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Finite lattice calculation of the quantum mechanical n-vector model

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Abstract. The truncated quantum mechanical n-vector model in one dimension is studied by means of the phenomenological renormalisation group (PRG) and the block renormalisation group (BRG) for general values of n. Particular emphasis is put on the extrapolation of the finite size results using the finite size scaling hypothesis. Accurate estimates of the critical properties can be made for $0 \leqslant n \leqslant 2$. The two methods used are critically compared.

1. Introduction

Recently, Hamiltonian versions of classical systems have received considerable attention. Besides being interesting in their own right, these models are connected to lattice formulations of gauge theories (Kogut 1979). For systems with a classical analogue, the relationship between the classical and its corresponding quantum mechanical model can be investigated. Presumably both formulations describe the same critical phenomena, allowing for the most convenient choice in actual calculations.

The quantum mechanical n-vector model has many applications in thermodynamics through its classical analogue (Stanley 1974) or its connection with field theory (Migdal 1975). The classical n-vector model corresponds for various values of n to models which have interesting critical properties: $n = 1$ is the well studied Ising model, $n = 2$ the planar or XY model (Kosterlitz and Thouless 1973) and $n = 0$ is connected with the statistics of polymers (de Gennes 1972). If n is continued to $n = -2$, the critical properties become gaussian (Balian and Toulouse 1973).

Thermodynamic properties of quantum mechanical systems can be studied with the same methods used for classical ones, notably perturbation expansions (Hamer *et al* 1978), exact solution of finite systems (Hamer and Barber 1981) and the renormalisation group (Drell *et al* 1976). In all these calculations it is important to estimate how fast the results converge with increasing order.

In the present calculation, we have looked at the n-vector model using two different kinds of renormalisation group transformations. Particular attention has been paid to the convergence and the validity of the extrapolations. Comparing the two conceptually very different approaches gives us more confidence in our results. Varying n continuously lets us link up with the exactly known values. We have chosen finite

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lattice renormalisations as they give numerical estimates which frequently converge extremely fast (Derrida 1981).

This work serves as a guide to more interesting (and more complicated) systems, notably those with fermions (Pfeuty *et al* 1982), as the methods used are not specific to the n-vector model. Higher-dimensional systems may be considered, as has been done for the transverse Ising model using block methods (Friedman 1976, 1978, Subbarao 1976) and the phenomenological RG (dos Santos *et al* 1981). Other generalisations include the study of crossover phenomena (dos Santos and Stinchcombe 1981).

In § 2, we introduce the model and perform the necessary analytic continuation in n. In § 3, the finite lattice methods are analysed with the finite size scaling ansatz; in appendix 1, the consequences of this assumption are derived in detail. Section 4 presents the results of the phenomenological renormalisation transformation and in § 5 we apply the block renormalisation group. In appendix 2 the transformations are given explicitly for arbitrary n and the smallest lattice sizes.

2. Quantum mechanical n-vector model

The classical n-vector model on a lattice is given by the Hamiltonian (Stanley 1974)

$$H = -K \sum_{\langle ij \rangle} \sum_{\alpha=1}^{n} S_i^\alpha S_j^\alpha, \qquad \sum_{\alpha=1}^{n} (S_i^\alpha)^2 = 1, \tag{1}$$

where $\langle ij \rangle$ sums over all nearest-neighbour pairs and each continuous variable $\boldsymbol{S}_i$ has n components. Via the transfer matrix, this model in d dimensions is related to the quantum mechanical n-vector model in $(d-1)$ dimensions where the time now plays the role of the extra dimension.

Thus the classical model on a square lattice, which we wish to study, is the analogue of the quantum mechanical model on a linear chain. The continuous variable $\boldsymbol{S}$ leads to an infinite number of states per site for the Hamiltonian system. It can be argued (Luther and Scalapino 1977) that the critical properties of the model are not altered if one truncates the number of states by retaining only the lowest singlet and n-fold degenerate multiplet at each site. With these simplifications, our model is given by the Hamiltonian, for N sites,

$$\hat{H} = \sum_{m=1}^{N} \hat{A}_m - x \sum_{m=1}^{N} \sum_{\beta=1}^{n} \hat{B}_{m-1}^{\beta} \hat{B}_m^{\beta}, \qquad \hat{B}_0^{\beta} \equiv \hat{B}_N^{\beta}, \tag{2}$$

where the single site operators $\hat{A}_m$ and $\hat{B}_m^{\beta}$ act on site m. We denote the singlet state by $|0\rangle_m$ and the n-multiplet by $|\alpha\rangle_m$, $\alpha = 1, 2, \ldots, n$. The model is completed by defining

$$\begin{aligned} &\hat{A}_m|\alpha\rangle_m = \delta_{\alpha,0}|\alpha\rangle_m, && \alpha = 0, 1, 2, \ldots, n, \\ &\hat{B}^{\beta}|\alpha\rangle_m = \delta_{\alpha,\beta}|0\rangle_m, && \alpha, \beta = 1, 2, \ldots, n, \\ &\hat{B}^{\beta}|0\rangle_m = |\beta\rangle_m, && \beta = 1, 2, \ldots, n, \end{aligned} \tag{3}$$

where $\delta_{\alpha,\beta}$ is the Kronecker delta function. Periodic boundary conditions are imposed and the parameter x takes the role of the temperature. This is a consequence of the fact that the thermodynamic properties of the two-dimensional system map into the ground state properties of the Hamiltonian model (Kogut 1979). We note that the

symmetries of the classical model have been preserved in the truncated version. A number of calculations indicate that the critical properties are indeed unaffected by the truncation (Hamber and Richardson 1981, Jullien and Pfeuty 1981).

