Continuously varying exponents in magnetic hard squares

1987 J. Phys. A: Math. Gen. 20 6471

(http://iopscience.iop.org/0305-4470/20/18/044)

J. Phys. A: Math. Gen. **20** (1987) 6471-6485. Printed in the UK

Continuously varying exponents in magnetic hard squares

Paul A Pearce† and Doochul Kim‡

† Mathematics Department, University of Melbourne, Parkville, Victoria 3052, Australia
‡ Department of Physics, Seoul National University, Seoul, 151, South Korea

Received 30 April 1987

Abstract. The commuting row-to-row transfer matrices of magnetic hard squares on the multicritical T manifold are shown to satisfy a special functional equation called an inversion identity. For strip widths up to $N=32$, these equations are solved numerically for the transfer matrix eigenvalues. The central charge or conformal anomaly $c=1$ is obtained from $1/N^2$ corrections to the exact bulk free energy and scaling dimensions are obtained from the eigenvalue gaps. The magnetic scaling dimension is $x_{\mathrm{m}}=\frac{1}{8}$ and the sublattice density difference scaling dimension is $x_{\mathrm{e}}=1/9(2-y)$, where $y=2\lambda/\pi$ and the interaction-dependent crossing parameter λ varies between 0 and $2\pi/3$. Scaling dimensions for further operators fall in the sequence $x_n=n^2x_{\mathrm{e}}$ where $n=1,2,3,4$. The critical exponents also vary continuously along the multicritical line and are given by $\alpha=(14-9y)/(16-9y)$, $\beta_{\mathrm{m}}=9(2-y)/16(16-9y)$, $\beta_{\mathrm{e}}=1/2(16-9y)$, $\nu=9(2-y)/2(16-9y)$ and $\delta=15$. These exponents are simply related to the exponents of the critical eight-vertex and Ashkin-Teller models, which also exhibit $Z_2\times Z_2$ symmetry, and we argue that these models lie in the same universality class.

1. Introduction

In statistical mechanics the universality hypothesis asserts that generally critical exponents of lattice models should depend on the dimension and symmetries of the model but not on the microscopic interactions. In sharp constrast, however, there exist a few models which exhibit a critical line along which the scaling dimensions and exponents vary continuously. Most notable amongst these are the symmetric eight-vertex, or Baxter model, and the Ashkin-Teller model. These models are defined in terms of Ising spins. They both have two independent spin-reversal symmetries and four-spin interactions and they both possess a special decoupling point. There exist simple relations between the critical exponents of these two models. Indeed, the critical behaviour of both models can be comprehensively understood, within the renormalisation group, by 'mapping' them onto the completely solvable Gaussian model (Kadanoff and Brown 1979, Knops 1980, den Nijs 1981, Nienhuis 1984). From the theory of conformal invariance (Friedan *et al* 1984, Cardy 1987) we now know that the critical exponents of many two-dimensional lattice models are in fact quantised and fall into various universality classes characterised by the central charge or conformal anomaly c. An important exception is the special case $c=1$ which is precisely the value which occurs for the eight-vertex and Ashkin-Teller models.

In this paper we consider the magnetic hard-square lattice gas. This model is exactly solvable (Pearce 1985, 1987a) on certain manifolds in the thermodynamic space, one of which, the T manifold, contains a multicritical surface TII. We show that, on this T manifold, the commuting row-to-row transfer matrices satisfy a special functional equation called an inversion identity (Pearce 1987b). Similar inversion identities have been derived for the eight-vertex (Pearce 1987b) and Ashkin-Teller (Pearce 1987c) models. The T manifold of magnetic hard squares is divided into two physical regimes which are naturally parametrised in terms of hyperbolic (TI) or trigonometric (TII) functions. Regime TII of concern here is a surface of multicritical points. We solve the inversion identity numerically for the largest eigenvalues in the critical regime TII for strip widths up to $N=32$. This allows us to accurately determine the conformal anomaly c and various scaling dimensions of the model. We find that the exponents vary continuously along the critical line and accordingly the conformal anomaly is $c=1$. We obtain the leading exponents as functions of y, where $y=2\lambda/\pi$ and the interaction-dependent crossing parameter λ varies between 0 and $2\pi/3$. These leading exponents are simply related to those of the eight-vertex and Ashkin-Teller models.

The layout of the paper is the following. In § 2 we describe the model and its phase diagram. We also state our results for the scaling dimensions and critical exponents of the isotropic model and discuss the scaling behaviour along the multicritical line. In § 3 we derive the inversion identity satisfied by the row-to-row transfer matrix on the T manifold. Finally, in § 4 we present the details of the numerical solution on the multicritical manifold TII of the functional equations derived in § 3.

2. The model: phase diagram, exponents and scaling

Magnetic hard squares (Pearce 1985, 1987a) is a three-state interaction-round-a-face or IRF model (Baxter 1982) that generalises and incorporates the two-dimensional magnetic Ising model and the hard-square (hexagon) lattice-gas models. The model describes hard core particles with spin and to each site i of a square lattice is assigned a spin variable $\sigma_i=0,\ \pm1$. If the site is empty $\sigma_i=0$ and if the site is full $\sigma_i=+1$ or -1 as the spin of the particle is up or down respectively. The occupation number of site i is then $\sigma_i^2=0,1$. The Boltzmann weight of a face (a,b,c,d), where the four spins a,b,c,d round a face are taken in anticlockwise order starting at the bottom left, is given by

$$W(a,b,c,d)=\begin{cases}(z/2)^{(a^2+b^2+c^2+d^2)/4}\exp(La^2c^2+Mb^2d^2+Jac+Kbd) & \\ \qquad\qquad\qquad\qquad\qquad\qquad ab=bc=cd=da=0 \\ 0 \qquad\qquad\qquad\qquad\qquad\qquad \text{otherwise.}\end{cases} \tag{2.1}$$

Here z is the total activity of the particles, L and M are diagonal lattice-gas interactions and J and K are diagonal magnetic interactions. The face weights are invariant under reversal of the spins on either of the two independent sublattices. Moreover, by reversing the spins on alternate pairs of diagonals on a periodic lattice we can assume that the magnetic interactions are ferromagnetic ($J, K\geqslant 0$).

