Universal amplitudes in finite-size scaling: the antiperiodic 3D spherical model

1992 J. Phys. A: Math. Gen. 25 L207

(http://iopscience.iop.org/0305-4470/25/4/010)

J. Phys. A: Math. Gen. 25 (1992) L207–L211. Printed in the UK

LETTER TO THE EDITOR

Universal amplitudes in finite-size scaling: the antiperiodic 3D spherical model

Malte Henkel†§ and Robert A Weston‡||

† Département de Physique Théorique, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genève 4, Switzerland

‡ Centre for Particle Theory, Department of Mathematical Sciences, University of Durham, South Road, Durham DH1 3LE, UK

Received 28 October 1991

Abstract. The antiperiodic 3D spherical model is studied on a hypercubic lattice, two sides of which are finite and the other infinite. The universal correlation length finite-size scaling amplitude in the conjectured relationship $\xi/L = A/x$ is calculated exactly and found to be $A = 0.1361\ldots$, which should be compared with the antiperiodic 3D Ising model value of $A \simeq 0.12$.

It is well known that the finite-size scaling amplitude $\mathcal{A}_i$ of the correlation length $\xi_i = L\mathcal{A}_i$ of a spin system (below its upper critical dimension), evaluated in a finite geometry of linear extent L and at its bulk critical point, is a universal number (Privman and Fisher 1984, Privman *et al* 1991). In two dimensions, on an infinitely long strip of finite width L with periodic boundary conditions, $\mathcal{A}_i$ can be related to the critical exponent x_i through $\mathcal{A}_i^{-1} = 2\pi x_i$ as a consequence of conformal invariance (Cardy 1984) (x_i is the scaling dimension, or critical exponent, of the field whose two-point function decays with correlation length ξ_i).

The same relationship $\mathcal{A}_i \sim 1/x_i$ has been observed for some 3D systems (at their bulk critical temperature), defined on hypercubic lattices in the 'pillar geometry', where two sides of the lattice are finite and the other infinite†. Two 3D models have been studied in detail so far: the spherical model model and the Ising model. For the spherical model this inverse relationship holds for both periodic and antiperiodic boundary conditions across the finite dimensions (Henkel 1988). For the Ising model it is *only* true for *antiperiodic* boundary conditions (Henkel 1986, 1987). A Monte Carlo study of the antiperiodic Ising model (Weston 1990) has found the scaling amplitude in the conjectured relationsip $\xi_i/L = A/x_i$ to be $A = 0.117$ (3)‡. In this letter, we find from an exact calculation for the antiperiodic spherical model $A = 0.1361\ldots$.

§ email: Henkel@CGEUGE52.BITNET

|| email: R.A. Weston@uk.ac.durham

† A similar behaviour has been predicted from conformal field theory for models defined on the geometry $S^2 \times \mathbb{R}$ (Cardy 1985). See Alcaraz and Herrmann (1987) for an attempted verification.

‡ The value $A = 0.117$ (3) was an average over measurements on $L = 6$, 8, 10 lattices. Its associated error does not take into account the uncertainties involved in extrapolating to $L \to \infty$. See Weston (1990) for details.

0305-4470/92/040207+05$04.50

The partition function formulation of the spherical model has been discussed in detail in the literature (see e.g. Joyce 1972, Barber and Fisher 1973, Baxter 1982, Brézin 1982, Luck 1985, Singh and Pathria 1985a, b). Here, for simplicity, the model is discussed in terms of its quantum Hamiltonian (Kogut 1979, Henkel 1990). Then the pillar geometry defined above is automatic. The quantum Hamiltonian of the $d=r+1$ dimensional spherical model (Srednicki 1979, Henkel and Hoeger 1984, Henkel 1988) is:

$$H=-\tfrac{1}{2}\Delta+\tfrac{1}{2}(\chi\lambda r\boldsymbol{x}^2-\tfrac{1}{2}\lambda\boldsymbol{x}\mathcal{M}\boldsymbol{x}) \qquad (1)$$

where $\boldsymbol{x}$ is a vector of position operators (one for each of N spatial sites), Δ is the Laplacian and $\mathcal{M}$ is the spatial interaction matrix. There is a canonical constraint which fixes χ in terms of the coupling $\lambda=2/T^2$ (where T is the temperature of the isotropic model)

$$N=\langle 0|\boldsymbol{x}^2|0\rangle. \qquad (2)$$

If $\mathcal{M}$ is taken to allow only nearest neighbour interactions, then on an antiperiodic hypercubic lattice of sides $L_1,\ldots,L_r$ the eigenvalues are

$$\mu_k=2\sum_{j=1}^{r}\cos(k_j) \qquad k_j=\frac{2\pi(n+\frac{1}{2})}{L_j} \qquad n=0,1,\ldots,L_j-1. \qquad (3)$$

