Anisotropic cubic lattice Potts ferromagnet: renormalisation group treatment

This article has been downloaded from IOPscience. Please scroll down to see the full text article.
1984 J. Phys. A: Math. Gen. 173209
(http://iopscience.iop.org/0305-4470/17/16/022)
View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 129.252.86.83
The article was downloaded on 31/05/2010 at 07:49

Please note that terms and conditions apply.

# Anisotropic cubic lattice Potts ferromagnet: renormalisation group treatment 

Luciano Rodrigues da Silva, $\dagger \ddagger$ Constantino Tsallis $\dagger$ and Georges Schwachheim $\dagger$<br>$\dagger$ Centro Brasileiro de Pesquisas Físicas/CNPq, Rua Xavier Sigaud 150, 22290 Rio de Janeiro, Brazil.<br>$\ddagger$ Departmento de Física Teórica e Experimental, Universidade Federal do Rio Grande do Norte, Campus Universitário, 59000 Natal-RN, Brazil

Received 14 December 1983, in final form 2 April 1984


#### Abstract

Within a real space renormalisation group framework, we discuss the criticality of the fully anisotropic (arbitrary $J_{x}, J_{y}$ and $J_{z}$ ) $q$-state Potts ferromagnet in the simple cubic lattice. Several previously known exact results for the $d=1$ and $d=2$ particular cases are recovered. Furthermore we obtain: (i) the $q$-dependence of the $d=3$ correlation length critical exponent $\nu_{3}$ (in particular, if $q \rightarrow 0, \nu_{3}(q) \sim \nu_{3}(0)+\nu_{3}^{\prime}(0) q$ where the present approximate values are $\nu_{3}(0) \simeq 1.105$ and $\nu_{3}^{\prime}(0) \simeq-0.66$; (ii) the $q$-dependence of the $d=2 \leftrightarrow d=3$ crossover critical exponent $\phi_{23}$ (in particular, $\phi_{23} \propto 1 / \sqrt{q}$ if $q \rightarrow 0$ ); (iii) through a convenient numerical extrapolation, a quite accurate proposal for the critical temperatures corresponding to arbitrary ratios $J_{y} / J_{x}$ and $J_{z} / J_{x}$ and values of $q$.


## 1. Introduction

During recent years much work has been devoted to the $q$-state Potts model, both because of its theoretical richness and its experimental utility (for an excellent review see Wu 1982). However most of this work has been focused on the two-dimensional ( $d=2$ ) case (see Wu 1982, and de Oliveira and Tsallis 1982 and references therein). Some effort has also been devoted to the isotropic $d=3$ ferromagnet (Blöte and Swendsen 1979), but we are not aware of any systematic study of the anisotropic $d=3$ case and its crossovers to lower dimensions. This is the purpose of the present work (restricted however to the discussion of the critical temperature $T_{\mathrm{c}}$ and correlation length and crossover critical exponents $\nu$ and $\phi$ ) which follows along the real space renormalisation group ( RG ) lines of de Oliveira and Tsallis (1982; which is herein recovered as a particular case). By noting $q_{c}(d)$ the limiting value of $q$ above which the phase transition is a first-order one (we recall that $\lim _{d \rightarrow 1+0} q_{\mathrm{c}}(d)=\infty, q_{\mathrm{c}}(2)=4$ and $q_{c}(3) \leqslant 3$; see Wu (1982) and de Magalhães and Tsallis (1981) and references therein), the present work is restricted to $q \leqslant q_{\mathrm{c}}(d)$. We present in $\S 2$ the model and the formalism, in $\S 3$ the RG results, and in $\S 4$ the extrapolation procedure which provides accurate values for $T_{c}$ corresponding to models with arbitrary anisotropy.

## 2. Model and formalism

Let us consider the $q$-state Potts ferromagnet whose Hamiltonian is given by
where $(i, j, k)$ runs over all sites of a simple cubic lattice and $\sigma_{t, j, k}=1,2, \ldots, q, \forall(i, j, k)$. We briefly recall the present status of knowledge of the critically ( $T_{\mathrm{c}}, v$ and $\phi$ ) of this
a

$b=?$
(b)

$b=i$
(c)

$b=2$
(d)
(e)
(f)

$b=1$

$b=1$

$\equiv i_{i}^{i}$
$D=1$

Figure 1. RG cells and their equivalent two-rooted graphs; the arrows indicate the entrance and exit points of the cells: $\bigcirc$ and respectively denote terminal and internal nodes of the graphs; $t_{x}, t_{y}$ and $t_{z}$ are the transmissivities along the three crystal-axes. $(a),(b)$ and (c) have been used (de Oliveira and Tsallis 1982) for the $d=2$ case (the cluster (c) is renormalised into the cluster $(a)$ ). ( $d$ )-( $h$ ) correspond to the $d=3$ case (the cluster ( $g$ ), or equivalently the graph $(h)$, is renormalised into the cluster $(d)$ ). $(g)$ is the $d=3$ extension of the central cluster of $(c) ;(h)$ is the $d=3$ extension of the right graph of (c); because of its complexity, we have omitted the indication of the $d=3$ extension of the left cluster of $(c)$.