Remarkably, magnetic hard squares is exactly solvable on four separate manifolds in the five-dimensional thermodynamic space spanned by the interactions J, K, L, M and the activity z. Let

$$\alpha=\tanh J \qquad \beta=\tanh K. \tag{2.2}$$

Then the exact solution manifolds, which are denoted by the letters I (Ising), H (interacting hard squares), E (elliptic) and T (trigonometric), are given by

$$
\begin{aligned}
&\mathrm{I} \quad z\,\mathrm{e}^{L+M} \to \infty \qquad L-M \text{ fixed} \\
&\mathrm{H} \quad \alpha=\beta=0 \qquad z=(1-\mathrm{e}^{-L})(1-\mathrm{e}^{-M})/(\mathrm{e}^{L+M}-\mathrm{e}^{L}-\mathrm{e}^{M}) \\
&\qquad \Delta_{\mathrm{H}} = z^{-1/2}(1-z\,\mathrm{e}^{L+M}) \\
&\mathrm{E} \quad \mathrm{e}^{L}=(\alpha+\beta)/\beta(1-\alpha^2)^{1/2} \qquad \mathrm{e}^{M}=(\alpha+\beta)/\alpha(1-\beta^2)^{1/2} \qquad (2.3)\\
&\qquad z=\alpha\beta(1-\alpha^2)(1-\beta^2)(1+\alpha\beta)/(\alpha+\beta)^4 \qquad \Delta_{\mathrm{E}}=(1-\alpha^2)(1-\beta^2)/\alpha\beta(1+\alpha\beta) \\
&\mathrm{T} \quad \mathrm{e}^{L}=(1-\alpha^2)^{1/2}/\beta^2 \qquad \mathrm{e}^{M}=(1-\beta^2)^{1/2}/\alpha^2 \qquad z=\alpha^2\beta^2 \\
&\qquad \Delta=(1-\alpha^2-\beta^2)/2\alpha\beta.
\end{aligned}
$$

On the I and H manifolds the model reduces to two-state spin models ($\sigma_i=\pm1$, $\sigma_i=0$, 1 respectively). For isotropic interactions ($\alpha=\beta$, $L=M$) the manifolds H, E and T reduce to curves and I to two 'planes at infinity' in a three-dimensional thermodynamic space. These manifolds are shown in figure 1. Also shown in figure 1 is the complete phase diagram, for the isotropic model, using the topology as determined by a corner transfer matrix variational approximation (Pearce and Seaton 1986). In this figure the point h denotes the critical point of pure hard squares ($\alpha=L=0$), the lines de and ef are the Ising critical lines of the I manifold and the curve ST is a locus of tricritical points. The surfaces cdef and cSTh are presumably critical surfaces, whereas the surfaces dgTS (respectively abdc) appear to be first-order coexistence surfaces between the fluid and the paramagnetic (respectively ferromagnetic) solid phases.

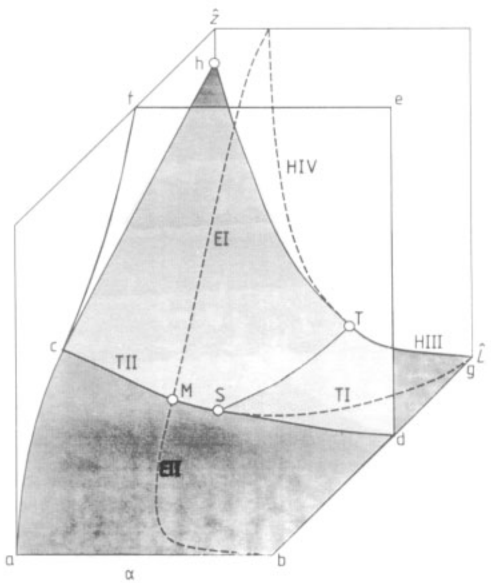

Figure 1. Schematic phase diagram of the isotropic magnetic hard-square model showing the exact solution curves H, E and T and incorporating the topology determined by Pearce and Seaton (1986). For convenience in plotting, the coordinates are $\alpha=\tanh J$, $\hat{L}=\mathrm{e}^{L}/(\mathrm{e}^{L}+3)$ and $\hat{z}=5z/(5z+2)$. These coordinates vary between 0 and 1 but only the portion of the phase diagram for $L\geqslant0$ is shown. The curve cMs is the multicritical regime TII. The crossing parameter is given by $\lambda=0$ at the point S and $\lambda=\pi/3$ at the multicritical point M, which lies at the intersection of the T and E solution curves. Regimes EI and HIV lie entirely in the paramagnetic solid phase. All the other exact solution regimes lie on phase boundaries.

There are two order parameters for magnetic hard squares, the sublattice density difference $R=\rho_1-\rho_2$ and the total magnetisation $m=(m_1+m_2)/2$, but only three phases are observed in the phase diagram. These phases are fluid ($R=0$, $m=0$), paramagnetic square-ordered solid ($R>0$, $m=0$) and ferromagnetic square-ordered solid ($R>0$, $m>0$). There is no indication of a ferromagnetic fluid ($R=0$, $m>0$) either in the exact solution or in the variational approximation. It therefore appears that spin-reversal symmetry is broken only on the sublattice that is preferentially occupied and hence $m=m_1/2$ and $m_2=0$. So, although magnetic hard squares has $Z_2\times Z_2$ symmetry, these symmetries are not on an equal footing as for the eight-vertex and Ashkin–Teller models. Here, one Z_2 symmetry corresponds to the spontaneous breaking of translational symmetry into two sublattices and the other to spontaneous breaking of spin-reversal symmetry on the preferentially occupied sublattice. What is more, unlike the eight-vertex and Ashkin–Teller models, magnetic hard squares does not have a decoupling point.