We are interested in physical quantities (like the ground state energy) depending continuously on n. Hence, analytical continuation must be performed starting from the positive integers, for which the model is well defined. We propose to perform the continuation at the level of the Hamiltonian. In addition to the obvious advantage of a continuation at an early stage, it will make the practical calculations easier.

The basic idea is to work with vectors which are independent of n and to introduce the n-dependence explicitly. The Hamiltonian itself suggests this representation. We proceed in two steps. Let the states of the system be written as

$$|\alpha\beta\ldots\omega|, \qquad \alpha,\beta\ldots\omega = 0, 1, 2, \ldots, n, \tag{4}$$

where α = state of first site, ..., ω = state of Nth site. Starting with the state $|0\ldots0|$ and applying $\Sigma_{\beta=1}^{n} \hat{B}_{m-1}^{\beta}\hat{B}_{m}^{\beta}$, one creates states of the form

$$\sum_{\beta=1}^{n} |0\ldots\dot{\beta}\beta\ldots0|. \tag{5}$$

This procedure generates invariant subspaces in a very natural way, for example

$$|0\ldots0|, \quad |0\ldots11\ldots0|, \quad |\ldots11\ldots11\ldots|, \quad |\ldots11\ldots22\ldots| \quad \text{etc (singlet)} \tag{6}$$

or

$$|1\ldots0|, \quad |1\ldots11\ldots|, \quad |1\ldots22\ldots| \quad \text{etc } (n\text{-multiplet}) \tag{7}$$

and so forth.

The notation adopted is to sum over all paired labels, whereby distinct labels stand for distinct components. Single labels stand for arbitrary but fixed components $\alpha \neq 0$. The distinction between singlet, n-multiplet etc comes from the fact that the Hamiltonian leaves these subspaces invariant. Thus

$$\begin{aligned} &|\ldots11\ldots22\ldots| \quad \text{stands for} \quad \sum_{\substack{\alpha,\beta=1\\ \alpha\neq\beta}}^{n} |\ldots\alpha\alpha\ldots\beta\beta\ldots|, \\ &|\ldots1\ldots22\ldots| \quad \text{stands for} \quad \sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{n} |\ldots\alpha\ldots\beta\beta\ldots|, \qquad \text{etc.} \end{aligned} \tag{8}$$

In this representation n appears only in the matrix elements of the Hamiltonian and in the normalisation of the states. The states are orthogonal, but their norm is not necessarily positive definite. In the present case this does not pose any problems. Also, the Hamiltonian is no longer symmetric (for general n), though it stays real for all real n.

Practical considerations lead us to use still another representation. What we gain is that the total number of states is smaller. However, the states are not orthogonal any more. The difference with the above representation consists in allowing the components of different labels in the notation of equation (8) to be the same. For

example, $|\ldots 11\ldots 11\ldots|$ is incorporated in $|\ldots 11\ldots 22\ldots|$ and now

$$|\ldots 11\ldots 22\ldots| \quad \text{stands for} \quad \sum_{\alpha,\beta=1}^{n} |\ldots \alpha\alpha\ldots \beta\beta\ldots| \quad \text{etc.} \tag{9}$$

To give an idea of the economy using these vectors, the ca 3000 symmetrised states for $n=2$ (or 30 000 for $n=3$) and $N=10$ reduce to 150 singlet and 435 n-multiplet states, independent of n. As for finite lattice methods the limiting size is dictated by the number of states, this reduction is most welcome.

3. Finite lattice methods

The quantum mechanical n-vector model can be solved exactly for $n=1$, the Ising model (Pfeuty 1970, Hamer and Barber 1981). For other values of n there exists no exact solution. A number of calculations have succeeded in extracting critical properties for several values of n. Perturbation calculations in x (strong coupling expansion) have been performed for the full (Hamer *et al* 1978, 1979) and the truncated (Moore and Wilson 1980, Barber and Richardson 1981, Hamber and Richardson 1981) model. Also, the renormalisation group has been applied to the problem in the form of the phenomenological (Hamer and Barber 1981) and the block transformation (Drell *et al* 1976, Jullien *et al* 1978, 1979).

Here, we wish to apply these methods to the case of general n, with emphasis on the improvements obtained when N, the system size, is increased and the possibility of extrapolation to $N=\infty$. The important assumption for this kind of calculation is the finite size scaling hypothesis (Fisher and Barber 1972). Given a physical quantity $F(x)$: if $F(x)$ behaves like

$$F(x)\sim \Delta x^{-\omega}, \qquad \Delta x = |x - x_c|, \tag{10}$$

near the critical point x_c, then $F(x, N)$ has the form

$$F(x,N)\sim N^{\omega/\nu}(a_0 + a_1 \Delta x N^{1/\nu} + \ldots), \qquad a_0, a_1 = \text{constant}, \tag{11}$$

for $\Delta x \to 0$, $N\to\infty$. The most direct way to estimate the critical properties (x_c, ω, ν) from finite N calculations uses

$$F(x_c, N)\sim N^{\omega/\nu}, \qquad \frac{1}{F(x,N)}\frac{\mathrm{d}F(x,N)}{\mathrm{d}x}\bigg|_{x=x_c} \sim N^{1/\nu}, \tag{12}$$

and ν is the correlation length exponent, $\xi \sim \Delta x^{-\nu}$. The quantities which we use are the energy gap

$$g(x,N) = E_1 - E_0 \tag{13}$$

between the energies of the ground state $|0\rangle$ and the first excited state $|1\rangle$ of the finite system, and the matrix element

$$a(x,N) = \langle 1|\hat{B}_1^1|0\rangle / \langle 1|1\rangle^{1/2}\langle 0|0\rangle^{1/2} \tag{14}$$

of the operator $\hat{B}$, equation (3).