Figure 1. (contd.).
model: (i) for $d=1$ (i.e., $J_{y}=J_{z}=0$ ) the critical temperature $T_{c}$ vanishes, and the correlation length critical exponent satisfies $\nu_{1}=1, \forall q$; (ii) for $d=2$ (i.e., $J_{z}=0$ and $J_{y}>0$ ) $T_{c}$ is exactly known (Baxter et al 1978, Burkhardt and Southern 1978 and Hintermann et al 1978); (iii) the $d=1$ to $d=2$ and $d=1$ to $d=3$ crossover critical exponents (respectively $\phi_{12}$ and $\phi_{13}$ ) are commonly believed to satisfy (Redner and Stanley 1979, de Oliveira and Tsallis 1982 and references therein) $\phi_{12}=\phi_{13}=1, \forall q$; (iv) for the isotropic $d=3$ case (i.e., $J_{x}=J_{y}=J_{z}$ ), $T_{c}$ is given by
$k_{\mathrm{B}} T_{\mathrm{c}} / q J_{x}= \begin{cases}3.52 \pm 0.05 & \text { for } q=1 \text { (from Gaunt and Ruskin 1978) } \\ 2.2556 \pm 0.0002 & \text { for } q=2 \text { (from Zinn-Justin 1979) } \\ 1.8169 & \text { for } q=3 \text { (from Jensen and Mouritsen 1979) }\end{cases}$
where the $q=1$ value has been obtained from $p_{c}=0.247$ @ 0.003 by using the Kasteleyn and Fortuin (1969) isomorphism ( $p=1-\mathrm{e}^{-J_{x} / k_{\mathrm{B}} T}$ ) with bond percolation, and where we recall that the $q=3$ case might be slightly first order; the corresponding critical exponent is given by
$\nu_{3} \simeq \begin{cases}0.88 & \text { for } q=1 \text { (Heerman and Stauffer 1981) } \\ 0.630 \pm 0.0015 & \text { for } q=2(\text { Le Guillou and Zinn-Justin 1980) } ;\end{cases}$
(v) For the $d=2$ to $d=3$ crossover exponent $\phi_{23}$ the following results are available $\phi_{23} \simeq\left\{\begin{array}{l}1.75 \\ 7 / 4 \text { (exact) }\end{array}\right.$ for $q=1$ (Redner and Stanley 1979)
for $q=2$ (Liu and Stanley 1972, 1973, Citteur and Kasteleyn 1972, 1973).

Before presenting our RG formalism, let us define a few convenient variables (Tsallis and Levy 1981, Tsallis 1981):

$$
\begin{equation*}
t_{\alpha} \equiv \frac{1-\exp \left(-q J_{\alpha} / k_{\mathrm{B}} T\right)}{1+(q-1) \exp \left(-q J_{\alpha} / k_{\mathrm{B}} T\right)} \in[0,1] \quad(\alpha=x, y, z) \tag{5a}
\end{equation*}
$$

(referred to as thermal transmissivity) and

$$
\begin{equation*}
s_{\alpha}^{(d)} \equiv s^{(d)}\left(t_{\alpha}\right) \equiv \frac{\ln \left[1+(q-1) h(d) t_{\alpha}\right]}{\ln [1+(q-1) h(d)]} \in[0,1] \quad(\alpha=x, y, z) \tag{5b}
\end{equation*}
$$

where (Tsallis and de Magalhães 1981, de Magalhães and Tsallis 1981) the pure number $h(d)$ sensibly depends on dimensionality $d$ and very slightly on the particular $d$ dimensional lattice $(h(2)=1$ for square lattice, and $h(3)=0.377 \pm 0.044$ for simple cubic lattice).

If we have a series (or parallel) array of two bonds with transmissivities $t_{1}$ and $t_{2}$, the overall transmissivities (respectively $t_{\mathrm{s}}$ and $t_{\mathrm{p}}$ ) are given by $t_{\mathrm{s}}=t_{1} t_{2}$ (series) and $t_{\mathrm{p}}^{\mathrm{D}}=t_{1}^{D} t_{2}^{\mathrm{D}}$ (parallel) where

$$
\begin{equation*}
t_{\mathrm{i}}^{\mathrm{D}} \equiv \frac{1-t_{\mathrm{i}}}{1+(q-1) t_{\mathrm{i}}} \quad(i=1,2, \mathrm{p}) \tag{6}
\end{equation*}
$$

(D stands for dual). We can also verify that $h=1$ (squared lattice) implies $s^{(2)}\left(t^{\mathrm{D}}\right)=$ $1-s^{(2)}(t)$.

We can now introduce our rg framework. Following along the lines of the de Oliveira and Tsallis (1982) treatment of the square lattice case, we establish the rg recursive relations by renormalising the $b=2$ cell indicated in figures $1(g),(h)$ into the $b=1$ cell in figure $1(d)$ ( $b$ denotes the size of the cell, and coincides with the linear scaling factor). The recurrence is based upon the preservation of the partition function, and can be economically established by using the break-collapse method (Tsallis and Levy 1981). We obtain

$$
\begin{equation*}
t_{x}^{\prime}=R_{b}\left(t_{x}, t_{y}, t_{z} ; q\right) \tag{7}
\end{equation*}
$$

where $R_{b}\left(t_{x}, t_{y}, t_{z} ; q\right)=R_{b}\left(t_{x}, t_{z}, t_{y} ; q\right)$ is a ratio of polynomials (in the $t$ 's) too lengthy to be reproduced herein (the numerator and denominator contain more than 1600 terms each). The sum of the coefficients of the numerator coincides with that corresponding to the denominator and is given (Tsallis and Levy 1981, Essam 1982) by $q^{\kappa}$ where $\kappa \equiv$ cyclomatic number $=[($ number of bonds $)-($ number of sites $)+1]$ (for the two-terminal graph of figure $1(h)$ it is $\kappa=20)$. It is worth noting that $R_{b}\left(t_{x}, t_{y}, 0 ; q\right)$ recovers equation (12) of de Oliveira and Tsallis (1982).