Most of the thermodynamic quantities of interest have already been calculated on the I (see, for example, Baxter 1982), H (Baxter 1980, 1981, Baxter and Pearce 1982, 1983, Pearce and Baxter 1984) and E (Jimbo and Miwa 1985, Pearce 1985, 1987a) manifolds. Not so much is known about the T manifold (Pearce 1985), although the free energy and the order parameters in the non-critical regime TI have been calculated. In this paper we focus on the multicritical regime TII. The T manifold (2.3) is a two-dimensional manifold in the full five-dimensional thermodynamic space. The curve $\Delta=1$ separates the multicritical regime TII ($|\Delta|<1$) from the regime TI($\Delta>1$) which is a first-order surface of three-fold phase coexistence between the fluid and the two paramagnetic square-ordered solid phases. Let us define

$$s(u)=\begin{cases}\sinh u & \text{TI}\\ \sin u & \text{TII}\end{cases} \tag{2.4a}$$

and set

$$\alpha=s_-=s(\lambda-u)/s(\lambda) \qquad \beta=s=s(u)/s(\lambda) \qquad s_+=s(\lambda+u)/s(\lambda) \tag{2.4b}$$

where $0<u<\lambda$ and

$$\Delta=\begin{cases}\cosh\lambda & \text{TI}\\ \cos\lambda & \text{TII.}\end{cases} \tag{2.4c}$$

Then the seven independent face weights can be written as

$$\begin{aligned}
\omega_1 &= W(0,0,0,0)=1\\
\omega_2 &= W(\sigma,0,0,0)=W(0,0,\sigma,0)=s/\sqrt{2}\\
\omega_3 &= W(0,\sigma,0,0)=W(0,0,0,\sigma)=s_-\\
\omega_4 &= W(\sigma,0,\sigma,0)=(1+s_-)/2\\
\omega_6 &= W(\sigma,0,-\sigma,0)=(1-s_-)/2\\
\omega_5 &= W(0,\sigma,0,\sigma)=1+s\\
\omega_7 &= W(0,\sigma,0,-\sigma)=1-s
\end{aligned} \tag{2.5}$$

where $\sigma=\pm1$. These weights are entire functions of the spectral parameter u. In the case of isotropic interactions $u=\lambda/2$ and, within regime TII, λ varies in the range $0<\lambda<2\pi/3$ to ensure positivity of the Boltzmann weights.

The inversion identity for the T manifold is derived in § 3 and solved numerically for regime TII in § 4. The solution of the inversion identity for regime TI will be considered elsewhere. In the remainder of this section we summarise our main results for the critical exponents and briefly discuss the scaling behaviour. For the conformal anomaly c we find $c = 1$. The scaling dimensions of various primary operators obtained by solving the inversion identity are presented in table 1(a). These exponents vary continuously along the multicritical line with

$$y = 2\lambda/\pi \qquad \cos\lambda = \tfrac{1}{4}[-3 + (1 + 4e^{2L})^{1/2}]. \tag{2.6}$$

The identification of operators corresponding to these exponents is also shown in table 1(a). As explained in § 4, some of these identifications are tentative. The identifications summarised in table 1(a) lead to the results for the standard critical exponents shown in table 1(b). The critical exponents of the eight-vertex and Ashkin–Teller models are also shown for comparison. Here the model parameters y_{8V} and y_{AT}, which depend on the four-spin interactions, are as defined in Baxter (1982). Notice that the critical exponents of all three models satisfy the relations

$$\begin{aligned} \delta &= (2 - \alpha - \beta_m)/\beta_m = 15 \\ \beta_e &= (1 - \alpha)/4 \end{aligned} \tag{2.7}$$

Table 1. (a) Identification of various primary operators and their scaling dimensions ($y = 2\lambda/\pi$). The spins on the corners of a unit square are denoted by a, b, c, d. The operators in the even (odd) sector are invariant (change sign) under spin reversal of all the spins. The odd operators appear in doublets because spin-reversal symmetry is not spontaneously broken on the sublattice (containing the b and d spins) that is not preferentially occupied. (b) The continuously varying exponents of magnetic hard squares along the multicritical line ($y = 2\lambda/\pi$). The exponents of the eight-vertex and Ashkin–Teller models are shown for comparison.

(a)

Name	Symbol	Operator	Scaling dimension	Conjugate field
		Even sector singlets		
Sublattice density difference	R	$a^2 - b^2$	$x_1 = x_e = 1/9(2-y)$	k
Total energy	E_+	$a^2c^2 + b^2d^2$	$x_2 = x_\varepsilon = 4/9(2-y)$	$L+M$
Marginal	λ	$ac + bd$	$x = 2$	$J+K$
Sublattice energy difference	E_-	$a^2c^2 - b^2d^2$	$x_3 = 1/(2-y)$	$L-M$
Anisotropy	u	$ac - bd$	$x = 2$	$J-K$
Total density	ρ	$a^2 + b^2$	$x_4 = 16/9(2-y)$	z
		Odd sector doublets		
Magnetisation	m	$a \pm b$	$x_{-1} = x_m = \frac{1}{8}$	h
Correlation	C_{mp}	$ac(a+c) \pm bd(b+d)$	$x_{-2} = \frac{9}{8}$	

(b)

Model	λ	α	β_m	β_e	ν	δ
Magnetic squares TII	$0-2\pi/3$	$(14-9y)/(16-9y)$	$9(2-y)/16(16-9y)$	$1/2(16-9y)$	$9(2-y)/2(16-9y)$	15
Eight-vertex	$0-\pi$	$2-2/y_{8V}$	$1/8y_{8V}$	$(2-y_{8V})/4y_{8V}$	$1/y_{8V}$	15
Ashkin–Teller	$0-2\pi/3$	$2(1-y_{AT})/(3-2y_{AT})$	$(2-y_{AT})/8(3-2y_{AT})$	$1/4(3-2y_{AT})$	$(2-y_{AT})/(3-2y_{AT})$	15

in addition to the usual scaling relations. This is due to the fact that the magnetic and energy scaling dimensions satisfy $x_{\mathrm{m}} = \frac{1}{8}$ and $x_{\varepsilon} = 4x_{\mathrm{e}}$ for all three models. If we equate the leading thermal exponents for these models we find that

$$4/9(2-y) = 2 - y_{8\mathrm{V}} = 1/(2-y_{\mathrm{AT}}). \tag{2.8}$$

With this identification, all of the exponents in table 1(*b*) correspond for the three models. This strongly suggests that the three models just give different manifestations of the same universal critical line.