Define $\boldsymbol{s}_i$ as the position vector of site i, and p_i as the operator conjugate to x_i such that $[x_i,p_j]=\mathrm{i}\delta_{ij}$ and $-\Delta=\boldsymbol{p}\cdot\boldsymbol{p}$. Making the mode expansion

$$x_i=\lambda^{-1/4}L^{-r/2}\sum_k\frac{1}{\sqrt{2w_k}}(a_k\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{s}_i}+a_k^\dagger\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{s}_i}) \qquad (4)$$

$$p_i=-\mathrm{i}\lambda^{1/4}L^{-r/2}\sum_k\sqrt{\frac{w_k}{2}}(a_k\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{s}_i}-a_k^\dagger\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{s}_i}) \qquad (5)$$

with $[a_k,a_{k'}^\dagger]=\delta_{kk'}$ and $w_k=[\chi r-\Sigma_{j=1}^r\cos(k_j)]^{1/2}$, gives the Hamiltonian as

$$H=\lambda^{1/2}\sum_k w_k(a_k^\dagger a_k+\tfrac{1}{2}). \qquad (6)$$

The constraint (2) becomes

$$L_1\ldots L_r=\lambda^{-1/2}\sum_k\frac{1}{2w_k} \qquad (7)$$

and can be solved (Henkel and Hoeger 1984, Singh and Pathria 1985, Henkel 1988) to give χ as a function of the L_j and λ.

In what follows, we shall consider the $r=2$ cases of the '*pillar geometry*' with $L_1=L_2=L$ and of the '*film geometry*' with $L_1=L$ and L_2 infinite. We define the 'thermogeometric parameter' $y=L\sqrt{(\chi-1)r/2}$ (see Pathria 1983). Then the spherical constraint for the pillar geometry becomes to leading order in $1/L$ (see Singh and Pathria 1985b)†

$$\sqrt{\lambda}-\sqrt{\lambda_c}=(2\pi^{r+1})^{-1/2}\left(\frac{y}{L}\right)^{r-1}\times\left(\frac{1}{2}\Gamma\left(\frac{1-r}{2}\right)+\sum_q{}'(-1)^{q_x+q_y}(qy)^{(1-r)/2}K_{(r-1)/2}(2qy)\right) \qquad (8)$$

† We correct numerical errors for the constraint in the Hamiltonian limit case (Henkel 1988).

where K_ν is a modified Bessel function, $q=\sqrt{q_x^2+q_y^2}$; $q_x, q_y \in \mathbb{Z}$, and the prime indicates that the term with $q=0$ should be excluded. For the film geometry $\Sigma'_q(-1)^{q_x+q_y} \to \Sigma'_{q_x}(-1)^{q_x}$ and $q=|q_x|$.

At the critical point $\lambda=\lambda_c$ the universal number y is obtained, in the case $r=2$

$$2y=\sum_q{}'(-1)^{q_x+q_y}q^{-1}\exp(-2yq). \tag{9}$$

In contrast with the cases of periodic or free boundary conditions (where $y>0$), (9) does not have a real solution. For the pillar geometry, we define the functions

$$\begin{aligned} S(v)&=\sum_{q_x=1}^{\infty}\sum_{q_y=0}^{\infty}(-1)^{q_x+q_y}q^{-1}\sin(2vq) \\ C(v)&=\sum_{q_x=1}^{\infty}\sum_{q_y=0}^{\infty}(-1)^{q_x+q_y}q^{-1}\cos(2vq) \end{aligned} \tag{10}$$

and from numerical studies we obtain the conjectures

$$S(v)=-v/2 \qquad \text{if } -\frac{\pi}{\sqrt{2}}\leqslant v\leqslant\frac{\pi}{\sqrt{2}} \qquad C(v)=0 \text{ if } v=\pm\tfrac{5}{4} \tag{11}$$

yielding $y=\mathrm{i}v=\pm\mathrm{i}5/4$. For the film geometry (see e.g. Singh and Pathria 1985b) the functions analogous to $S(v)$ and $C(v)$ can be evaluated exactly and $y=\pm\mathrm{i}\pi/3$. It was this exact result in the film geometry which triggered us to consider the imaginary y-axis for the pillar geometry as well.

