Finite-size corrections and numerical calculations for long spin 1/2 Heisenberg chains in the critical region

1987 J. Phys. A: Math. Gen. 20 L97

(http://iopscience.iop.org/0305-4470/20/2/010)

J. Phys. A: Math. Gen. **20** (1987) L97–L104. Printed in the UK

LETTER TO THE EDITOR

Finite-size corrections and numerical calculations for long spin-$\frac{1}{2}$ Heisenberg chains in the critical region

F Woynarovich† and H-P Eckle

Fachbereich Physik, Freie Universität Berlin, Animallee 14, 1000 Berlin 33, West Germany

Received 5 September 1986

Abstract. Leading and next-to-leading-order finite-size corrections to the ground and first excited states are calculated for the spin-$\frac{1}{2}$ anisotropic Heisenberg model in the critical region. The analytic results are compared to numerical data obtained for chains up to a length of $N = 1024$. It is found that, near the isotropic point, the asymptotic region where the results obtained for $N \to \infty$ are applicable sets in at very large N values, and for obtaining good accuracy in fitting the numerical data one has to take into account several correction terms, even at large ($N > 100$) chain lengths.

The widely used method of finite-size scaling for studying the properties of lower-dimensional statistical and quantum systems makes it desirable to have reliable methods for drawing conclusions about the behaviour of infinite systems from that of finite systems, i.e. to know more about the effects of finite size. Important steps in this direction have been made by Cardy (1984, 1986a, b) and by others (Blöte *et al* 1986, Affleck 1986) observing that, in conformally invariant systems, the leading corrections to the bulk (infinite-size) results have a universal character and are connected to the critical behaviour of the system, namely (in the language of 1D quantum systems) for large size (L)

$$E_n - E_0 \simeq \frac{2\pi x_n}{L} \qquad E_0 \simeq AL - \frac{\pi c}{6L} \tag{1}$$

where E_n are the energy eigenvalues, x_n the scaling dimensions of the scaling operators of the theory and c is the conformal anomaly number. The next corrections are powers of $1/L$, or under certain circumstances, logarithmic in L.

In the present letter we have studied both analytically and numerically the finite-size behaviour of the 1D anisotropic Heisenberg model

$$H = \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \rho S_i^z S_{i+1}^z) \tag{2}$$

in the region $0 \leqslant \rho = \cos\theta \leqslant 1$. Our main aim has been twofold: to check the above relations by independent analytic methods and, by performing numerical calculations for long chains, to find the range of sizes for which the above behaviour can be expected to set in. We based our study on the solution of the Bethe ansatz (BA) equations.

In our analytic calculation we extended the method introduced by de Vega and Woynarovich (1985) to calculate the finite-size corrections in systems with zero mass

† Permanent address: Central Research Institute for Physics, POB 49, H-1525 Budapest 114, Hungary.

0305-4470/87/020097+08\$02.50

gap. Simpler versions of this extension have already been applied to the present system (Avdeev and Dörfel 1985, Hamer 1985) to obtain the leading corrections. Our present treatment enables one to calculate systematically the higher ones as well. These higher-order corrections are needed to achieve reasonable accuracy in extrapolating small-size results to the infinite-size limit. This is clearly demonstrated by our numerical findings. We solved the BA equations for chain lengths increasing from $N=4$ to $N=20$ in steps of two and from $N=32$ always doubling the length up to $N=256$, for the isotropic case even up to $N=1024$. The results show that linear extrapolation in $1/N$ based on the small N data is misleading. The asymptotic region near to the isotropic point starts at very large N, and to reproduce the analytic results one needs to take into account several higher-order corrections. These numerical results also provide an explanation why the finite-size scaling method fails in reproducing correctly the phase boundary between the antiferromagnetic and XY phase of the model (as demonstrated by Sólyom and Ziman (1984)).

As is well known the BA equations for the Heisenberg Hamiltonian (2) are

$$N2\tan^{-1}\left(\cot\frac{\theta}{2}\tanh\frac{\eta_\alpha}{2}\right)=2\pi J_\alpha+\sum_{\beta=1}^{M}2\tan^{-1}\left(\cot\theta\tanh\frac{\eta_\alpha-\eta_\beta}{2}\right). \tag{3}$$

The solution of these equations describes an eigenstate with an energy per site

$$E_N^{(S)}=-\frac{1}{N}\sum_\alpha\frac{\sin^2\theta}{\cosh\eta_\alpha-\cos\theta} \tag{4}$$

and spin

$$S=\tfrac{1}{2}N-M. \tag{5}$$

To obtain the lowest energy state at a given S one must choose for J_α the set

$$J_\alpha:\ -\tfrac{1}{2}(\tfrac{1}{2}N-(S+1));\ -\tfrac{1}{2}(\tfrac{1}{2}N-(S+1))+1;\ldots\tfrac{1}{2}(\tfrac{1}{2}N-(S+1)). \tag{6}$$

The ground and first excited states are determined by (6) with $S=0$ and $S=1$, respectively.