Using the critical exponents of tables 1(*a*) and (*b*) gives the following alternative scaling forms for the singular part of the free energy:

$$\begin{aligned} f_{\mathrm{sing}}(t, q, h, k, u, \lambda, \ldots) &= b^{-2} f_{\mathrm{sing}}(b^{y_2} t, b^{y_4} q, b^{y_{-1}} h, b^{y_1} k, u, \lambda, \ldots) \\ &= t^{2/y_2} f_{\pm}\left(\frac{q}{|t|^{y_4/y_2}}, \frac{h}{|t|^{y_{-1}/y_2}}, \frac{k}{|t|^{y_1/y_2}}, u, \lambda, \ldots\right) \\ &= q^{2/y_4} F_{\pm}\left(\frac{t}{|q|^{y_2/y_4}}, \frac{h}{|q|^{y_{-1}/y_4}}, \frac{k}{|q|^{y_1/y_4}}, u, \lambda, \ldots\right). \end{aligned} \tag{2.9}$$

Here b is an arbitrary scale factor, t is the leading thermal non-linear scaling field, q is the next-to-leading thermal non-linear scaling field, h is the magnetic symmetry-breaking non-linear scaling field and k is the sublattice symmetry-breaking non-linear scaling field. The scaling exponents y_n are related to the scaling dimensions x_n given in table 1(*a*) by

$$y_n = 2 - x_n. \tag{2.10}$$

In Pearce (1985, 1987a) the critical behaviour and critical exponents have been discussed at the special point $M(\lambda = \pi/3)$ where the E manifold intersects the multicritical TII manifold. In these papers the critical exponents were calculated with q as the deviation from criticality variable and the last scaling form in (2.9) was taken as the starting point for discussing the scaling behaviour. However, as q varies the exact free energy varies analytically on the E manifold even across the multicritical line. In fact the dominant singularity is obtained by crossing the point M in a different direction corresponding to the leading thermal field t. Thus t should be taken as the deviation from criticality variable and not the next-to-leading thermal field q. Doing this we obtain the critical exponents

$$\alpha = \tfrac{4}{5} \qquad \beta = \beta_{\mathrm{m}} = \tfrac{3}{40} \qquad \beta_1 = \beta_{\mathrm{e}} = \tfrac{1}{20} \qquad \nu = \mu = \tfrac{3}{5} \qquad \delta = 15 \tag{2.11}$$

at the special point M common to the E and T manifolds.

3. The inversion identity

The elements of the row-to-row transfer matrix $\boldsymbol{V}$ are given by

$$V_{\sigma,\sigma'} = \prod_{j=1}^{N} W(\sigma_j, \sigma_{j+1}, \sigma'_{j+1}, \sigma'_j) \tag{3.1}$$

where σ and σ' are the configurations of two successive periodic rows of N spins. The matrix $\boldsymbol{V}$ is an $A_N \times A_N$ matrix with $A_N = 2^N + (-1)^N$. We will show in this section that on the T manifold, where the face weights are given by (2.5), the row-to-row transfer matrix $V(u)$ satisfies the functional equation or inversion identity (Pearce 1987b)

$$V(u)V(u+\lambda)=\phi(\lambda+u)\phi(\lambda-u)I+\phi(u)P(u) \tag{3.2}$$

where $P(u)$ is an auxiliary matrix which commutes with $V(u)$, I is the identity matrix and $\phi(u)=s^N$ with s given by (2.3) and (2.4). The transpose matrices are given by $V(u)^{\mathrm{T}}=V(\lambda-u)$ and $P(u)^{\mathrm{T}}=(-1)^N P(-u)$ and both $V(0)$ and $V(\lambda)$ are shift operators. The matrices $V(u)$ and $P(u)$ commute with the spin-reversal operator $\boldsymbol{R}$ with elements

$$R_{\sigma,\sigma'}=\prod_{j=1}^{N}\delta(\sigma_j,-\sigma'_j). \tag{3.3}$$

Their eigenvalues can therefore be labelled by the eigenvalues $R=\pm 1$ of $\boldsymbol{R}$. The matrices $V(u)$ and $P(u)$ must also satisfy the periodicity conditions

$$\begin{aligned} &V(u+\pi\mathrm{i})=RV(u) \qquad P(u+\pi\mathrm{i})=(-1)^N P(u) \qquad \mathrm{TI}\\ &V(u+\pi)=RV(u) \qquad P(u+\pi)=(-1)^N P(u) \qquad \mathrm{TII}. \end{aligned} \tag{3.4}$$

In general, the inversion identity (3.2) admits many solutions subject to the constraints (3.4). In Pearce (1985) it was conjectured that the row-to-row transfer matrix $V(u)$ on the T manifold satisfies a similar functional equation to that of the six-vertex model. In fact (Pearce 1987b) the six-vertex model satisfies precisely the inversion identity (3.2). The even sector ($R=1$) corresponds to the six-vertex model with periodic boundary conditions while the odd sector ($R=-1$) corresponds to the six-vertex model with boundary conditions such that horizontal arrows are reversed at the boundary. As is discussed in § 4, the inversion identity (3.2) is sufficient to determine the eigenvalues $V(u)$ in the odd sector, while in the even sector, additional information (4.9) on the behaviour of $V(u)$ as $u\to\lambda/2-\mathrm{i}\infty$ is required to obtain the eigenvalues.