The exponent ω/ν is related to the dynamical critical exponent for the gap and to the correlation function exponent for the matrix element:

$$\begin{aligned} z &= -\omega/\nu \qquad \text{gap,} \\ \eta/2 &= -\omega/\nu \qquad \text{matrix element.} \end{aligned} \tag{15}$$

We assume (and verify) that the dynamical exponent $z = 1$, which holds true for models with a classical analogue.

A more powerful way to analyse the finite lattice results is with the renormalisation group. First, let us consider the phenomenological renormalisation group (PRG) which is based on the equation

$$N^{-\omega_0/\nu}F(x, N) = M^{-\omega_0/\nu}F(x', M), \qquad M < N. \tag{16}$$

This defines $x' = x'(x, M, N)$ (Nightingale 1976, Sneddon and Stinchcombe 1979). Finite size scaling asserts that this transformation becomes exact when $M, N \to \infty$. In appendix 1 we derive the consequences of this hypothesis on the convergence. It is advantageous to choose $M = N - 1$ and $\omega_0 = \omega$, if possible. We find

$$x_c = x_N^* + O(N^{-1/\nu}), \qquad \omega \neq \omega_0, \tag{17}$$

$$x_c = x_N^* + O(N^{-\alpha-1/\nu}), \qquad \omega = \omega_0, \tag{18}$$

$$\left(\frac{dx'}{dx}\right)_{x=x_N^*} = \left(\frac{N}{N-1}\right)^{1/\nu}(1 + O(N^{-\alpha-1})), \qquad \omega = \omega_0, \tag{19}$$

where x_N^* is the fixed point, $x_N^* = x'(x_N^*, N-1, N)$, and α the exponent characterising the leading correction to the asymptotic scaling.

The second method used is the block renormalisation group (BRG) (Drell *et al* 1976). The spirit of this approach is very different from the PRG. Here, the ground state properties are calculated iteratively. The approximation consists in retaining only the lowest few energy levels in each block in order to avoid proliferation of the renormalisation group parameters. If the BRG is truncated to the lowest two levels at each iteration, the transformation becomes (Jullien *et al* 1978)

$$x'(x, N) = xa^2(x, N)/g(x, N) \tag{20}$$

where the gap g and the matrix element a are given by equations (13) and (14) but now for a system with free ends. As with increasing N the BRG becomes exact, the results can also be analysed in terms of finite size scaling. In appendix 1 we determine how x_c and ν are obtained from the BRG for $N \to \infty$, namely

$$x_c = x_N^* + O(N^{-1/\nu}), \tag{21}$$

$$\left(\frac{dx'}{dx}\right)_{x=x_N^*} = N^{1/\nu}(a + O(N^{-1/\nu})), \qquad a = \text{constant}. \tag{22}$$

The usefulness of the finite lattice methods depends on the validity of the asymptotic expansions. Equations (17)–(19), (21) and (22) provide self-consistency conditions for the asymptotic region. By extrapolating the finite N results to $N = \infty$, better estimates of the critical properties can be obtained. Finally, comparing PRG and BRG lets us judge how well the two methods perform.

The results presented in the next two sections have, for all but the smallest sizes, been obtained numerically. The main task is the calculation of the lowest lying

eigenstates and their energies. In order to be able to handle the matrices for N up to $N = 10$ (PRG) resp $N = 9$ (BRG) with relative ease, we used the Lanczos scheme (Paige 1972, Roomany *et al* 1980). The method, ordinarily used for Hermitian matrices, has been generalised to be applicable to the present non-symmetric case (see also Wilkinson 1965).

4. The phenomenological renormalisation group

We have applied the fundamental PRG equation (16) to the gap g and the matrix element a for a selection of values of n in the range $-8 \leq n \leq 8$.

Firstly, for $n = 1$, the Ising model, the critical properties have been determined using the different methods and compared with the exact results. The results are listed in table 1 for sizes up to $N = 7$. As always, unless indicated otherwise, $M = N - 1$. The convergence sets in for N as small as $N = 3$ but one has to keep in mind that $n = 1$ is a rather special case. The matrix element $a(x)$ with the exact value of $\omega_0 = \omega$ gives slightly better results than the gap $g(x)$.

Next, the case $n = 2$ is considered. The results (together with those of the BRG) are given in table 2. There are strong odd/even fluctuations in N and the asymptotic analysis of § 3 cannot be applied to the series. We have also tried $M = N - 2$, but the

Table 1. PRG of the transverse Ising model ($n = 1$). x_c is the critical coupling and z, ν, η are the critical exponents. For both the gap $g(x)$ and the matrix element $a(x)$ (equations (13) and (14)) we compare finite size scaling (equation (12)) with the PRG for $N = 7$ and its extrapolation. α is the correction-to-scaling exponent (the exact value of α for the gap is $\alpha = 2$). In this and the following tables, the number of decimals retained for the finite N results are such that only the last one changes when comparing $N - 1$ and N. For a comparison of these results with other RG calculations, classical and quantum mechanical, see for example table II of Hirsch and Mazenko (1979).