Introducing the density of roots for the finite system in the form

$$z_N(\eta)=\frac{1}{2\pi}\left(2\tan^{-1}(\cot\tfrac{1}{2}\theta\tanh\tfrac{1}{2}\eta)-\frac{1}{N}\sum_\beta 2\tan^{-1}[\cot\theta\tanh\tfrac{1}{2}(\eta-\eta_\beta)]\right) \tag{7}$$

$$\sigma_N(\eta)=\mathrm{d}z_N(\eta)/\mathrm{d}\eta \tag{8}$$

leads to an equation for $\sigma_N(\eta)$:

$$\begin{aligned}\sigma_N(\eta)&=\frac{1}{4\theta}\frac{1}{\cosh(\eta\pi/2\theta)}-\int_{-\infty}^{\infty}F(\eta-\eta')S(\eta')\,\mathrm{d}\eta'\\ F(x)&=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\exp(\mathrm{i}\omega x)\sinh\omega(\pi-2\theta)}{2\cosh\omega\theta\sinh\omega(\pi-\theta)}\,\mathrm{d}\omega\end{aligned} \tag{9}$$

and an energy per site

$$E_N^{(S)}=E_\infty-\int_{-\infty}^{\infty}\varepsilon(\eta)S_N(\eta)\,\mathrm{d}\eta. \tag{10}$$

Here E_∞ is the energy per site for an infinite system in the ground state

$$E_\infty=-\sin\theta\int_0^\infty\left(1-\frac{\tanh(\omega\theta)}{\tanh(\omega\pi)}\right)\mathrm{d}\omega \tag{11}$$

and $\varepsilon(\eta)$ is the same function as the excitation energy of a hole (Woynarovich 1982):

$$\varepsilon(\eta)=\frac{\pi}{2}\frac{\sin\theta}{\theta}\frac{1}{\cosh(\eta\pi/2\theta)} \qquad \left(\sim\pi\frac{\sin\theta}{\theta}\exp(-|\eta|\pi/2\theta) \qquad \text{if } |\eta|\gg 1\right). \tag{12}$$

$S_N(\eta)$ stands for the expression

$$S_N(\eta)=\frac{1}{N}\sum_\beta \delta(\eta-\eta_\beta)-\sigma_N(\eta). \tag{13}$$

Replacing $\sigma_N(\eta)$ by $\sigma_\infty(\eta)$ and the η_β set by that obtained through the relation $z_\infty(\eta_\beta)=J_\beta/N$ corresponds to the approximation used by other authors (Avdeev and Dörfel 1985, Hamer 1985). This gives the right first corrections, but does not enable one to get the next set of corrections. Here we approximte the effect of the $S_N(\eta)$ by the formula

$$\frac{1}{2N}\left[f\left(\frac{n_1}{N}\right)+2\sum_{n_1+1}^{n_2-1}f\left(\frac{n}{N}\right)+f\left(\frac{n_2}{N}\right)\right]=\frac{1}{12N^2}\left[f'\left(\frac{n_2}{N}\right)-f'\left(\frac{n_1}{N}\right)\right]+\mathrm{O}\left(\frac{\max(f'''')}{N^4}\right) \tag{14}$$

where the prime means the derivative according to the argument. In our present case the application of (14) leads to expressions like

$$\int_{-\infty}^{\infty} g(\eta)S_N(\eta)\simeq-\left(\int_{-\infty}^{-\Lambda}+\int_{\Lambda}^{\infty}\right)g(\eta)\sigma_N(\eta)\,\mathrm{d}\eta+\frac{1}{2N}(g(\Lambda)+g(-\Lambda))$$
$$+\frac{1}{12N^2\sigma_N(\Lambda)}(g'(\Lambda)-g'(-\Lambda)) \tag{15}$$

where Λ is the largest root and is determined by the relation $z_N(\Lambda)=\frac{1}{2}[N/2-(S+1)]/N$, or what is equivalent to it:

$$\int_\Lambda^\infty \sigma_N(\eta)\,\mathrm{d}\eta=(1-\theta/\pi)S/N+1/2N. \tag{16}$$