We now derive the inversion identity (3.2). Let $V=V(u)$, $V'=V(u+\lambda)$, and similarly for the face weights W and W'. Then it follows that

$$[VV']_{\sigma,\sigma'}=\mathrm{Tr}\, S(\sigma_1,\sigma_2,\sigma'_2,\sigma'_1)S(\sigma_2,\sigma_3,\sigma'_3,\sigma'_2)\ldots S(\sigma_N,\sigma_1,\sigma'_1,\sigma'_N) \tag{3.5}$$

where the twenty-five S matrices have elements

$$[S(\sigma_1,\sigma_2,\sigma'_2,\sigma'_1)]_{\tau_1,\tau_2}=W(\sigma_1,\sigma_2,\tau_2,\tau_1)W'(\tau_1,\tau_2,\sigma'_2,\sigma'_1) \tag{3.6}$$

with τ being the intermediate row of spins. If $\sigma_j=\sigma'_j=0$, then τ_j can assume the values $0,\pm 1$ and the corresponding S matrices have three rows or columns. Otherwise we must have $\tau_j=0$ and the corresponding S matrices have one row or column. Thus $S(0,0,0,0)=A$ is a 3×3 matrix and all the other S matrices are 1×3 row vectors, 3×1 column vectors or 1×1 scalars. Now let

$$x=\tfrac{1}{2}\begin{bmatrix}\sqrt{2}\\ 1\\ 1\end{bmatrix} \qquad y=\tfrac{1}{2}\begin{bmatrix}\sqrt{2}\\ -1\\ -1\end{bmatrix} \qquad z=\frac{1}{\sqrt{2}}\begin{bmatrix}0\\ 1\\ -1\end{bmatrix} \tag{3.7}$$

be the orthonormal eigenvectors of

$$A=\frac{1}{\sqrt{2}}\begin{bmatrix}\sqrt{2} & -s^2 & -s^2\\ s_+s_- & 0 & 0\\ s_+s_- & 0 & 0\end{bmatrix} \tag{3.8}$$

corresponding to the eigenvalues s_+s_-, s^2 and 0, respectively, so that

$$Ax = s_+s_-x \qquad y^TA = s^2y^T \qquad Az = z^TA = 0. \tag{3.9}$$

Then the twenty-four other S matrices are given by

$$\begin{aligned}
&S(0, \sigma, \sigma, 0) = s_+s_-x\\
&S(0, \sigma, -\sigma, 0) = x - s^2y + \sqrt{2}\sigma sz\\
&S(0, 0, \sigma, 0) = (s_+ + s_-)x/2 + \Delta sy - \sigma ss_-z/\sqrt{2}\\
&S(0, \sigma, 0, 0) = (s_+ + s_-)x/\sqrt{2} - \sqrt{2}\Delta sy + \sigma ss_+z\\
&S(\sigma, 0, 0, \sigma) = s_+s_-x^T - y^T + \sigma(s_+ + s_-)z^T/\sqrt{2}\\
&S(\sigma, 0, 0, -\sigma) = -s^2y^T - \sqrt{2}\sigma\Delta sz^T\\
&S(0, 0, 0, \sigma) = -\sqrt{2}sy^T + \sigma ss_+z^T\\
&S(\sigma, 0, 0, 0) = sy^T - \sigma ss_-z^T/\sqrt{2}\\
&S(\sigma_1, 0, \sigma_2, 0) = ss_+/2\\
&S(0, \sigma_1, 0, \sigma_2) = -ss_-
\end{aligned} \tag{3.10}$$

where $\sigma, \sigma_1, \sigma_2 = \pm 1$. It is now straightforward to evaluate the following inner products ($\sigma, \sigma_1, \sigma_2 = \pm 1$):

$$\begin{aligned}
&S(\sigma_1, 0, 0, \sigma_2)S(0, \sigma, \sigma, 0) = 0 \qquad \sigma_1 \neq \sigma_2\\
&S(\sigma_1, 0, 0, \sigma_1)S(0, \sigma_2, \sigma_2, 0) = (s_+s_-)^2\\
&S(\sigma_1, 0, 0, -\sigma_1)S(0, \sigma_2, -\sigma_2, 0) = s^2(s^2 - 2\Delta\sigma_1\sigma_2)\\
&S(\sigma_1, 0, 0, -\sigma_1)S(0, \sigma_2, 0, 0) = \sqrt{2}\Delta s^2(s - \sigma_1\sigma_2s_+)\\
&S(\sigma_1, 0, 0, -\sigma_1)S(0, 0, \sigma_2, 0) = -\sqrt{2}\Delta s^2(s - \sigma_1\sigma_2s_-)\\
&S(\sigma_1, 0, 0, 0)S(0, \sigma_2, 0, 0) = -s^2(2\Delta + \sigma_1\sigma_2s_+s_-)/\sqrt{2}\\
&S(0, 0, 0, \sigma_1)S(0, 0, \sigma_2, 0) = -s^2(2\Delta + \sigma_1\sigma_2s_+s_-)/\sqrt{2}.
\end{aligned} \tag{3.11}$$

Because of the periodic boundary conditions, the above observations suffice to show that the non-zero elements of $[VV']_{\sigma,\sigma'}$ fall into two categories: either $\sigma_j = \sigma'_j$ for all j (these are the diagonal elements), or else $\sigma_j\sigma'_j = 0$ for all j. The vacuum element ($\sigma_j = \sigma'_j = 0$ for all j) of VV' is given by

$$\mathrm{Tr}\, A^N = (s_+s_-)^N + s^{2N}. \tag{3.12}$$

The non-vacuum elements break up into scalar segments. For diagonal elements the segments of length n are of the form

$$S(\sigma_1, 0, 0, \sigma_1)S(0, 0, 0, 0)^{n-2}S(0, \sigma_2, \sigma_2, 0) = (s_+s_-)^n. \tag{3.13}$$

For off-diagonal elements the various segments of length n are all of the form

$$s^n \times \text{entire function of } u. \tag{3.14}$$

This follows directly for segments of length 1 or 2 from (3.10) and (3.11). For longer segments it is easier to use the facts that for $\sigma_1 \neq \sigma_2$

$$\begin{aligned}
&S(\sigma_1, 0, 0, \sigma_2)S(0, 0, 0, 0) = s^2y^T \times \text{entire function of } u\\
&y^TS(0, \sigma_1, \sigma_2, 0) = s \times \text{entire function of } u.
\end{aligned} \tag{3.15}$$

In all cases we conclude that the elements of VV' are of the form given by the inversion identity (3.2) with the elements of $P(u)$ entire functions of u.