The rest of the rG recursive relations are given by

$$
\begin{align*}
& t_{y}^{\prime}=R_{b}\left(t_{y}, t_{z}, t_{x} ; q\right)  \tag{8}\\
& t_{z}^{\prime}=R_{b}\left(t_{z}, t_{x}, t_{y} ; q\right) \tag{9}
\end{align*}
$$

where the equivalence of the $x, y$ and $z$ axes has been taken into account. By studying, for fixed $q$, the RG flow (in the ( $t_{x}, t_{y}, t_{z}$ )-space) determined by equations (7)-(9) we can obtain the fixed points, the para-ferromagnetic separatrix, as well as the relevant Jacobians $\partial\left(t_{x}^{\prime}, t_{y}^{\prime}, t_{z}^{\prime}\right) / \partial\left(t_{x}, t_{y}, t_{z}\right)$, which in turn determine the critical exponents $\nu$ and $\phi$.

## 3. Results

Our results are illustrated in figure 2. Equations (7)-(9) provide the following fixed points: (i) $\left(s_{x}^{(2)}, s_{y}^{(2)}, s_{z}^{(2)}\right)=(0,0,0)$ and $(1,1,1)$ are fully stable, and correspond respectively to the para- and ferromagnetic phases; (ii) $(1,1,0),(1,0,1)$ and $(0,1,1)$ are


Figure 2. Para( P )-ferro( F ) magnetic critical surface in the $\left(s_{x}^{(2)}, s_{y}^{(2)}, s_{z}^{(2)}\right)$ space. The arrows indicate the RG flow. The main fixed points are indicated: $\triangle$ (ferromagnetic) and $\boldsymbol{\Delta}$ (paramagnetic) attract all the points respectively above and below the critical surface; $\square, \bigcirc$ and - respectively are the $d=1, d=2$ and $d=3$ critical fixed points.


Figure 3. $q$-dependence of the RG critical point corresponding to the isotropic $d=3$ model (notice the ordinate scale). The dots are series results: $q=1$ (Gaunt and Ruskin 1978), $q=2$ (Zinn-Justin 1979) and $q=3$ (Jensen and Mouritsen 1979).
semi-stable ones, and belong to the ferromagnetic region; (iii) ( $1,0,0$ ), ( $0,1,0$ ) and $(0,0,1)$ are fully unstable ones, and correspond to the $d=1$ case; (iv) $\left(\frac{1}{2}, \frac{1}{2}, 0\right),\left(\frac{1}{2}, 0, \frac{1}{2}\right)$ and ( $0, \frac{1}{2}, \frac{1}{2}$ ) are semi-stable ones, and correspond to the $d=2$ isotropic case; (v) ( $s_{\mathrm{c}}^{(3)}, \mathrm{s}_{\mathrm{c}}^{(3)}, s_{\mathrm{c}}^{(3)}$ ) is a semi-stable one, and corresponds to the $d=3$ isotropic case ( $s_{\mathrm{c}}^{(3)}$ softly depends on $q$; see figure 3 ).

The RG critical surface contains the line $s_{x}^{(2)}+s_{y}^{(2)}=1$ at $s_{z}^{(2)}=0$ (and the equivalent ones), thus reproducing the exact $d=2$ result. The performance at the isotropic $d=3$ fixed point is not comparable to the $d=2$ case, as the RG provides, for $q=1, t_{\mathrm{c}} \simeq 0.2260$ (instead of 0.247 , corresponding to equation $2(a)$ ), for $q=2, t_{c} \simeq 0.1949$ (instead of 0.21811 , corresponding to equation $2(b)$ ), and, for $q=3, t_{c} \simeq 0.1750$ (instead of 0.1966 , corresonding to equation $2(c)$ ). The results obtained for $T_{c}$ for arbitrary anisotropy ratios $J_{y} / J_{x}$ and $J_{z} / J_{x}$ are indicated in table 1.

The Jacobian at the $d=1$ fixed points is fully degenerate and its unique eigenvalue $\lambda^{(1)}$ equals 3. It can be shown that $\lambda^{(1)}=2 b-1$ for arbitrary values of $b$, therefore $\nu_{1}=\lim _{b \rightarrow \infty} \ln b / \ln (2 b-1)=1$, thus recovering the exact result. The degeneracy of this Jacobian implies that both $d=1 \leftrightarrow d=2$ and $d=1 \leftrightarrow d=3$ crossover exponents $\phi_{12}$ and $\phi_{13}$ equal unity, thus recovering the exact answer.

At the $d=2$ fixed points the Jacobians are as follows. Let us analyse for instance the $\left(s_{x}^{(2)}, s_{y}^{(2)}, s_{z}^{(2)}\right)=\left(\frac{1}{2}, \frac{1}{2}, 0\right)$ fixed point (the others are analogous); its Jacobian has the following form

$$
\left(\begin{array}{ccc}
a(q) & b(q) & c(q)  \tag{10}\\
b(q) & a(q) & c(q) \\
0 & 0 & d(q)
\end{array}\right)
$$

Table 1. Critical points ( $k_{\mathrm{B}} T_{\mathrm{c}} / q J_{x}$ ) for the anisotropic $d=3$ model: RG (top) and extrapolated (bottom) values. + indicates exact results (see for example $W u$ 1982) for the isotropic $d=2$ case; $\ddagger, \S$ and $\|$ are series results (see the text and figure 3 ) for the isotropic $d=3$ case.