Finally introducing the functions

$$\sigma_N^+(\eta)=\begin{cases}\sigma_N(\eta+\Lambda) & \text{if } \eta>0\\ 0 & \text{if } \eta<0\end{cases}$$
$$\sigma_N^-(\eta)=\begin{cases}0 & \text{if } \eta>0\\ \sigma_N(\eta+\Lambda) & \text{if } \eta<0\end{cases} \tag{17}$$

and taking Fourier transforms leads to the closed set of equations

$$\tilde\sigma^-(\omega)+\frac{\sinh\omega\pi}{2\cosh(\omega\theta)\sinh\omega(\pi-\theta)}\tilde\sigma^+(\omega)$$
$$=\frac{1}{2\pi}\frac{1}{2\cosh(\omega\theta)}\exp(\mathrm{i}\omega\Lambda)-\frac{1}{2\pi}\frac{\sinh\omega(\pi-2\theta)}{2\cosh(\omega\theta)\sinh\omega(\pi-\theta)}$$
$$\times\left[\left(\frac{1}{2N}-\frac{\mathrm{i}\omega}{12N^2\sigma_N(\Lambda)}\right)\right.$$
$$\left.+\left(\frac{1}{2N}+\frac{\mathrm{i}\omega}{12N^2\sigma_N(\Lambda)}-2\pi\tilde\sigma^+(-\omega)\right)\exp(\mathrm{i}\omega 2\Lambda)\right] \tag{18}$$

$$2\pi\tilde\sigma^+(0)=(1-\theta/\pi)S/N+1/2N \tag{19}$$

$$\sigma_N(\Lambda)=2\int_{-\infty}^{\infty}\tilde\sigma^+(\omega)\,\mathrm{d}\omega \tag{20}$$

$$E_N^{(S)} - E_\infty = (2\pi)^2 \frac{\sin\theta}{\theta} \exp(-\Lambda\pi/2\theta)\left[\tilde{\sigma}^+\left(-\frac{i\pi}{2\theta}\right) - \frac{1}{2\pi}\left(\frac{1}{2N} - \frac{\pi/2\theta}{12N^2\sigma_N(\Lambda)}\right)\right]$$
$$+ O(\exp(-3\Lambda\pi/2\theta)). \tag{21}$$

The equations for the isotropic case can be obtained by the $\theta \to 0$, $\eta/\theta \to \nu$ limit, which in the case of (18)-(21) means taking the $\theta \to 0$ limit after making the substitutions $\sigma(\Lambda) \to \sigma_i(\Lambda_i)/\theta$, $\tilde{\sigma}^\pm(\omega) \to \tilde{\sigma}_i^\pm(\omega\theta)$ and $\Lambda \to \Lambda_i\theta$.

Equation (18) is analogous to that which arose when calculating the magnetisation for the model and can be treated in the same way (Griffiths 1964, Yang and Yang 1966a, b). Here we do not give details of the solution, but rather our findings.

In the first approximation, when we neglect the terms in (18) which are proportional to $\exp(2i\omega\Lambda)$, we get the already known result

$$E_N^{(S)} - E_\infty = (2\pi)^2 \frac{\sin\theta}{\theta}\left(\frac{(1-\theta/\pi)S^2}{8N^2} - \frac{1}{48N^2}\right) \tag{22}$$

which in the $\theta \to 0$ limit reproduces the energy per site for the isotropic chain. Normalising the Hamiltonian appropriately (von Gehlen *et al* 1986) (22) coincides with (1) with $x_1 = \frac{1}{2}(1-\theta/\pi)$ and $c = 1$.

The next approximation is obtained when the terms proportional to $\exp(2i\omega\Lambda)$ are also taken into account with the $\tilde{\sigma}^+(-\omega)$ of the first approximation in it. This generates corrections proportional to $(1/N)^{n4\theta/(\pi-\theta)}$ and $(1/N^2)^m$. But corrections containing $(1/N^2)^m$ are also generated by the neglected $O(\exp(-3\Lambda\pi/2\theta))$ terms in the energy, by higher-order terms in (14) (and therefore in (15)) and by the first-order solution of (18) (by the poles of $1/\cosh(\omega\theta)$ at $\omega = i(2n+1)\pi/2$, $n \geq 1$). Finally the corrections can be compiled into a double series

$$E_N^{(S)} - E_\infty = (2\pi)^2 \frac{\sin\theta}{\theta}\left(\frac{1-\theta/\pi)S^2}{8N^2} - \frac{1}{48N^2}\right) + \frac{1}{N^2}\sum_{n,m} A_{nm}^{(S)}\left(\frac{1}{N}\right)^{(n4\theta/(\pi-\theta)+2m)}. \tag{23}$$

In this double series all n and $m \geq 0$ can be present except for $n = m = 0$. Which term is the dominant one depends on the value of θ.