4. Numerical solution in TII

In this section we discuss the numerical solution of the inversion relation (3.2) in regime TII. Let

$$V_n = \exp(-E_n) \qquad n = 0, 1, 2, \ldots \tag{4.1}$$

be the eigenvalues of the row-to-row transfer matrix $\boldsymbol{V}$ for a strip of even width N with periodic boundary conditions. Then, for the isotropic model, the conformal anomaly c and the scaling dimensions x_n are given by the limiting values of the estimators (Blöte *et al* 1986, Cardy 1986, 1987):

$$c(N) = -(6N/\pi)(E_0 - Nf) \tag{4.2}$$

$$x_n(N) = (N/2\pi)(\mathrm{Re}\, E_n - E_0) \tag{4.3}$$

where E_0 is the ground-state energy, E_n are the low-lying energy levels and f is the exact bulk free energy (Pearce 1985)

$$f = \int_{-\infty}^{\infty} \mathrm{d}t \frac{\cosh(\pi - 2\lambda)t \sinh ut \sinh(\lambda - u)t}{t \sinh \pi t \cosh \lambda t}. \tag{4.4}$$

For a discussion of the anisotropic model see Kim and Pearce (1987).

In TII the critical Boltzmann weights (2.5) are polynomials in the variable

$$v = \exp(-\mathrm{i}u + \mathrm{i}\lambda/2). \tag{4.5}$$

Each element of the transfer matrix $\boldsymbol{V}(u) = \boldsymbol{V}(v)$ is a product of N of these weights. Hence $\boldsymbol{V}(v)$ can be written in the polynomial form

$$\boldsymbol{V}(v) = \sum_{k=0}^{2N} \boldsymbol{V}_k v^{-N+k} \tag{4.6}$$

where the matrices $\boldsymbol{V}_k$ are independent of u. Since the Boltzmann weights are real for real u, we must have $\boldsymbol{V}_k^* = \boldsymbol{V}_{2N-k}$. Similarly, since taking the transpose is equivalent to replacing u with $\lambda - u$, we have $\boldsymbol{V}_k^{\mathrm{T}} = \boldsymbol{V}_{2N-k}$. Hence $\boldsymbol{V}_k$ are Hermitian matrices. Furthermore, since the $\boldsymbol{V}_k$ commute with each other and possess u-independent eigenvectors, each eigenvalue $V(u)$ of $\boldsymbol{V}(v)$ is also a polynomial in v with real coefficients. The eigenvalues $V(u)$ are either symmetric or antisymmetric under spin reversal, i.e. $V(u+\pi) = RV(u)$ where $R = \pm 1$ is the spin-reversal quantum number. We can therefore write $V(v)$ in the form

$$V(v) = \begin{cases} (2v \sin\lambda)^{-N} \displaystyle\sum_{k=0}^{N} A_{2k} v^{2k} & R = 1 \\ (2v \sin\lambda)^{-N} \displaystyle\sum_{k=0}^{N-1} A_{2k+1} v^{2k+1} & R = -1 \end{cases} \tag{4.7}$$

where the coefficients A_k are real and the leading factors are included for convenience.

The eigenvalue $P(u)$ of the auxiliary matrix $\boldsymbol{P}(u)$ can similarly be written as a polynomial in the variable v

$$P(v) = (-2\mathrm{i} \sin\lambda)^{-N} \sum_{k=0}^{N} B_k [v \exp(-\mathrm{i}\lambda/2)]^{2k-N}. \tag{4.8}$$

Again the coefficients B_k must be real since $\boldsymbol{P}(u)$ is real for real u and $\boldsymbol{P}^{\mathrm{T}}(u) = (-1)^N \boldsymbol{P}(-u)$. Inserting (4.7) and (4.8) into the inversion identity (3.2) and equating powers of v, we obtain $(2N+1)$ equations for the unknowns A_k and B_k. The functional equation can therefore be solved immediately in the odd sector $(R=-1)$ for the $(2N+1)$ unknowns. In the even sector $(R=1)$, however, there are $(2N+2)$ unknowns and an extra condition must be imposed. The condition we impose is

$$A_0 = \lim_{v\to 0} (2v \sin\lambda)^N V(v) \tag{4.9}$$

where the limit $v \to 0$ or $u \to \lambda/2 - \mathrm{i}\infty$ is obtained by direct diagonalisation of the limiting row-to-row transfer matrix. For all the low-lying levels in the even sector of interest here it is found that either $A_0 = 2$ or $A_0 = -1$ independent of N and λ. Specifically, for $E_0, E_1, \ldots, E_4$ we find $A_0 = 2, -1, -1, 2, -1$ respectively.

For small values of N ($N \leqslant 10$), the eigenlevels can be obtained by direct diagonalisation of $\boldsymbol{V}(u)$. In this method the eigenvalues are found by using the common eigenvectors of $\boldsymbol{V}_k$ to evaluate the A_k in the polynomials (4.7). The levels for different N are identified and classified according to the spin-reversal quantum number R, the momentum $p = 2\pi j/N$ ($j = 0, 1, \ldots, N-1$) and the degeneracy of the eigenstate. For larger values of N ($10 \leqslant N \leqslant 32$) the inversion identity can be solved for the A_k. In practice, however, it is more convenient to solve for the complex zeros of the polynomials (4.7) because they behave in a systematic and predictable way as N increases. The initial patterns of zeros are inferred from the results of direct diagonalisation. This is of practical importance because the inversion identity admits many solutions. By iterating from the initial zero patterns we have obtained the estimators $c(N)$ and $x_n(N)$ given by (4.2) and (4.3) for many values of λ and for several eigenlevels. The lengths of the sequences are limited by numerical uncertainties. We stop the sequences whenever the ninth digit in the estimators becomes uncertain.

Tables 2(a) and (b) show the $c(N)$ sequences obtained for $\lambda = \pi/3$ and $2\pi/3$ respectively. To analyse our sequences we use the alternating-ε algorithm (Hamer and Barber 1981). In the second columns of table 2, we show the accelerated sequences obtained by one iteration of the alternating-ε algorithm. Here and below we take the last entry to be our extrapolated value. Thus, for the central charge, we find the estimates $c = 1.000\,001$ and 1.0001 for $\lambda = \pi/3$ and $\lambda = 2\pi/3$ respectively. We also obtain $c(N)$ sequences for N up to 16, 26 and 20 for $\lambda = \pi/6$, $\pi/4$ and $7\pi/12$ respectively. The extrapolated values for c obtained from them are 1.001, 1.0002 and 1.000 01 respectively. For other values of λ the results of direct diagonalisation were all consistent with $c = 1$. We therefore conjecture that $c = 1$ exactly for all λ between 0 and $2\pi/3$.