		Gap $g(x)$			
	Exact	Equations (12)	$N = 7$	Extrapolation $N = \infty$	Correction exponent α
x_c	0.5	0.505	0.4988	0.4998	2.2
z	1	1.01			
ν	1	1.1	0.87	0.96	1.9
$\eta/2$	0.125		0.1261	0.1252	1.8
		Matrix element $a(x)$			
	Exact	Equations (12)	$N = 7$	Extrapolation $N = \infty$	Correction exponent α
x_c	0.5	0.49	0.4996	0.5001	2.6
z	1	1.05			
ν	1	1.1	0.83	0.97	1.8
$\eta/2$	0.125	0.12	0.125 (imposed)		

Table 2. Comparison of PRG and BRG for $n = 2$. The PRG estimates a transition at $x_c = 3.5$ whereas for the BRG $x^*(N)$ grows logarithmically. η for the BRG is estimated from the even N results.

	x_c ($x^*(N)$)		$1/\nu$		$\eta/2$	
N	PRG	BRG	PRG	BRG	PRG	BRG
2		0.66		0.206		
3	0.66	0.69	−1.76	0.326	0.184	
4	1.00	0.73	−0.37	0.358	0.156	
5	1.15	0.76	−0.30	0.375	0.148	
6	1.37	0.78	−0.18	0.385	0.143	
7	1.42	0.80	−0.14	0.393	0.140	
8	1.52	0.82	−0.11	0.398	0.137	
9	1.60	0.84	−0.08	0.401	0.135	
10	1.67		−0.07		0.134	
Extrapolation $N = \infty$	3.5 ± 1.0	$\ln N$	$\lvert 1/\nu \rvert < 0.03$		0.127 ± 0.005	0.14 ± 0.02

results are not conclusive either. Nevertheless there is qualitative agreement with the theory of Kosterlitz and Thouless (1973). For $n > 2$, the PRG has no longer a non-trivial fixed point. This is an indication that there is no phase transition.

Let us now turn to non-integer values of n. First, we determine the dynamical exponent z. Using equations (12) and (15), we conclude that $z = 1$ in the whole range $-2 \leqslant n \leqslant 2$. As an example, we show in figure 1 the gap as a function of N for $n = 1.5$.

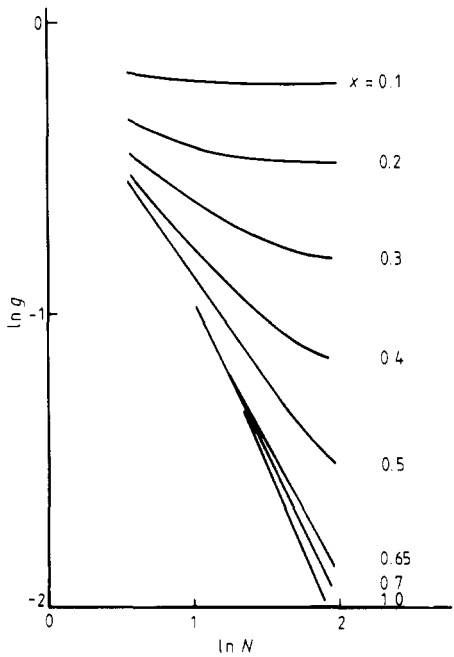

Figure 1. Log–log plot of the gap $g(x, N)$ against N for $n = 1.5$. At $x_c = 0.68$, $g \sim 1/N$, thus $z = 1$.

At the critical point $x_c \cong 0.68$, $g(x, N)$ scales with N and $z = 1$. In figure 2 the general form of $g(x)$ is shown for varying n.

Analysing the finite N results, one concludes that g is real for all x as long as $n \geqslant 0$. As long as $n > 1$ the gap stays positive and goes through a minimum. When $n < 1$, the gap vanishes at a value $x_0 > x_c$. This shows nicely how $n = 1$ is a very special situation, where $g(x \to \infty, N) = 0$. For $-2 < n < 0$, the gap is complex for $x > x_1$, where $x_1 > x_0$ varies with N. When $n < -2$, $g(x_1) > 0$ and there is no longer a real fixed point. Note that we define the gap always between the n-multiplet and the singlet. In the range $-2 \leqslant n \leqslant 2$, the singlet is always the ground state as long as $x \leqslant x_c$. The case $n = -2$ is a limiting situation where x_c, x_0 and x_1 all tend to the same value with increasing N. The matrix element $a(x)$ can be analysed similarly.

The PRG analyses for $n = 1.5$ and $n = 0.5$ are given in table 3. The results agree well with the scaling ansatz. The corrections indicate $\alpha \simeq 2$ independent of n. For $n = 0.5$, the equation $g(x_0, N) = 0$ provides another method to calculate the critical behaviour. The case $n = 0$ is of particular interest. In table 4, we list the results. For small values of N ($\leqslant 7$) the convergence is quite rapid. However, when $N \cong 10$, we