For $\pi/2 > \theta > \pi/3$ the dominant term in the double series is the one with $n = 0$, $m = 1$, i.e. the next correction to (22) is $\sim 1/N^4$. The next largest term is the one with $n = 1$, $m = 0$, i.e. $\sim(1/N)^{4\theta/(\pi-\theta)+2}$.

If $\pi/3 > \theta > 0$ the leading term of the double series is the one with $n = 1$ and $m = 0$ ($\sim(1/N)^{4\theta/(\pi-\theta)+2}$), while for $\theta > \pi/5$ the next term is the one with $n = 0$ and $m = 1$ ($\sim 1/N^4$), but for $\theta < \pi/5$ the term with $n = 2$, $m = 0$ ($\sim(1/N)^{8\theta/(\pi-\theta)+2}$) is the next largest one.

As $\theta \to 0$ at any fixed N an increasing number of terms of the type $n \neq 0$, $m = 0$ is to be taken into account, which in the $\theta = 0$ limit sums up to a logarithmic correction. Since the isotropic case, being the phase boundary between the critical and non-critical phases, is of special interest, we have studied it in more detail. By solving the $\theta \to 0$ limit of (18)-(21), we have found that

$$E_N^{(0)} - E_\infty = -\frac{(2\pi)^2}{48N^2}\left(1 + \frac{0.3433}{(\ln N)^3} + O\left(\frac{\ln(\ln N)}{(\ln N)^4}; \frac{1}{(\ln N)^4}\right)\right) \tag{24}$$

$$E_N^{(S)} - E_N^{(0)} = (2\pi)^2 \frac{S^2}{8N^2}\left(1 - \frac{1}{2}\frac{1}{\ln N} + O\left(\frac{\ln(\ln N)}{(\ln N)^2}; \frac{1}{(\ln N)^2}\right)\right) \tag{25}$$

where $O((\ln(\ln N))/(\ln N)^{2(4)}; 1/(\ln N)^{2(4)})$ stands for the next two terms, which for N not large enough are not different in order of magnitude. We note here that the term $(\ln(\ln N))/(\ln N)^{2(4)}$ was not expected by Cardy (1986b).

We have also solved the BA equations (3) numerically for the ground and first excited states. We have found the solution by iteration. The stability of the fixed point has been checked by starting the iteration from different initial η_α sets. This check proved also that the procedure does not accumulate numerical errors. In figure 1 we have plotted $(E_N^{(0)}-E_\infty)/|(E_N^{(0)}-E_\infty)_{as}| = (E_N^{(0)}-E_\infty)48N^2\theta/[\sin\theta(2\pi)^2]$. Figure 2 shows the scaled gap normalised to its theoretically expected value, i.e. $(E_N^{(1)}-E_N^{(0)})8N^2\theta/[(1-\theta/\pi)\sin\theta(2\pi)^2]$.

It is apparent that the correction to the ground state approaches its asymptotic value much faster than the scaled gap does (2% and 10% at around $N=10$, respectively). The linear approximation in $1/N$ based on the first few points, however, does not increase the accuracy in either case. The curves are power-like, but these powers, as long as θ and N are small, do not coincide with the theoretically expected ones. That can be attributed to the effect of various higher-order corrections (Privman and Fisher 1983). Assuming the power law behaviour