Above the ground state, we have identified four singlet states with $R = 1$ whose scaling dimensions x_n, $n = 1, 2, 3, 4$, labelled in increasing order, vary continuously with λ. These are associated with momentum $p = \pi(0)$ for n odd (even). The estimators $x_n(N)$ for these levels are shown in table 3 for $\lambda = \pi/3$. The extrapolated values are again the last entry given by one iteration of the alternating-ε algorithm. We show only the significant digits in the extrapolated values. Extrapolated values of x_n for other values of λ are shown in table 4. The maximum strip widths used are 16, 26, 32, 20 and 16 for $\lambda = \pi/6$, $\pi/4$, $\pi/3$, $7\pi/12$ and $2\pi/3$, respectively, except for x_3 where we used 22 and 16 for $\lambda = \pi/3$ and $7\pi/12$ respectively. We find that the data for x_n fit perfectly the simple formula

$$x_n = n^2 x_e \qquad n = 1, 2, 3, 4 \tag{4.10}$$

Table 2. Conformal anomaly estimator sequences $c(N)$ for (*a*) $\lambda = \pi/3$ and (*b*) $\lambda = 2\pi/3$. The adjacent columns are the accelerated sequences given by one application of the alternating-ε algorithm.

(*a*)

N	$c(N)$	Accelerated
2	0.852 345 578	
4	0.949 225 973	
6	0.975 512 468	1.000 029 12
8	0.985 873 262	1.000 027 31
10	0.990 901 650	1.000 019 53
12	0.993 689 289	1.000 013 12
14	0.995 384 050	1.000 008 83
16	0.996 486 475	1.000 006 07
18	0.997 241 588	1.000 004 28
20	0.997 780 277	1.000 003 10
22	0.998 177 403	1.000 002 30
24	0.998 478 198	1.000 001 75
26	0.998 711 256	1.000 001 36
28	0.998 895 343	1.000 001 09
30	0.999 043 181	
32	0.999 163 631	

(*b*)

N	$c(N)$	Accelerated
2	0.899 796 112	
4	0.961 538 584	
6	0.979 224 410	0.997 245 04
8	0.987 380 709	1.000 702 25
10	0.991 623 400	1.000 439 86
12	0.994 063 666	1.000 112 98
14	0.995 583 875	
16	0.996 591 025	

where

$$x_e = 1/9(2-y) \qquad y = 2\lambda/\pi. \tag{4.11}$$

For comparison, we also list in table 4, the values of $n^2 x_e$. These, together with less accurate estimates from direct diagonalisation, lead us to conjecture that the formulae (4.10) and (4.11) are exactly correct.

From the exact solution along the E manifold (Pearce 1985) we expect, at $\lambda = \pi/3$ where it intersects the T manifold, to find scaling operators in the even sector with scaling dimensions $\frac{1}{12}$, $\frac{1}{3}$ and $\frac{4}{3}$. This is in excellent agreement with the results of table 4 and, accordingly, we identify without ambiguity the corresponding operators as the sublattice density difference, the total energy and the total density for $n = 1$, 2 and 4 respectively as shown in table 1(*a*). For $n = 3$ we propose the sublattice energy difference operator as a likely candidate. This is the only remaining even operator that can be formed from the four spins on a unit square.

In the odd ($R = -1$) sector the lowest lying states are a doublet of momentum 0 and π near $\frac{1}{8}$. Above this, near $\frac{9}{8}$, we find another doublet of momentum 0 and π. We

Table 3. Scaling dimension estimator sequences $x_n(N)$ for the first four singlet levels in the even ($R = 1$) sector at $\lambda = \pi/3$. The extrapolated values are the last entry of the accelerated sequence given by the alternating-ε algorithm.

N	$x_1(N)$	$x_2(N)$	$x_3(N)$	$x_4(N)$
2	0.071 028 798	0.291 664 398		
4	0.079 102 164	0.317 639 423	0.961 644 565	1.402 915 77
6	0.081 292 706	0.325 199 056	0.870 712 593	1.347 214 06
8	0.082 156 105	0.328 362 964	0.835 852 127	1.334 762 56
10	0.082 575 137	0.329 977 332	0.817 063 854	1.331 046 09
12	0.082 807 441	0.330 911 058	0.805 201 918	1.329 897 77
14	0.082 948 671	0.331 499 829	0.796 989 520	1.329 645 89
16	0.083 040 540	0.331 895 242	0.790 948 354	1.329 730 41
18	0.083 103 466	0.332 173 855	0.786 308 893	1.329 938 81
20	0.083 148 356	0.332 377 717	0.782 629 254	1.330 184 45
22	0.083 181 450	0.332 531 492	0.779 636 818	1.330 431 01
24	0.083 206 517	0.332 650 428		1.330 663 64
26	0.083 225 938	0.332 744 368		1.330 877 02
28	0.083 241 279	0.332 819 898		1.331 070 12
30	0.083 253 598	0.332 881 565		1.331 243 79
32	0.083 263 636	0.332 932 586		1.331 399 63
Extrapolated				
	0.083 333 4	0.333 334	0.750 0	1.333

Table 4. Numerically determined values of the scaling dimensions x_n, $n = 1, 2, 3, 4$, for various values of λ. Only significant digits are shown. The conjectured exact values $n^2 x_e$ are shown alongside for comparison.

	x_1		x_2		x_3		x_4	
λ	Extrapolated	x_e	Extrapolated	$4x_e$	Extrapolated	$9x_e$	Extrapolated	$16x_e$
$\pi/6$	0.068	$0.0\dot{6}$	0.266 7	$0.2\dot{6}$				
$\pi/4$	0.074 1	$0.\dot{0}7\dot{4}$	0.296 29	$0.\dot{2}9\dot{6}$			1.183	$1.\dot{1}8\dot{5}$
$\pi/3$	0.083 333 4	$0.08\dot{3}$	0.333 334	$0.\dot{3}$	0.750 0	0.75	1.333	$1.\dot{3}$
$7\pi/12$	0.133 334	$0.1\dot{3}$	0.533 333	$0.5\dot{3}$	1.200	1.2		
$2\pi/3$	0.166 67	$0.1\dot{6}$	0.666 67	$0.\dot{6}$				

Table 5. Numerically determined values of the scaling dimensions x_{-1} and x_{-2} in the odd sector ($R = -1$) for several values of λ.