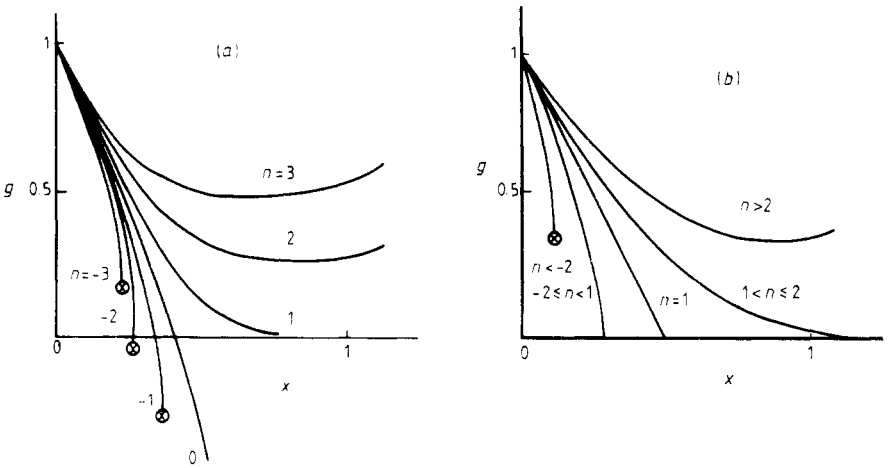

Figure 2. Gap $g(x, N)$ against x for $-3 < n < 3$. In (a) the results for $N = 7$ are shown, in (b) the extrapolation to $N = \infty$. For $n < 0$ the gap is complex for $x > x_1$, indicated by ($\otimes$).

Table 3. PRG for $n = 1.5$ and $n = 0.5$. The results converge well and are consistent with a correction exponent $\alpha = 2$. For $n = 0.5$, $g(x_0) = 0$ has been analysed with finite size scaling. The convergence $x_0(N) \to x_c$ is expected to be like $N^{-1/\nu}$.

n		x^*	ν	$\eta/2$	Convergence exponent
1.5	$N = 10$ Extrapolation	0.6650 0.6660 ± 0.0005	0.87 1.36 ± 0.04	0.134 0.132 ± 0.001	2.2 ± 0.3
0.5	$N = 10$ Extrapolation	0.418 02 $0.418\,15 \pm 0.0001$	0.830 0.845 ± 0.005	0.1144 0.1152 ± 0.0004	2.05 ± 0.1
0.5	$\{g(x_0) = 0\}, N = 7$ Extrapolation	0.472 0.421 ± 0.05	0.843	0.080	1.2 ± 0.1

Table 4. PRG for $n = 0$ (polymers).

N	x^*	ν	$\eta/2$
3	0.361 06	0.6741	0.083 78
4	0.364 56	0.7134	0.093 89
5	0.365 71	0.7303	0.096 89
6	0.366 22	0.7392	0.098 37
7	0.366 50	0.7444	0.099 27
8	0.366 66	0.7478	0.099 87
9	0.366 77	0.7500	0.100 31
10	0.366 85	0.7516	0.100 65

cannot exclude a maximum for ν, and $\nu = 0.75$ is a possible exact value. In table 5, we present the various analyses performed. Again, the convergence of the PRG is characterised by $\alpha \cong 2$ and x_0 tends towards x_c like $N^{-1/\nu}$.

In order to understand the behaviour of $n = 0$ better, we look at $n = -1$ and $n = -2$. We expect the effects which slow the convergence to appear more clearly. In table 6, the relevant data are collected. For $n = -2$, the exponent ν actually reaches a maximum at $N = 6$ and then approaches $\nu = 0.5$. η shows a similar trend. The

Table 5. Comparison of various methods for $n = 0$. The PRG is applied to the gap $g(x)$ and the matrix element $a(x)$ (with $\omega_0 = 0$). Analysis of the equation $g(x_0) = 0$ gives results that match those of the PRG.

	x_c	ν	$\eta/2$	Convergence exponent
PRG, gap, $z = 1$				
$N = 10$	0.366 85	0.7516	0.100 65	$2.2 \pm 0.3(\alpha)$
Extrapolation	0.3672 ± 0.0002			
PRG, matrix element, $\omega_0 = 0$				
$N = 7$	0.378	0.71 ± 0.1		
Extrapolation	0.365 ± 0.008			
$g(x_0) = 0, N = 7$	0.387	0.737	0.063	$1.4 \pm 0.3(1/\nu)$
Extrapolation	0.369 ± 0.004		0.100 ± 0.002	

Table 6. PRG for $n = -1$ and $n = -2$. The presence of another fixed point very close to the physical one prevents us from making a reliable extrapolation. $\nu(N)$ goes through a maximum at $N = 6$ and then approaches $\nu = 0.5$.

		x_c	ν	$\eta/2$	Comments
PRG $n = -1$	$N = 10$	0.303 67	0.6299	0.064	No convergence
PRG $n = -2$	$N = 10$	0.264 76	0.536 ($\nu = 0.540$ at $N = 6$)	0.010	Unphysical fixed point at $x^* = 0.266$

estimates for x_c do not go through an extremum, but the asymptotic region has not been reached yet. The reason for these difficulties is the presence of a second fixed point at $x \cong 0.266$ very close to the physical one at $x \cong 0.265$.

In all, the PRG proves to be a valid method to calculate critical properties for general n. The convergence is satisfactory for values of n away from the limiting cases $n = -2$ and $n = 2$. The critical point x_c behaves much more regularly than the exponents for all values of n.

5. Block renormalisation group

In this section, we present the results of the block renormalisation transformation, equation (20). The calculation is slightly more involved than the PRG as the blocks are not translationally invariant any more. Also, the definition of the matrix element $a(x)$ contains some ambiguity. In accordance with Jullien *et al* (1978), we choose to evaluate $\hat{B}$ in the middle of the block, in order to minimise edge effects. The qualitative picture for the energies and the matrix element is the same as for the PRG. For $x \lesssim x_c$ the states of lowest energy are symmetric under the symmetry operations of the block.