| (a) | $q=1$ |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | 0.1 | 0,2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 |
| 0 | 0 | 0.5548 | 0.7112 | 0.8349 | 0.9421 | 1.0390 | 1.1287 | 1.2129 | 1.2928 | 1.3692 | 1.4427 |
|  | 0 | 0.5548 | 0.7112 | 0.8349 | 0.9421 | 1.0390 | 1.1287 | 1.2129 | 1.2928 | 1.3692 | $1.4427 \dagger$ |
| 0.1 | - | 1.0592 | 1.2643 | 1.4255 | 1.5646 | 1.6896 | 1.8047 | 1.9125 | 2.0145 | 2.1117 | 2.2049 |
|  | - | 1.0229 | 1.2104 | 1.3612 | 1.4934 | 1.6139 | 1.7260 | 1.8317 | 1.9322 | 2.0284 | 2.1210 |
| 0.2 | - | - | 1.4912 | 1.6689 | 1.8216 | 1.9584 | 2.0840 | 2.2013 | 2.3121 | 2.4174 | 2.5183 |
|  | - | - | 1.4061 | 1.5636 | 1.7024 | 1.8293 | 1.9479 | 2.0601 | 2.1670 | 2.2696 | 2.3686 |
| 0.3 | - | - | - | 1.8592 | 2.0223 | 2.1682 | 2.3019 | 2.4266 | 2.5440 | 2.6557 | 2.7625 |
|  | - | - | - | 1.7259 | 1.8690 | 2.0002 | 2.1231 | 2.2394 | 2.3506 | 2.4575 | 2.5607 |
| 0.4 | - | - | - | - | 2.1942 | 2.3476 | 2.4882 | 2.6190 | 2.7421 | 2.8591 | 2.9708 |
|  | - | - | - | - | 2.0158 | 2.1504 | 2.2766 | 2.3963 | 2.5107 | 2.6209 | 2.7273 |
| 0.5 | - | - | - | - | - | 2.5078 | 2.6543 | 2.7905 | 2.9186 | 3.0402 | 3.1563 |
|  | - | - | - | - | - | 2.2882 | 2.4172 | 2.5397 | 2.6569 | 2.7698 | 2.8789 |
| 0.6 | - | - | - | - | - | - | 2.8061 | 2.9472 | 3.0798 | 3.2055 | 3.3256 |
|  | - | - | - | - | - | - | 2.5489 | 2.6739 | 2.7935 | 2.9088 | 3.0203 |
| 0.7 | - | - | - | - | - | - | - | 3.0927 | 3.2294 | 3.3590 | 3.4826 |
|  | - | - | - | - | - | - | - | 2.8012 | 2.9232 | 3.0406 | 3.1543 |
| 0.8 | - | - | - | - | - | - | - | - | 3.3699 | 3.5031 | 3.6300 |
|  | - | - | - | - | - | - | - | - | 3.0472 | 3.1667 | 3.2824 |
| 0.9 | - | - | - | - | - | - | - | - | - | 3.6395 | 3.7696 |
|  | - | - | - | - | - | - | - | - | - | 3.2882 | 3.4057 |
| 1.0 | - | - | - | - | - | - | - | - | - | - | 3.9026 |
|  | - | - | - | - | - | - | - | - | - | - | $3.5250 \ddagger$ |
| (b) | $q=2$ |  |  |  |  |  |  |  |  |  |  |



Table 1-continued


The eigenvalues $\lambda_{1}^{(2)}=a(q)+b(q)$ and $\lambda_{2}^{(2)}=a(q)-b(q)$ recover the results of de Oliveira and Tsallis (1982) and $\lambda_{3}^{(2)}=d(q)$ (too lengthy to be reproduced herein; it monotonically decreases from about 8.1 to about 3.3 when $q$ increases from 0 to 3 ). The respective eigenvectors are $(1,1,0)(1,-1,0)$ and $\left(1,1,\left(\lambda_{3}^{(2)}(q)-\lambda_{1}^{(2)}(q)\right) / c(q)\right)$. We verify that $\lambda_{1}^{(2)}(q) \geqslant 1 \geqslant \lambda_{2}^{(2)}(q)>0, V q \geqslant 0$, and that $\lambda_{3}^{(2)}(q) \geqslant \lambda_{1}^{(2)}(q)\left(\lambda_{3}^{(2)}(q)<\right.$ $\left.\lambda_{1}^{(2)}(q)\right)$ if $q \leqslant q^{*}\left(q>q^{*}\right)$ where $q^{*} \simeq 5$. The coefficient $c(q)$ monotonically increases from roughly zero to roughly 10 when $q$ varies from zero to infinity; consistently the eigenvector associated with $\lambda_{3}^{(2)}(q)$ is roughly along the $(1,1,1)$ direction for $q$ varying let us say between 1 and 3. Within the present $b=2 \mathrm{RG}$ approximation the critical exponents are given by $\nu_{2}=\ln 2 / \ln \lambda_{1}^{(2)}$ and $\phi_{23}=\ln \lambda_{3}^{(2)} / \ln \lambda_{1}^{(2)}$ : see figures 4 and 5 and table 2.


Figure 4. $q$-dependence of the $d=2$ correlation length critical exponent $\nu_{2}: \operatorname{RG}(-)$ and exact ( $-\cdots$; den Nijs 1979).


Figure 5. $q$-dependence of the $d=2 \leftrightarrow d=3$ RG crossover exponent $\phi_{23}$. The dots are series ( Redner and Stanley 1979) and exact ( $O$; Liu and Stanley 1979, 1973, Citteur and Kasteleyn 1972, 1973).

