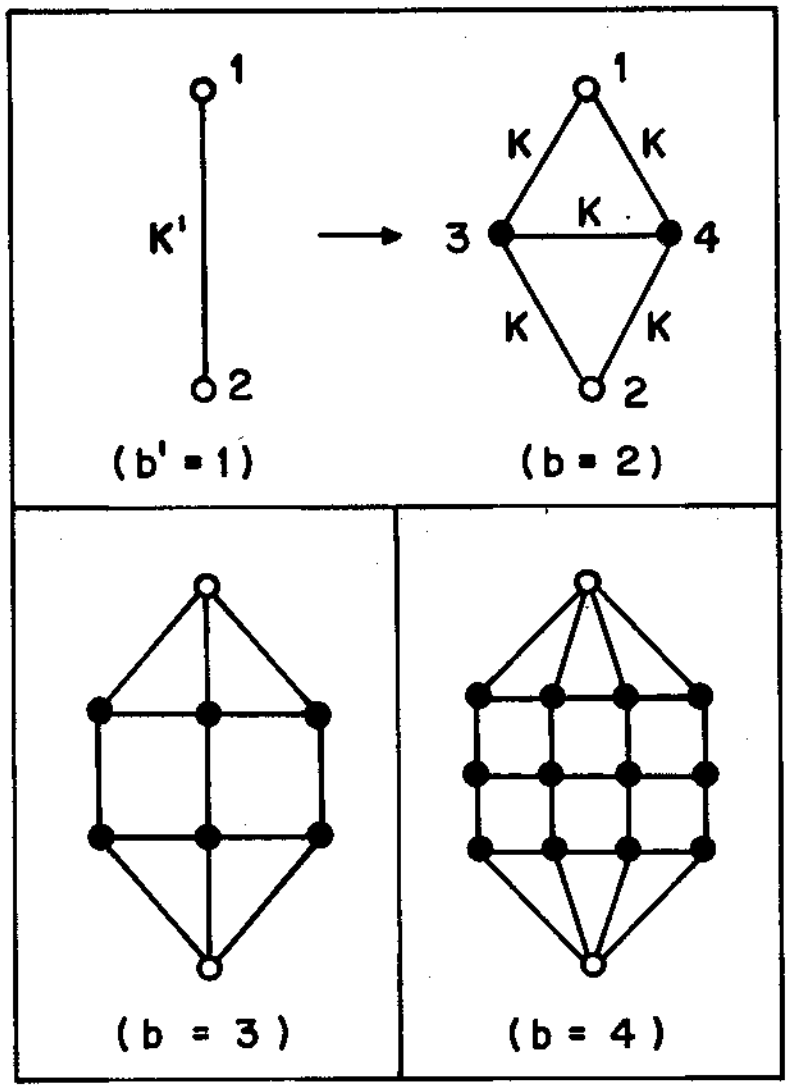


FIG.1

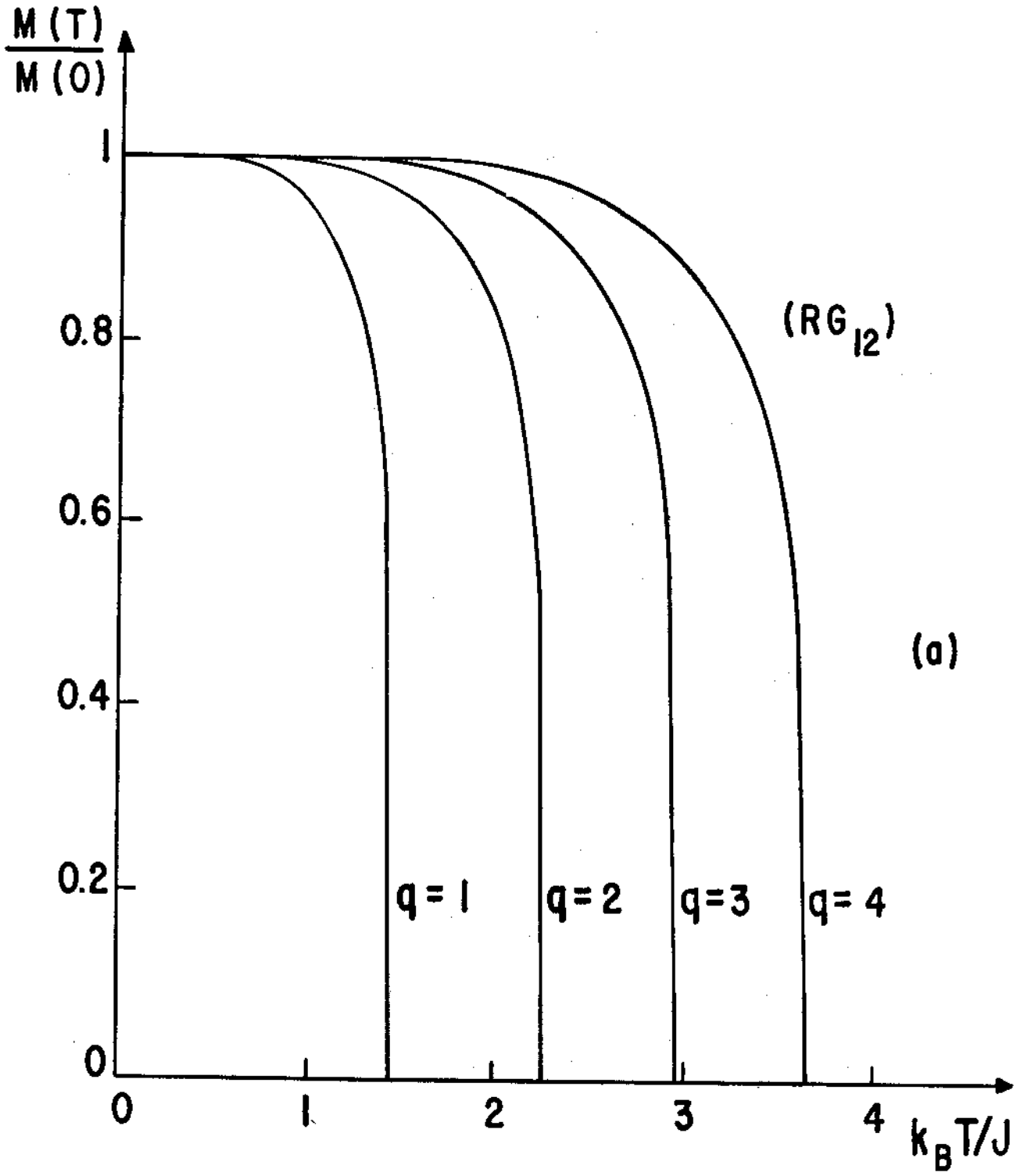