$$1+a(1/N)^\alpha \qquad \text{and} \qquad 1+b(1/N)^\beta \tag{26}$$

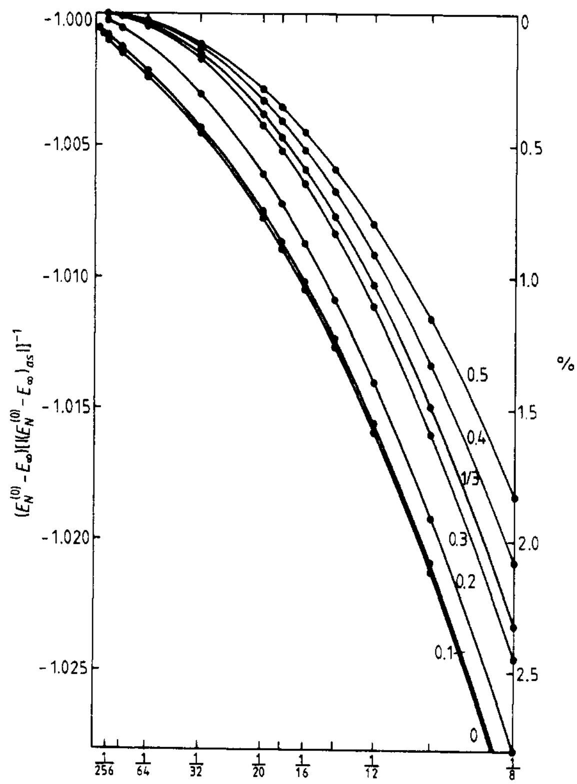

Figure 1. Corrections to the ground-state energy per site obtained numerically and normalised to the expected asymptotic values, i.e. $(E_N^{(0)}-E_\infty)(\pi^2\sin\theta/12\theta N^2)^{-1}$ plotted against $1/N$. The individual curves are labelled by the value of θ/π.

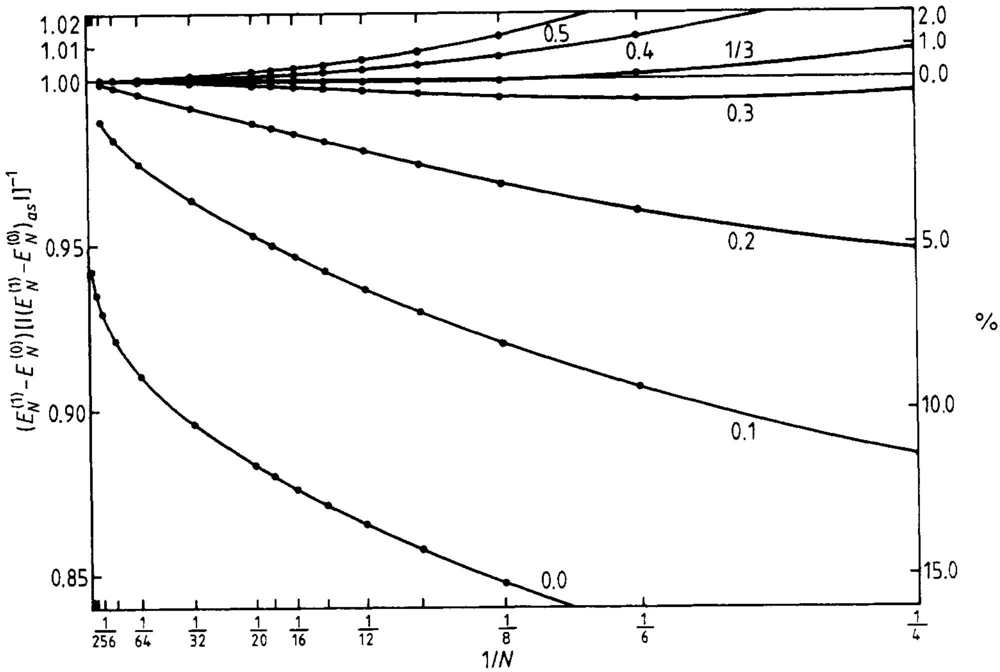

Figure 2. The scaled gap normalised to the theoretically expected $N \to \infty$ value, i.e. $(E_N^{(1)} - E_N^{(0)})(\pi \sin \theta(\pi - \theta)/2\theta N^2)^{-1}$ plotted against $1/N$. The individual curves are labelled by the value of θ/π.

for the curves of figures 1 and 2, respectively, table 1 lists the α and β exponents (obtained by graphical methods) best fitting the different regions of these curves.

For the scaled gap in the isotropic point we have made several least square fits to find the region where the asymptotic form is already applicable. According to (25) the normalised scaled gap has the form

$$a_0 + a_1 \frac{1}{\ln N} + a_2 \frac{\ln(\ln N)}{(\ln N)^2} + a_3 \frac{1}{(\ln N)^2} \tag{27}$$

with $a_0 = 1$ and $a_1 = -\frac{1}{2}$. In table 2 we give the results of three kinds of fits for the a coefficients. In the first we ignored the terms with a_2 and a_3, whereas in the third we

Table 1.