The Jacobian at the $d=3$ fixed point $\left(t_{x}=t_{y}=t_{z}=t_{\mathrm{c}}^{(3)}(q)\right)$ is as follows:

$$
\left(\begin{array}{lll}
e(q) & f(q) & f(q)  \tag{11}\\
f(q) & e(q) & f(q) \\
f(q) & f(q) & e(q)
\end{array}\right)
$$

The eigenvalues are

$$
\begin{equation*}
\lambda_{1}^{(3)}=e(q)+2 f(q) \tag{12}
\end{equation*}
$$

and

$$
\begin{equation*}
\lambda_{2}^{(3)}=\lambda_{3}^{(3)}=e(q)-f(q) \tag{13}
\end{equation*}
$$

and the eigenvectors are respectively $(1,1,1)$ and any vector perpendicular to $(1,1,1)$. We verify $\lambda_{1}^{(3)}(q) \geqslant 1 \geqslant \lambda_{2}^{(3)}(q)>0, \forall q \geqslant 0$. The corresponding approximated critical exponent is given by $\nu_{3}=\ln 2 / \ln \lambda_{1}^{(3)}$ (see figure 6 and table 2 ); $\lambda_{2}^{(3)}(q)$ monotonically increases from roughly zero to 1 when $q$ varies from zero to infinity.

Table 2. Present RG and exact (or series) results for the critical point $t_{\mathrm{c}}$ and exponents $\nu$ and $\phi$ for the isotropic $d$-dimensional models. ${ }^{(a)} \mathrm{Wu}$ (1982) and references therein; ${ }^{\text {(b) }}$ den Nijs (1979); ${ }^{(c)}$ Redner and Stanley (1979); ${ }^{(d)}$ Liu and Stanley (1972, 1973), Citteur and Kasteleyn (1972, 1973); ${ }^{(e)}$ Gaunt and Ruskin (1978); ${ }^{(f)}$ Zinn-Justin (1979); ${ }^{(\mathrm{g})}$ Jensen and Mouritsen (1979); ${ }^{(h)}$ Heerman and Stauffer (1981); ${ }^{(1)}$ Le Guillou and Zinn-Justin (1980).

|  |  |  | $q \rightarrow 0$ | $q=1$ | $q=2$ | $q=3$ | $q=4$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $d=1$ |  | $\mathrm{RG}(\forall b)$ exact | $\begin{aligned} & 1 \\ & 1^{a} \end{aligned}$ | $\frac{1}{1^{\mathrm{a}}}$ | $\begin{aligned} & 1 \\ & 1^{a} \end{aligned}$ | $\begin{aligned} & 1 \\ & 1^{\mathrm{a}} \end{aligned}$ | $\begin{aligned} & 1 \\ & 1^{a} \end{aligned}$ |
|  | $\nu_{1}$ | RG( $\quad$ ( $b$ ) | $\frac{\ln b}{\ln (2 b-1)}$ | $\frac{\ln b}{\ln (2 b-1)}$ | $\frac{\ln b}{\ln (2 b-1)}$ | $\frac{\ln b}{\ln (2 b-1)}$ | $\frac{\ln b}{\ln (2 b-1)}$ |
|  |  | exact | $1^{\text {a }}$ | $1^{\text {a }}$ | $1^{\text {a }}$ | $1^{\text {a }}$ | $1^{\text {a }}$ |
|  | $\phi_{1 d}$ | $\mathrm{RG}(\forall b)$ exact | $\begin{aligned} & 1 \\ & 1^{a} \end{aligned}$ | $\begin{aligned} & 1 \\ & 1^{a} \end{aligned}$ | $\begin{aligned} & 1 \\ & 1^{\mathrm{a}} \end{aligned}$ | $\begin{aligned} & 1 \\ & 1^{a} \end{aligned}$ | $\begin{aligned} & 1 \\ & 1^{\mathrm{a}} \end{aligned}$ |
| $d=2$ | $t_{\text {c }}^{(2)}$ | $\operatorname{RG}(\forall b)$ <br> exact | $\begin{aligned} & \sim 1-\sqrt{q} \\ & \sim 1-\sqrt{q^{a}} \end{aligned}$ | $\begin{aligned} & 1 / 2 \\ & 1 / 2^{\mathrm{a}} \end{aligned}$ | $\begin{aligned} & \sqrt{2}-1 \\ & \sqrt{2}-1^{\mathrm{a}} \end{aligned}$ | $\begin{aligned} & 1 /(\sqrt{3}+1) \\ & 1 /(\sqrt{3}+1)^{a} \end{aligned}$ | $\begin{aligned} & 1 / 3 \\ & 1 / 3^{a} \end{aligned}$ |
|  | $\nu_{2}$ | $\operatorname{RG}(b=2)$ exact | $\begin{aligned} & \frac{45 \ln 2}{52 \sqrt{q}} \simeq \frac{0.600}{\sqrt{q}} \\ & \frac{\pi}{3 \sqrt{q}} \simeq \frac{1.047^{\mathrm{b}}}{\sqrt{q}} \end{aligned}$ | 1.042 $\frac{4}{3} \simeq 1.333^{\mathrm{b}}$ | 0.864 $1^{\text {b }}$ | 0.785 $\frac{5}{6} \simeq 0.833^{\text {b }}$ | 0.738 $\frac{2}{3} \simeq 0.667^{\text {b }}$ |
|  | $\phi_{23}$ | $\mathrm{RG}(b=2)$ <br> exact or series | $=\frac{2}{\sqrt{q}}$ | 2.258 $1.75{ }^{\text {c }}$ | 1.637 $1.75{ }^{\text {d }}$ | 1.346 - | 1.163 - |
| d=3 | $t_{\mathrm{c}}^{(3)}$ | $\mathbf{R G}(b=2)$ <br> series | $\begin{aligned} & \approx 0.294-0.11 q \\ & - \end{aligned}$ | $\begin{aligned} & 0.2260 \\ & 0.247^{e} \end{aligned}$ | $\begin{aligned} & 0.1949 \\ & 0.21811^{f} \end{aligned}$ | $\begin{aligned} & 0.1750 \\ & 0.1966^{8} \end{aligned}$ | - |
|  | $\nu_{3}$ | $\operatorname{RG}(b=2)$ <br> series | $\approx 1.105-0.66 q$ | $\begin{aligned} & 0.756 \\ & 0.88^{\mathrm{h}} \end{aligned}$ | $\begin{aligned} & 0.657 \\ & 0.630^{1} \end{aligned}$ | 0.606 | $-$ |