FIG. 2

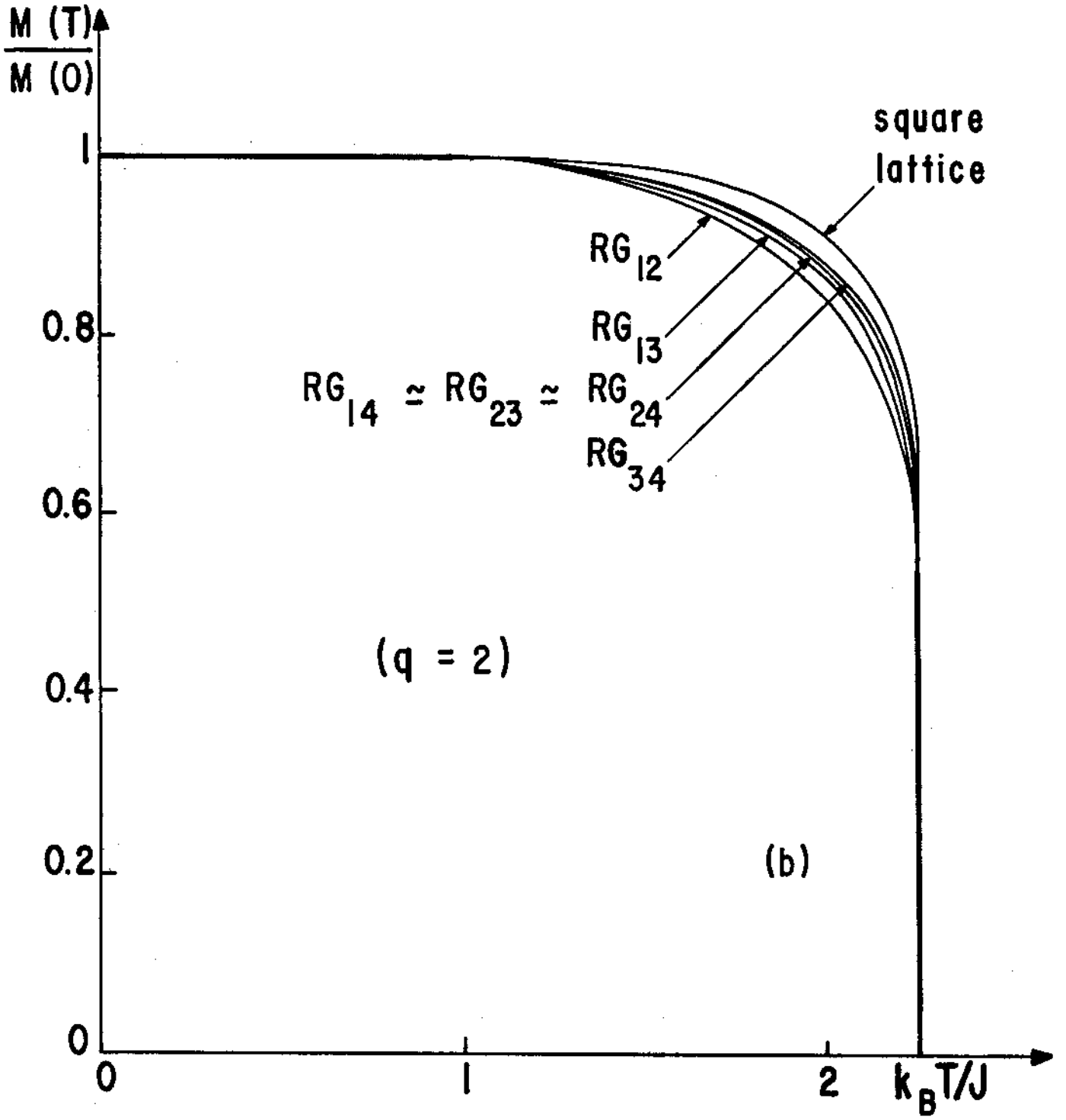

M (T)
M (0)
1
0.8
0.6
0.4
0.2
0
0
1
2
$k_B T/J$
square lattice
RG_{12}
RG_{13}
$RG_{14} \simeq RG_{23} \simeq RG_{24}$
RG_{34}
(q = 2)
(b)