It might seem surprising to find an imaginary value for y. This new possibility arises from the discretization equation (3) which implies that the eigenvalues μ_k always remain separated from their bulk upper limit $2r$ by a term of order $O(1/L^2)$. Since only y^2 enters into physical quantities, it is enough to demand that the partition function exists, which is guaranteed as long as the masses obtained from H stay real. This is the case if $|v|\leqslant\pi/\sqrt{2}$.

Substituting into (6) gives the mass gap of the theory as a function of L, and its inverse, the spin-spin correlation length ξ_σ. Since the quantum Hamiltonian is obtained from the transfer matrix by taking an extreme anisotropic limit in the spatial and temporal coupling constants, the normalization of H is arbitrary (Kogut 1979, Henkel 1990). This normalization must be fixed consistently in order to obtain the universal scaling amplitude A. The natural way to do this is to demand that the spin-spin correlation be symmetric in the thermodynamic limit, or equivalently to require that energy and momentum should be measured in the same units so as to obtain the linear dispersion relation $E=|\boldsymbol{k}|$, where the 'speed of light' is unity. It is important to realize that changing the normalization of the Hamiltonian is not equivalent to simply rescaling λ. The values λ_c and y are independent of this normalization (y is even universal).

The operators x_i become time-dependent through the normal relationship

$$\begin{aligned} x_i(t)&=\mathrm{e}^{\mathrm{i}Ht}x_i\,\mathrm{e}^{-\mathrm{i}Ht} \\ &=\lambda_c^{-1/4}L^{-r/2}\sum_k\frac{1}{\sqrt{2w_k}}\left(a_k\,\mathrm{e}^{-\mathrm{i}(\lambda_c^{1/2}w_kt-\boldsymbol{k}\cdot\boldsymbol{s}_i)}+a_k^\dagger\,\mathrm{e}^{\mathrm{i}(\lambda_c^{1/2}w_kt-\boldsymbol{k}\cdot\boldsymbol{s}_i)}\right). \end{aligned} \tag{12}$$

The spin correlation function of the statistical mechanical system is given by

$$\langle x_i(t)x_j(0)\rangle=\langle 0|T(x_i(-\mathrm{i}t)x_j(0))|0\rangle \tag{13}$$

where the meaning of time-ordering is extended to imaginary time. This may be worked out from the mode expansion, and is

$$\langle x_i(t)x_j(0)\rangle = \lambda_c^{1/2}L^{-r}\sum_k \frac{e^{-\lambda_c^{1/2}w_k|t|+ik\cdot(s_i-s_j)}}{2w_k} \tag{14}$$

$$= \lambda_c L^{-r}\sum_k \int \frac{dw}{2\pi}\frac{e^{i(wt+k\cdot(s_i-s_j))}}{(w^2+\lambda_c w_k^2)}. \tag{15}$$

Altering the normalization of the Hamiltonian $H \to \gamma^{1/2}H$ changes this expression to

$$\langle x_i(t)x_j(0)\rangle_\gamma = \gamma^{1/2}\lambda_c L^{-r}\sum_k \int \frac{dw}{2\pi}\frac{e^{i(wt+k\cdot(s_i-s_j))}}{(w^2+\gamma\lambda_c w_k^2)}. \tag{16}$$

It follows from the definition of w_k, that in the thermodynamic limit (the combined limit $La\to\infty$, $a\to 0$, where a is the lattice spacing)

$$\langle x_i(t)x_j(0)\rangle_\gamma \to \gamma^{1/2}\lambda_c \int \frac{dw}{2\pi}\frac{d^rk}{(2\pi)^r}\frac{e^{i(wt+k\cdot(s_i-s_j))}}{(w^2+\gamma\lambda_c k^2/2)}. \tag{17}$$