Figure 6. $q$-dependence of the $d=3$ correlation length critical exponent $\nu_{3}$ : RG ( - ) and series ( - Heerman and Stauffer 1981 for $q=1$; Le Guillou and Zinn-Justin 1980 for $q=2$ ).

## 4. Extrapolation for the critical point

In this section we describe an ad hoc extrapolation procedure for the critical temperature $T_{c}$ for an arbitrary value of $q$. We take advantage from the fact that the anisotropic $d=2$ RG result is the exact one for all $q$, and that the isotropic $d=3$ RG result is not too bad (at least for $q=1,2,3$, where comparison with other results is possible). It essentially consists in 'pushing' the centre ( $s_{x}^{(2)}=s_{y}^{(2)}=s_{z}^{(2)}=s_{\mathrm{c}}^{(2)}$ ) of the RG critical surface in the ( $s_{x}^{(2)}, s_{y}^{(2)}, s_{z}^{(2)}$ )-space (see figure 2 ), until it coincides (by imposition) with the best value (noted $s_{0}$; usually from series) available in the literature for that particular value of $q$; the effects of this 'pushing' monotonically and softly decrease while going from the centre of the critical surface to its periphery, eventually vanishing on the anisotropic $d=2$ limiting case (i.e. $s_{x}^{(2)}=0$ or $s_{y}^{(2)}=0$ or $s_{z}^{(2)}=0$ ) where, as said before, the exact result is reproduced by the RG. As no confusion can occur in the present section, we use $s_{\alpha} \equiv s_{\alpha}^{(2)}(\alpha=x, y, z)$, where $s_{\alpha}^{(2)}$ is given by equation ( 5 b ) with $h(2)=1$. Summarising, the input, for a given $q$, of the extrapolation procedure is the RG critical surface and the 'exact' value for the isotropic $d=3$ critical point.


Figure 7. Geometric constructions related to the extrapolation procedure (see §4): (a) the $\left(s_{x}^{(2)}, s_{y}^{(2)}, s_{z}^{(2)}\right)$ space; $(b)$ the triangle determined by the points $\mathrm{O}, \mathrm{P}$ and T of $(a)$.

We consider, in the ( $s_{x}, s_{y}, s_{z}$ ) -space (see figure $7(a)$ ), the point P (on the RG critical surface and not belonging to the trisectrix $s_{x}=s_{y}=s_{z}$ ) to be extrapolated; its coordinates are noted ( $s_{x}^{\mathrm{P}}, s_{y}^{\mathrm{P}}, s_{z}^{\mathrm{P}}$ ) and conventionally satisfy $1 \geqslant s_{x}^{\mathrm{P}} \geqslant s_{y}^{\mathrm{P}} \geqslant s_{z}^{\mathrm{P}} \geqslant 0$ (every other region is directly associated with this one through trivial symmetry transformations). This point and the trisectrix determine a unique plane whose equation is given by

$$
\begin{equation*}
\frac{s_{y}-s_{z}}{s_{x}-s_{z}}=\frac{s_{y}^{\mathrm{P}}-s_{z}^{\mathrm{P}}}{s_{x}^{\mathrm{P}}-s_{z}^{\mathrm{P}}} \equiv g \in[0,1] . \tag{14}
\end{equation*}
$$

This plane and the plane

$$
\begin{equation*}
s_{x}+s_{y}+s_{z}=1 \tag{15}
\end{equation*}
$$

(which contains all three exact $d=2$ critical lines, e.g., $s_{x}+s_{y}=1$ for $s_{z}=0$ ) determine a unique straight line. This line cuts the $s_{z}=0$ plane at the point $\left(s_{x}^{(z)}, s_{y}^{(z)}, 0\right)$ and the $s_{x}=0$ plane at the point $\left(0, s_{y}^{(x)}, s_{z}^{(x)}\right)$, where

$$
\begin{array}{ll}
s_{x}^{(z)}=1 /(1+g), & s_{y}^{(x)}=g /(1+g) . \\
s_{y}^{(x)}=(1-g) /(2-g), & s_{z}^{(x)}=1 /(2-g) .
\end{array}
$$

This line also cuts the trisectrix at the point $T$ with coordinates $\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$. If we consider now the triangle determined by the points $(0,0,0),\left(s_{x}^{(z)}, s_{y}^{(z)}, 0\right)$ and $\left(0, s_{y}^{(x)}, s_{z}^{(x)}\right)$ (see figure $7(b)$ ), we immediately obtain

$$
\begin{align*}
& r_{1}=+\left[\left(\frac{1}{3}\right)^{2}+\left(\frac{1}{3}-s_{y}^{(x)}\right)^{2}+\left(\frac{1}{3}-s_{z}^{(x)}\right)^{2}\right]^{1 / 2}  \tag{17a}\\
& r_{2}=+\left[\left(\frac{1}{3}-s_{x}^{(z)}\right)^{2}+\left(\frac{1}{3}-s_{y}^{(2)}\right)^{2}+\left(\frac{1}{3}\right)^{2}\right]^{1 / 2} \tag{17b}
\end{align*}
$$