FIG. 2

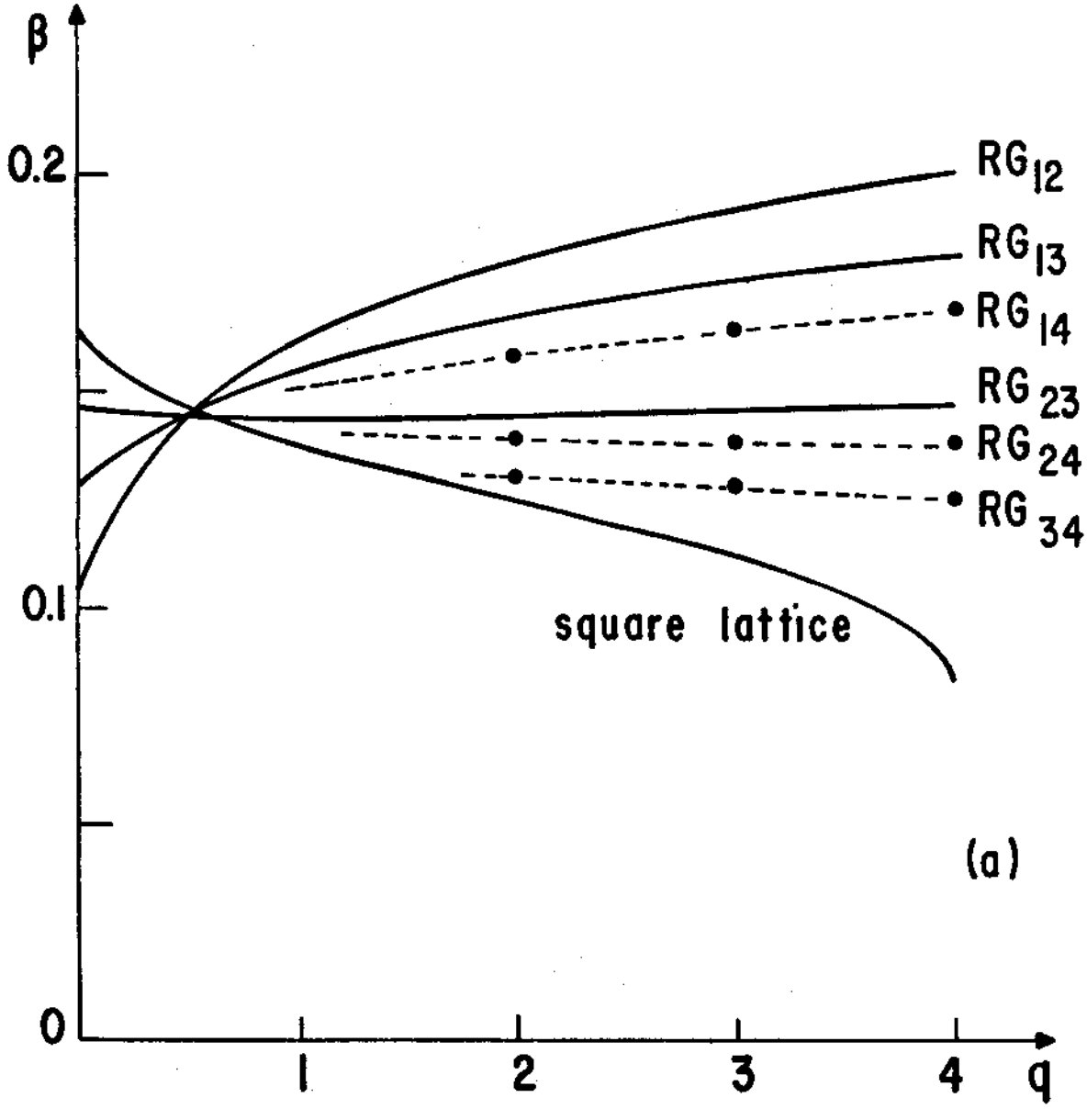


FIG. 3

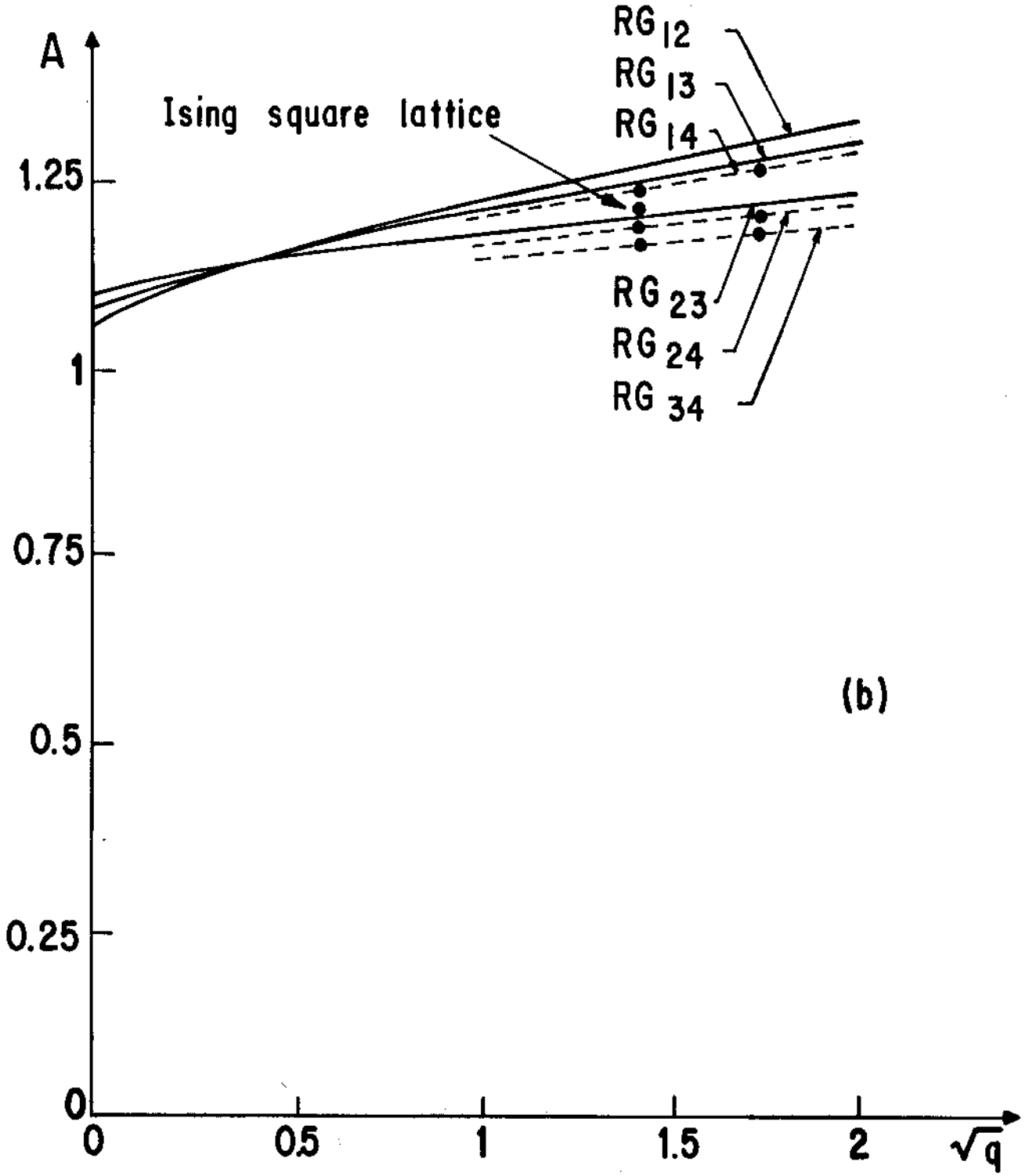
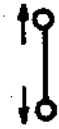

A
Ising square lattice
RG 12
RG 13
RG 14
RG 23
RG 24
RG 34
1.25
1
0.75
0.5
0.25
0
0
0.5
1
1.5
2
√q
(b)

FIG. 3

(a) G' configuration	weight	m
	$e^{K'}$	$2\mu'$
	$e^{-K'}$	0

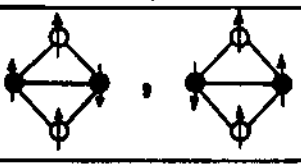
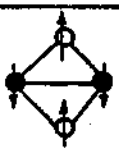
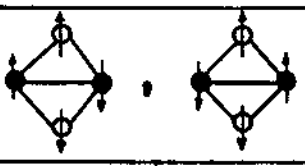
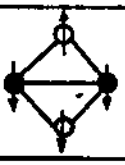
(b) G configuration	weight	m
	e^{5K}	10μ
	e^{K}	6μ
	e^{-K}	4μ
	e^{-3K}	-2μ
	e^{-K}	0
	e^{K}	-6μ

TABLE 1

		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	4/3 = 1.333...
	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	5/6 = 0.833...
	q=4	0.948	0.916	0.903	0.864	0.862	0.859	2/3 = 0.666...
β	q=1	0.161	0.154	—	0.144	—	—	5/36 = 0.139...
	q=2	0.180	0.166	0.159	0.145	0.139	0.131	1/8 = 0.125
	q=3	0.193	0.175	0.165	0.147	0.139	0.129	1/9 = 0.111...
	q=4	0.204	0.182	0.170	0.148	0.139	0.127	1/12 = 0.083...
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	—	—	?

TABLE 2

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