If we require that our quantum Hamiltonian describes an isotropic statistical mechanical system in this limit, then this function should be symmetric in t and each component of (s_i-s_j). This means choosing $\gamma = 2/\lambda_c$ and we see from (17) that this gives indeed the desired form of the dispersion relation. Then (6) gives the mass gap as

$$m = \xi_\sigma^{-1} = \sqrt{2}\, w_k^{\min}. \tag{18}$$

In the limit $L\to\infty$, this implies that for antiperiodic boundary conditions (see Henkel 1988)

$$\xi_\sigma/L = \frac{1}{2\pi}\left(\frac{y^2}{\pi^2}+\frac{d^*}{4}\right)^{-1/2} \tag{19}$$

where d^* is the number of finite dimensions. The scaling dimension of the spin operator of this model is the same as that of the Gaussian model, $x_\sigma = \frac{1}{2}$. So the scaling amplitude A for the antiperiodic† pillar geometry, defined through $\xi_\sigma/L = A/x_\sigma$, is

$$A = \frac{1}{\sqrt{2}\,2\pi}\left(1-\frac{25}{8\pi^2}\right)^{-1/2} \simeq 0.1361\ldots \tag{20}$$

and should be compared with the analogous 3D Ising model result $A \simeq 0.12$ (Weston 1990). The value $1/(\sqrt{2}\,2\pi)$ is the scaling amplitude of the Gaussian model—a model not immediately useful as a comparison because of its lack of a simple second-order phase transition.

To summarize, we have found that *the finite-size scaling amplitude of the correlation* length in some 3D models supports the conjectured form $\mathcal{A}_i = A/x_i$. The values of A obtained for the Ising and spherical models are quite close to each other. It remains an open question why imposing *antiperiodic* boundary conditions should be essential. It would be very interesting to know this amplitude for some other critical 3D models. Very recently, correlation functions in a 3D dimer model have been studied (Priezzhev and Brankov 1991).

† In the case of periodic boundary conditions, $y = 0.755\,9777\ldots$, which implies $A = 4y \simeq 3.0239\ldots$. This is in agreement with the Lagrangian results (see Brézin 1982, Luck 1985), confirming universality.

We thank V B Priezzhev and J G Brankov for useful correspondence. RAW thanks Andreas Ludwig for some useful discussions and the SERC for providing him with a research fellowship. MH is grateful to the Swiss National Science Foundation for financial support.

References

Alcaraz F Ç and Herrmann H J 1987 *J. Phys. A: Math. Gen.* **20** 5735
Barber M N and Fisher M E 1973 *Ann. Phys.* **77** 1
Baxter R E 1982 *Exactly Solved Models in Statistical Mechanics* (New York: Academic) p 60
Brézin E 1982 *J. Physique* **43** 15
Cardy J L 1984 *J. Phys. A: Math. Gen.* **17** L385
—— 1985 *J. Phys. A: Math. Gen.* **18** L757
Henkel M 1986 *J. Phys. A: Math. Gen.* **19** L247
—— 1987 *J. Phys. A: Math. Gen.* **20** L769
Henkel M 1988 *J. Phys. A: Math. Gen.* **21** L227
—— 1990 *Finite-Size Scaling and Numerical Simulation of Statistical Systems* ed V Privman (Singapore: World Scientific) ch VIII, p 353
Henkel M and Hoeger C 1984 *Z. Phys.* B **55** 67
Joyce G S 1972 *Phase Transitions and Critical Phenomena* vol 2 ed C Domb and M S Green (New York: Academic) p 375
Kogut J B 1979 *Rev. Mod. Phys.* **51** 659
Luck J M 1985 *Phys. Rev.* B **31** 3069
Pathria R K 1983 *Can. J. Phys.* **61** 228
Priezzhev V B and Brankov J G 1991 *J. Phys. A: Math. Gen.* submitted
Privman V and Fisher M E 1984 *Phys. Rev.* B **30** 322
Privman V, Hohenberg P C and Aharony A 1991 *Phase Transitions and Critical Phenomena* ed C Domb and J Lebowitz (New York: Academic)
Singh S and Pathria R K 1985a *Phys. Rev.* B **31** 4483
—— 1985b *Phys. Rev.* B **32** 4818
Srednicki M 1979 *Phys. Rev.* B **20** 3783
Weston R A 1990 *Phys. Lett.* **248B** 340