where $r_{1}$ and $r_{2}$ are defined in figure $7(b)$ ( $r_{1}$ and $r_{2}$ respectively correspond to ( $s_{x}^{(z)}, s_{y}^{(z)}, 0$ ) and $\left(0, s_{y}^{(x)}, s_{z}^{(x)}\right)$ ). The angle $\theta$ defined in figure $7(b)$ is determined by

$$
\begin{equation*}
\cos \theta=\frac{s_{x}^{\mathrm{P}}+s_{y}^{\mathrm{P}}+s_{z}^{\mathrm{P}}}{\sqrt{3} s^{\mathrm{P}}} \tag{18}
\end{equation*}
$$

where

$$
\begin{equation*}
s^{\mathrm{P}} \equiv+\left[\left(s_{x}^{\mathrm{P}}\right)^{2}+\left(s_{y}^{\mathrm{P}}\right)^{2}+\left(s_{z}^{\mathrm{P}}\right)^{2}\right]^{1 / 2} \tag{19}
\end{equation*}
$$

The quantity $r^{\mathrm{P}}$ defined in figure $7(b)$ is given by

$$
\begin{equation*}
r^{\mathrm{p}}=-(\tan \theta) / \sqrt{3} \in\left[-r_{2}, r_{1}\right] \tag{20}
\end{equation*}
$$

Obviously $s^{\mathrm{P}} \leqslant\left[\frac{1}{3}+\left(r^{\mathrm{P}}\right)^{2}\right]^{1 / 2}$.
The value $s^{P}$ is going to be extrapolated into $s^{e x}$ through the relation

$$
\begin{equation*}
s^{\mathrm{ex}}=s^{\mathrm{P}}\left[1+F\left(r^{\mathrm{P}}\right)\right] \tag{21}
\end{equation*}
$$

where the extrapolating function $F(r)$ is assumed to satisfy the following conditions:

$$
\begin{equation*}
F\left(r_{1}\right)=F\left(-r_{2}\right)=0 \tag{i}
\end{equation*}
$$

$$
\begin{equation*}
F(0)=\sqrt{3} s_{0} / s^{\mathrm{p}}-1 \tag{22a}
\end{equation*}
$$

(iii) $\quad F(r)$ maximal at $r=0$.

The simplest polynomial which satisfies these conditions is

$$
\begin{equation*}
F(r)=F(0)\left(1-A r^{2}-B r^{3}\right) \tag{23}
\end{equation*}
$$

where

$$
\begin{equation*}
A \equiv\left(r_{2}^{3}+r_{1}^{3}\right) /\left(r_{1}^{2} r_{2}^{3}+r_{1}^{3} r_{2}^{2}\right) \tag{24a}
\end{equation*}
$$

and

$$
\begin{equation*}
B \equiv\left(1-A r_{1}^{2}\right) / r_{1}^{3} \tag{24b}
\end{equation*}
$$

Finally the coordinates of the extrapolated point are given by

$$
\begin{equation*}
s_{\alpha}^{\mathrm{ex}}=\left(s^{\mathrm{ex}} / s^{\mathrm{P}}\right) s_{\alpha}^{\mathrm{P}} \quad(\alpha=x, y, z) \tag{25}
\end{equation*}
$$

In spite of its apparent complexity, the implementation in computer of this extrapolating algorithm is very simple. The operational steps are as follows: (i) given $\left(s_{x}^{\mathrm{P}}, s_{y}^{\mathrm{P}}, s_{z}^{\mathrm{P}}\right), g$ is calculated through equation (14), and also $s_{x}^{(z)}, s_{y}^{(z)}, s_{y}^{(x)}$ and $s_{z}^{(x)}$ through equations (16), hence $r_{1}$ and $r_{2}$ (through equations (17)) and finally $A$ and $B$ (through equations (24)) ; (ii) ( $s_{x}^{\mathrm{P}}, s_{y}^{\mathrm{P}}, s_{z}^{\mathrm{P}}$ ) also determine $\theta$ and $s^{\mathrm{P}}$ through equations (18) and (19), which in turn determine $r^{p}$ through equation (20); (iii) $s_{0}$ (taken from the literature) and $s^{\mathrm{P}}$ determine $F(0)$ through equation (22b); (iv) the knowledge of $A, B, r^{P}$ and $F(0)$ determines $F\left(r^{P}\right)$ through equation (23), hence $s^{e x}$ (through equation (21)) and finally ( $s_{x}^{\mathrm{ex}}, s_{y}^{\mathrm{ex}}, s_{z}^{\mathrm{ex}}$ ) through equation (25).

The results obtained by using the above algorithm are indicated in table 1. In order to test the reliability of our results we have compared them with series calculations available for $q=1$ (figure $8(a)$ ) and $q=2$ (figure $8(b)$ ) for the particular cases $0 \leqslant$ $J_{z} / J_{x} \leqslant J_{y} / J_{x}=1$ and $0 \leqslant J_{y} / J_{x}=J_{z} / J_{x} \leqslant 1$. The agreement is very satisfactory (the discrepancy in the $t$-variable is always smaller than 0.01 ).


Figure 8. Present extrapolated results (——) for the critical point corresponding to the particular anisotropic $d=3$ case where two coupling constants are assumed equal ( $\equiv J_{\perp}$ ) and the third one ( $\equiv J_{\|}$) eventually different. We have the isotropic $d=1, d=2$ and $d=3$ cases at the ordinate, abcissa and bisectrix respectively. (a) $q=1$; the dots are series results (Redner and Stanley 1979) ; (b) $q=2$; both dots (Oitmaa and Enting 1971) and circles (Paul and Stanley 1972) are series results.