For $n = 1$, we have reproduced the results of Jullien *et al* (1978). With the analysis of appendix 1, the estimates are considerably improved by extrapolating to $N = \infty$. It is interesting to note that an unbiased extrapolation of $\nu(N)$ would not favour a logarithmic convergence, but the $N = \infty$ value is more accurate with the logarithmic extrapolation. Table 7 gives the results. The matrix element $a(x)$ is afflicted by strong odd/even fluctuations requiring us to analyse the odd and the even N points separately. The even N series are much smoother.

Table 7. Results of BRG for $n = 1$. The exact values are compared with those for $N = 7$ and their extrapolation to $N = \infty$. η has been calculated with equations (12) and (15).

	x_c	ν	$\eta/2$
Exact	0.5	1.0	0.125
$N = 7$	0.474	1.16	
Extrapolation	0.505	0.98	0.100 odd/odd 0.123 even/even
Convergence exponent	1.05	log	

The same analysis has been done for $n \neq 1$ and is reported in table 8. For $n > 0$ the convergence of x_c is characterised by the exponent $1/\nu$, as expected. The thermal exponent $\nu(n)$ from the renormalisation group analysis converges very slowly and there is no clear advantage of a logarithmic extrapolation. η exhibits odd/even fluctuations which are even more pronounced than for $n = 1$. When $n < 0$, the maximum value $N = 9$ is too small to estimate the limiting values. As for the PRG, the best performance of the BRG is for $n = 0.5$ and $n = 1$. For $n = 2$, the BRG is completely inadequate to describe the transition (Jullien *et al* 1979). The series for x_c and ν in table 2 show that x_c grows logarithmically with N, thus missing the transition, and ν remains finite. Only η is consistent with the expected $\eta = 0.25$. When $n > 2$, there is no transition, as illustrated in figure 3. For $n < 0$ effects similar to the PRG are found; in particular, the series for x_c and ν go through a maximum.

Table 8. BRG for $n \neq 1$ $(-2 < n < 1.75)$ analysed as in table 7. When it was possible to extrapolate, the results are given along with the convergence exponent. ν was extrapolated logarithmically. For η, the better even/even results are quoted.

n	x_c $N=9$	x_c extrapolated	Convergence exponent	ν $N=9$	ν extrapolated	$\eta/2$
1.75 ($N=7$)	0.656	0.78 ± 0.1	0.6 ± 0.1	1.79		0.13 ± 0.01
1.5	0.586	0.66 ± 0.02	0.85 ± 0.1	1.45	1.28	0.135 ± 0.01
0.5	0.4169	0.420 ± 0.002	1.40 ± 0.2	0.96	0.88	0.097 ± 0.01
0	0.3724			0.84		
−1	0.3129			0.69		
−2	0.273			0.59		

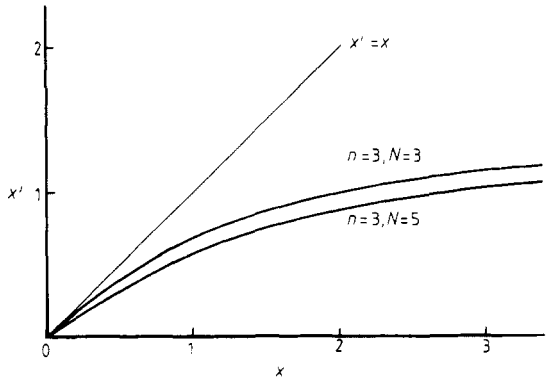

Figure 3. BRG for $n > 2$. $x'(x) > x$ for all $x > 0$, there is no transition.

The smaller n the sharper the maximum and the earlier (in N) it occurs. For $n < -2$, the BRG ceases to have a real fixed point.

The BRG supports a transition for $-2 \leqslant n < 2$ which is continuous in n. It is more sensitive to odd/even fluctuations in N and to the problem of slow convergence than the PRG.

6. Discussion

The purpose of this calculation has been to assess finite lattice methods and to extrapolate, when it is feasible, to $N = \infty$. The model studied, the truncated quantum mechanical n-vector model, is interesting for a number of reasons. It is believed—and the numerical evidence supports this—that this model exhibits the same critical phenomena as the classical n-vector model. For a number of values of n, the critical properties are known exactly, which allows one to assess the convergence of the results with increasing N. The variation of the critical properties with n is continuous, which permits interpolation between known limits.

The PRG, for the present model, proves to be the better of the two methods. As we compare neighbouring sizes N and $N-1$, the convergence is much improved. There is flexibility in defining the transformation; the matrix element $a(x)$ (equation (14)) works as well as the gap. As long as n is not too close to the border line situations

($n = -2, n = 2$), the asymptotic region in N starts for values as small as $N \simeq 4$, and the correction term to the scaling form behaves like N^{-2}. The consistency of the behaviour of the various quantities is a valid indicator of the asymptotic region.

The BRG is more sensitive to the difficulties encountered for $n = -2$ and $n = 2$. For $n = 2$, it does not predict the transition correctly. When $n = -2$, the series is too short to make accurate predictions. Figures 4–6 summarise the results and compare with other calculations.

The present treatment can be applied equally well to other systems, as it only uses the scaling hypothesis. Of course, it requires series which are sufficiently long ($N \simeq$ 8–10) to justify the extrapolation. For the block method, it would be desirable to find modifications (as suggested in appendix 1) to improve the answers for small N. Application to higher dimension is possible, though the shorter series make the conclusions more precarious.