	$N=6$-20		$N=64$-256		Theory
θ/π	α	β	α	β	$\alpha=\beta$
0.1	1.5	0.6	0.67	0.47	$\frac{4}{9} \simeq 0.44$
0.2	1.63	0.97	1.18	1	1.0
0.3	1.95	1.2	1.9	1.6	$\frac{12}{7} \simeq 1.71$
$\frac{1}{3}$	2	—	2	1.73	2.0
0.4	2	2.1	2	2.03	2.0
0.5	2	2	2	2	2.0

Table 2.

N	a_0	a_1	a_2	a_3
6-20	$1-4.19\times10^{-2}$	-0.228	—	—
32-1024	$1-1.30\times10^{-2}$	-0.317	—	—
6-24	$1+0.25\times10^{-2}$	-0.435	—	0.234
32-1024	$1-0.49\times10^{-2}$	-0.396	—	0.183
6-32	$1-1.17\times10^{-2}$	-0.303	-0.151	0.131
32-1024	$1-1.62\times10^{-3}$	-0.461	0.154	0.176
128-1024	$1-2.99\times10^{-4}$	-0.490	0.235	0.161

took all of them. The second fit, in which the a_2 term is omitted, is to demonstrate that involving the $(\ln(\ln N))/(\ln N)^2$ term improves the accuracy for large N. Strangely enough, the small N data can be fitted best when the third term is omitted. This, however, could be an accident, since fitting the same curve to the large N data reproduces the theoretically expected a_0 and a_1 with less accuracy. With the large N data the fits get better and better involving more and more terms and the four-parameter fits are actually very accurate.

When studying a system by direct diagonalisation of the Hamiltonian, usually only chains up to $N=20$ can be treated. In Monte Carlo simulations this upper limit in size can be raised up to about 30-40. That makes it especially important to know what kind of behaviour is expected for short chains. Our calculations show (tables 1 and 2) that for these chain lengths the behaviour of different quantities cannot be described accurately just by the leading correction terms; to achieve numerical accuracy a larger number of corrections is needed. This implies that fitting the numerical data to some simple curves and extrapolating by them can be misleading and naive scaling procedures can give the wrong results. A prime example of this is the present model, as was pointed out by Sólyom and Ziman (1984): the naive scaling procedure shows that the 'critical anisotropy' is around $\rho=0.5$. Our results provide an explanation for this. Figure 2 shows that the correction to the scaled gap changes sign around $\rho=0.5$. Thus the $1/N$ behaviour for the gap could be seen here already at small N. That the scaled gap would not blow up for $1\geqslant\rho\geqslant0.5$, but would saturate in all the region $1\geqslant\rho\geqslant-1$, could not be seen from the small N data. In the case of the present model we know from exact results that the true phase boundary point is at $\rho=1$, but in the case of models where not enough analytic results are available, similar finite-size behaviour can lead to the wrong conclusions. The difficulties are greatly enhanced by the fact that near to the end of the critical region the scaled gap terminates with infinite slope, and to locate the phase boundary point correctly one needs to study long chains, and in the extrapolation one needs to take into account several correction terms.

We would like to thank Professor I Peschel for many inspiring discussions. We also benefited from discussions with Professor K-D Schotte and Dr T Truong. This research has been supported by DFG under contract Scho 158/7-2.

References

Affleck I 1986 *Phys. Rev. Lett.* **56** 746
Avdeev L V and Dörfel B-D 1985 *J. Phys. A: Math. Gen.* **19** L13

Blöte H W J, Cardy J L and Nightingale M P 1986 *Phys. Rev. Lett.* **56** 742
Cardy J L 1984 *J. Phys. A: Math. Gen.* **17** L385
—— 1986a *Nucl. Phys.* B **270** 186
—— 1986b *Preprint no 79* University of California at Santa Barbara
de Vega H J and Woynarovich F 1985 *Nucl. Phys.* B **251** [FS13] 439
Griffiths R B 1964 *Phys. Rev.* **133** A768
Hamer C J 1985 *J. Phys. A: Math. Gen.* **18** L1133
Privman V and Fisher M E 1983 *J. Phys. A: Math. Gen.* **16** L295
Sólyom J and Ziman T A L 1984 *Phys. Rev.* B **30** 3980
von Gehlen G, Rittenberg V and Ruegg H 1986 *J. Phys. A: Math. Gen.* **19** 107
Woynarovich F 1982 *J. Phys. A: Math. Gen.* **15** 2985
Yang C N and Yang C P 1966a *Phys. Rev.* **150** 321
—— 1966b *Phys. Rev.* **150** 327