## 5. Conclusion

We have discussed, within a real space renormalisation group framework, the $q$-state Potts ferromagnet in the fully anisotropic (arbitrary $J_{x}, J_{y}$ and $J_{z}$ ) simple cubic lattice. The $q$-dependences of the critical temperature $T_{c}$, the one-, two- and three-dimensional correlation length critical exponents $\nu_{1}, \nu_{2}$ and $\nu_{3}$, and the $d=1 \leftrightarrow d>1$ and $d=2 \leftrightarrow d=3$ crossover critical exponents $\phi_{1 d}$ and $\phi_{23}$ are analysed in the second-order phase transition region ( $\forall q$ for $d=1, q \leqslant 4$ for $d=2$, and $q \leqslant q_{c}(3) \approx 3$ for $d=3$ ).

The present renormalisation group reproduces a considerable amount of already known exact results such as $t_{c}^{(1)}=\nu_{1}=\phi_{1 d}=1, \forall q$, for $d=1, t_{c}=1 /(\sqrt{q}+1)$ for $d=\underline{2}$, etc; it also recovers, in the $q \rightarrow 0$ limit, the correct asymptotic behaviour $\nu_{2} \propto 1 / \sqrt{q}$. Whenever our numerical results do not coincide with available exact or series ones, the discrepancies are acceptable. Furthermore the universality classes we obtain are as commonly expected, i.e. the $d=3$ one for all values of $J_{x}, J_{y}$ and $J_{z}$ as long as none of them vanishes, and the $d=2$ one when only one among them vanishes. The general picture inspires reasonable confidence, and therefore we tend to believe that the $q \rightarrow 0$
$d=3$ results $\phi_{23} \propto 1 / \sqrt{q}, t_{\mathrm{c}}^{(3)}(q) \sim t_{\mathrm{c}}^{(3)}(0)+t_{\mathrm{c}}^{(3) \prime}(0) q$ and $\nu_{3}(q) \sim \nu_{3}(0)+\nu_{3}^{\prime}(0) q$ (with finite values for $t_{\mathrm{c}}^{(3)}(0), t_{\mathrm{c}}^{(3)}(0), \nu_{3}(0)$ and $\left.\nu_{3}^{\prime}(0)\right)$ are correct.

We have also developed an extrapolation procedure for $T_{\mathrm{c}}$ which has proved to be quite satisfactory whenever comparison with other available results (typically from series) was possible, namely for the $0 \leqslant J_{z} / J_{x} \leqslant J_{y} / J_{x}=1$ and $0 \leqslant J_{y} / J_{x}=J_{z} / J_{x} \leqslant 1$ particular cases of the $q=1,2$ models. Through this procedure we have calculated $T_{c}$ for arbitrary ratios $J_{y} / J_{x}$ and $J_{z} / J_{x}$ and values of $q$ (the $q=3$ results are probably almost unaffected by the fact that the transition might be slightly first order). A theory which, enlarging the parameter space, would succeed in recovering the existence of first-order phase transitions would be very welcome. If alternatively the present RG is understood as referring to the hierarchical lattice defined by figure $1(h)$, then all the results it provides are exact for $q \geqslant 0$.

## Acknowledgments

Useful remarks from A C N de Magalhães, E M F Curado, M Schick, P M C de Oliveira, P R Hauser and W K Theumann are gratefully acknowledged. One of us (LRS) has benefited from a CNPq Fellowship (Brazilian Agency); CT acknowledges partial support through the tenure of a Guggenheim Fellowship.

## References

Baxter R J, Temperley H N V and Ashley S E 1978 Proc. R. Soc. A 358535
Blöte H W J and Swendsen R H 1979 Phys. Rev. Lett. 43799
Burkhardt T W and Southern B W 1978 J. Phys. A: Math. Gen. 11 L247
Citteur C A and Kasteleyn P W 1972 Phys. Lett. 42A 143
_- 1973 Physica 68491
de Magalhães A C N and Tsallis C 1981 J. Physique 421515
den Nijs M P M 1979 Physica 95 A 449
de Oliveira P M C and Tsallis C 1982 J. Phys. A: Math. Gen. 152865
Essam J W 1982 Preprint Some Combinatorial Interpretations of the Potts Model
Gaunt D S and Ruskin M 1978 J. Phys. A: Math. Gen. A 111369
Heerman D W and Stauffer D 1981 Z. Phys. B 44339
Hintermann A, Kunz H and Wu F Y 1978 J. Stat. Phys. 19623
Jensen S J K and Mouritsen O G 1979 Phys. Rev. Lett. 431736
Kasteleyn P W and Fortuin C M 1969 J. Phys. Soc. Japan (Suppl.) 2611
Le Guillou J C and Zinn-Justin J 1980 Phys. Rev. B 213976
Liu L L and Stanley H E 1972 Phys. Rev. Lett. 29927

- 1973 Phys. Rev. B 82279

Oitmaa J and Enting I G 1971 Phys. Lett. 36A 91
Paul G and Stanley H E 1972 Phys. Rev. B 52578
Redner S and Stanley H E 1979 J. Phys. A: Math. Gen. 121267
Tsallis C 1981 J. Phys. C: Solid State Phys. 14 L85
Tsallis C and de Magalhães A C N 1981, J. Physique Lett. 42 L227
Tsallis C and Levy S V F 1981 Phys. Rev. Lett. 47950
Wu F Y 1982 Rev. Mod. Phys. 54235
Zinn-Justin J 1979 J. Physique 40969