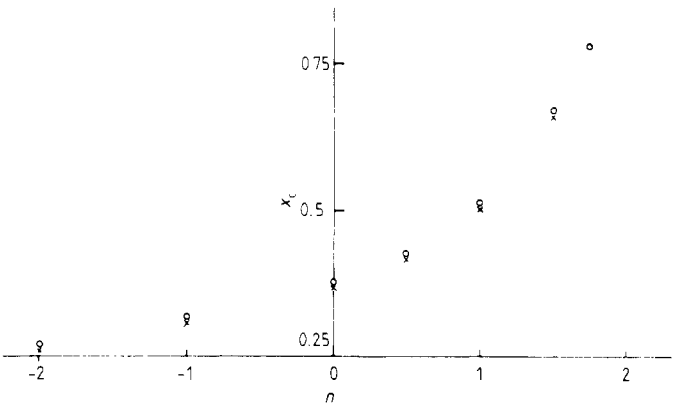

Figure 4. Best estimates of the critical coupling x_c as a function of n by the PRG (×) and the BRG (○). The strong coupling expansion of Hamber and Richardson (1981) coincides with the PRG for $n < 2$ to within the accuracy of the graph. The exact value for $n = 1$ is $x_c = 0.5$.

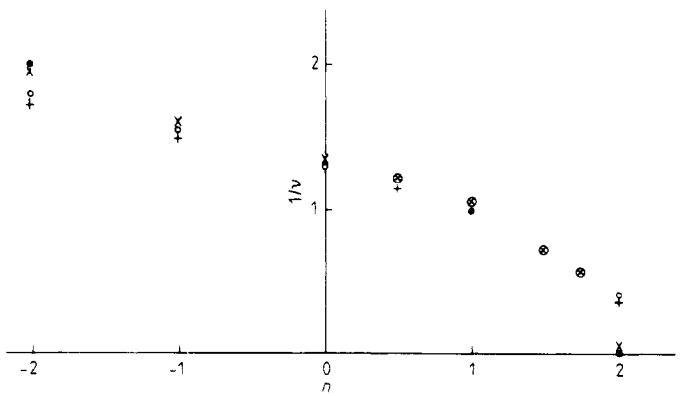

Figure 5. Thermal exponent ν against n by the PRG (×) and the BRG (○). Renormalisation calculation (●) (Cardy and Hamber 1980) and strong coupling results (+) (Hamber and Richardson 1981) have been indicated when they differ from the PRG.

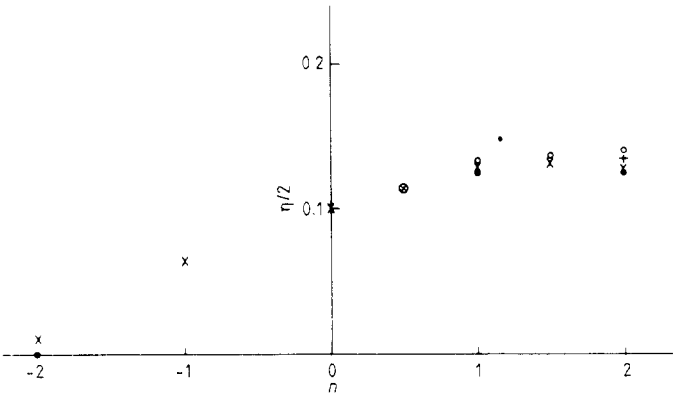

Figure 6. Correlation function exponent η against n by the PRG (×) and the BRG (○). Also indicated are $\eta = 0$ for $n = -2$ (●), $\eta = 0.25$ for $n = 1, 2$ (●) and the strong coupling estimate for $n = 2$ (+) (Hamber and Richardson 1981).

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Appendix 1.

In this appendix, we derive the asymptotic behaviour of the renormalisation group transformation when the size of the system is large.

Let $A(x)$ be a physical quantity which has the following form near the critical point x_c:

$$A(x) \sim \Delta x^{-\omega}, \qquad \Delta x = |x - x_c|. \tag{A1.1}$$

For a system of linear dimension N, the finite size scaling hypothesis postulates that

$$A(x, N) = N^{\omega/\nu}(A(z) + A_1(z)N^{-\alpha} + \ldots), \qquad z = \Delta x N^{1/\nu}, \tag{A1.2}$$

where $A(z)$ is a universal scaling function which can be expanded at $z = 0$. In order to recover (A1.1), $A(z \to \infty) \sim z^{-\omega}$.

ω is the critical exponent characteristic of A and ν is the correlation function exponent. We choose the leading correction to be a power in N, with an exponent $\alpha > 0$.

First, let us apply equation (A1.2) to a generalised phenomenological renormalisation transformation which defines $x' = x'(x, M, N)$ through

$$N^{-\omega_0/\nu}A(x, N) = M^{-\omega_0/\nu}A(x', M), \qquad N > M. \tag{A1.3}$$

In the limit $N, M \to \infty$, $\delta = N - M = \text{constant}$, the fixed point $x^* = x'(x^*)$ satisfies

$$\Delta\omega A(z^*) + z^* \, dA(z^*)/dz^* = 0 \tag{A1.4}$$

with

$$\Delta\omega = \omega - \omega_0, \qquad z^* = N^{1/\nu}(x^* - x_c). \tag{A1.5}$$

For $\Delta\omega$ small, $z^* = O(\Delta\omega)$. The derivative $(dx'/dx)_{x=x^*}$ then becomes

$$\left(\frac{dx'}{dx}\right)_{x=x^*} = 1 + \frac{\delta}{N}\frac{1}{\nu}(1 + O(\Delta\omega) + O(N^{-1}) + O(N^{-\alpha})). \tag{A1.6}$$

If ω/ν is exactly known, the convergence improves for $\Delta\omega = 0$, namely

$$x^* = x_c + O(N^{-\alpha-1/\nu}), \qquad (dx'/dx)_{x=x^*} = (1-\delta/N)^{-1/\nu}(1 + O(N^{-\alpha-1})). \tag{A1.7}$$

These arguments indicate that we can generalise the PRG to the case when ω/ν is not known exactly. The fixed point x^* still tends toward x_c, but at a slower rate, and the derivative is no longer related to ν in a simple fashion. The same finite size scaling analysis can be applied to the block renormalisation transformation. With increasing block size, the truncation of the states becomes negligible and the exact critical behaviour is approached in the defining equation of the BRG

$$x'(x, N) = xa^2(x, N)/g(x, N). \tag{A1.8}$$

We apply equation (A1.2) to the ratio a^2/g. The fixed point condition $x'(x^*) = x^*$ imposes $\omega = 0$. Then x^* satisfies for large N

$$x^* = x_c + N^{-1/\nu}(z^* + O(N^{-1}) + O(N^{-\alpha})) \tag{A1.9}$$

with z^* determined by the scaling function A,

$$A(z^*) = 1. \tag{A1.10}$$

The derivative is related to ν,

$$\left(\frac{dx'}{dx}\right)_{x=x^*} = x_c \frac{dA(z^*)}{dz^*} N^{1/\nu} + \text{constant}. \tag{A1.11}$$

This suggests that the BRG behaves similarly to the PRG, for $\Delta\omega \neq 0$. If $A(0) = 1$, we find

$$x^* = x_c + O(N^{-\alpha-1}), \qquad \frac{dx'}{dx} - 1 = x_c \frac{dA}{dz}(0) N^{1/\nu}(1 + O(N^{-\alpha-1/\nu})). \tag{A1.12}$$

Hence, the PRG gives better results than the BRG. The latter could be improved by modifying the transformation. Another possibility to speed up the convergence consists in comparing the BRG for different sizes.

Appendix 2.

Here explicit expressions for the renormalisation group equations for arbitrary n are presented. For the PRG, the situation when $N = 3$ and $M = N - 1 = 2$ can be solved analytically. In the representation of § 2, the states for the single (s) and n-multiplet

subspaces (m) and their normalisation are

N	State	Normalisation	Subspace
2	$\|00\|$	1	s
2	$\|11\|$	n	s
2	$\|10\|+\|01\|$	2	m
3	$\|000\|$	1	s
3	$\|110\|+\|011\|+\|101\|$	$3n$	s
3	$\|100\|+\|010\|+\|001\|$	3	m
3	$\|122\|+\|121\|+\|112\|$	$3n+6$	m

The Hamiltonian takes the form

$$H_2^{\mathrm{s}} = \begin{pmatrix} 0 & -2nx \\ -2x & 2 \end{pmatrix}, \qquad H_2^{\mathrm{m}} = (1-2x), \qquad N=2,$$

$$H_3^{\mathrm{s}} = \begin{pmatrix} 0 & -3nx \\ -x & 2-2x \end{pmatrix}, \qquad H_3^{\mathrm{m}} = \begin{pmatrix} 1-2x & (n+2)x \\ -x & 3 \end{pmatrix}, \qquad N=3.$$

The gap $g(x)$ then is

$$\begin{aligned} g_2 &= r-2x, \qquad r=(1+4nx^2)^{1/2}, \\ g_3 &= 1+[(1-x)^2+3nx^2]^{1/2}-[(1+x)^2+(n+2)x^2]^{1/2}, \end{aligned} \tag{A2.1}$$

and the matrix element $a(x)$, for $N=2$,

$$a_2 = (1+r+2x)/\sqrt{2}[(1+r)^2+4nx^2]^{1/2}. \tag{A2.2}$$

A number of properties found here remain valid for larger N. The Hamiltonian is real for all real values of n but is not symmetric. As long as $n \geqslant 0$, the gap and the matrix element stay real for all x. The PRG, $3g_3(x) = 2g_2(x')$, has a physical fixed point $0 < x^* < \infty$ for $-2 \leqslant n \leqslant 2$. The gap has a finite size transition $g(x_0) = 0$ at a value $x_0 > x^*$ for $n < 1$ and $g(x) < 0$ for $x > x_0$. Similarly $a(x) > 1$ for $n < 1$ and x sufficiently large.

The block renormalisation group, for $N=2$, is also represented by the states listed above. The Hamiltonian is

$$H_2^{\mathrm{s}} = \begin{pmatrix} 0 & -xn \\ -x & 2 \end{pmatrix} \qquad \text{resp } H_2^{\mathrm{m}} = (1-x). \tag{A2.3}$$

The BRG

$$x' = xa_2^2(x)/g_2(x) \tag{A2.4}$$

is determined by

$$\begin{aligned} g_2(x) &= s-x, \qquad s=(1+nx^2)^{1/2}, \\ a_2(x) &= (1+s+x)/\sqrt{2}[(1+s)^2+nx^2]^{1/2}. \end{aligned} \tag{A2.5}$$

The fixed point satisfies $a_2^2(x^*) = g_2(x^*)$ and is real for $-2 \leqslant n \leqslant 2$. For both transformations, for $x \leqslant x^*$, the ground state is a singlet and the first excited state an n-multiplet.

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