λ	x_{-1} extrapolated	x_{-2} extrapolated
$\pi/4$	0.127	1.12
$\pi/3$	0.125 3	1.125 0
$7\pi/12$	0.124 99	1.125 0
$2\pi/3$	0.125	1.125 0
Exact	0.125	1.125

label the scaling dimensions of these levels by x_{-1} and x_{-2} respectively. Table 5 shows our extrapolated values for these exponents for $\lambda = \pi/4$, $\pi/3$, $7\pi/12$ and $2\pi/3$ using maximum strip widths of 26, 32, 20 and 14 respectively. In general the convergence of sequences for smaller values of λ are poorer, as has been encountered in other models (Alcaraz *et al* 1987). Taking this into account we conjecture that

$$x_{-1} = \tfrac{1}{8} \qquad x_{-2} = \tfrac{9}{8} \tag{4.12}$$

for all λ, $0 < \lambda < 2\pi/3$. Again, the exact solution at $\lambda = \pi/3$ (Pearce 1985) allows us to identify the zero-momentum operator as the total magnetisation. The momentum-π partner is associated with the sublattice magnetisation operator. Since one sublattice magnetisation is always zero (even in the ferromagnetic solid phase) the critical exponents for the two order parameters are the same giving rise to the degeneracy of the level. To the second doublet x_{-2}, we tentatively associate the operators $ac(a+c) \pm bd(b+d)$ since, apart from $(a+c) \pm (b+d)$, these are the only odd sector operators that can be formed from the spins a, b, c, d on the corners of a unit square.

All operators discussed above are primary operators (Belavin *et al* 1984) with zero spin. The level diagram obtained by direct diagonalisation also shows two non-zero spin levels with x in the range $1.1 \sim 1.2$. One is a doublet with momentum $p = \pi \pm 2\pi/N$, $R = 1$ and the other is a quartet with $p = \pm 2\pi/N$, $\pi \pm 2\pi/N$ and $R = -1$. To each primary operator with scaling dimension x there is a conformal block of operators (descendents) whose scaling dimension and spin are $x + m + \bar{m}$ and $s + m - \bar{m}$, respectively, for $m, \bar{m} = 0, 1, 2, \ldots$ (Belavin *et al* 1984, Cardy 1987). For magnetic hard squares the momentum p of the eigenstate associated with the operator of spin $s + m - \bar{m}$

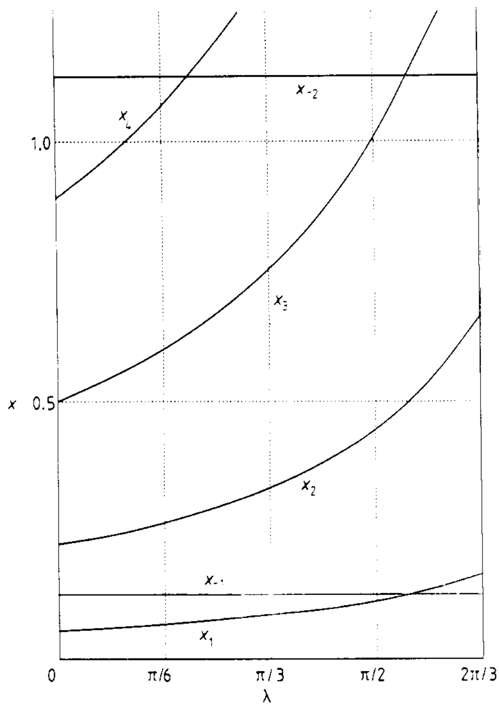

Figure 2. Variation of the primary operator scaling dimensions as a function of λ. We show the complete spectrum for $x \leqslant 1.35$.

is given by

$$p = 2\pi/N(s + m - \bar{m}) \qquad \text{mod } \pi. \tag{4.13}$$

The reason mod π appears here instead of the usual mod 2π is that in the adjoining $\sqrt{2}\times\sqrt{2}$ ordered phases the ordered structure repeats itself only after two translations along the side of the square edges, and hence V^2 should be regarded as the generator of unit translation. Therefore the doublet and quartet levels carry spin ± 1 and are naturally identified with $(m, \bar{m}) = (0, 1)$ and $(1, 0)$ levels descended from the singlet x_1 and the doublet x_{-1} respectively. The expected scaling dimensions $1 + x_e$ and $\frac{9}{8}$ for the doublet and quartet are also consistent with our results from direct diagonalisation. In this way we also identified the descendents of x_2 whose scaling exponents are $1 + 4x_e$.

This completes the analysis of the transfer matrix eigenenergy spectrum for regime TII for $0 < \lambda < 2\pi/3$ and for $x \leqslant 1.35$. We have not attempted to sort out the higher levels although it would be intriguing to know whether all even sector primary operators correspond to Gaussian model operators with dimensions

$$x_{n,m} = n^2 x_e + m^2/4x_e \qquad n, m = 0, 1, 2, \ldots \tag{4.14}$$

as in the *XXZ* results of Alcaraz *et al* (1987). Unfortunately, the vortex operators (Kadanoff and Brown 1979) would have dimensions $m^2/4x_e$ $(m = 1, 2, \ldots)$ that are outside of the range of our present analysis. Figure 2 shows the variation of the scaling dimensions x_n, $n = 1, 2, 3, 4$ and x_{-1}, x_{-2} as a function of λ. For $x \leqslant 1.35$ this is a complete set of energy levels associated with primary fields.

Acknowledgments

We thank Francisco C Alcaraz for useful discussions. This work was done while one of us (DK) was a visitor to the University of Melbourne and the support of the Mathematics Department and the hospitality of Colin J Thompson are gratefully acknowledged.

References

Alcaraz F C, Barber M N and Batchelor M T 1987 *Phys. Rev. Lett.* **58** 771-4
Baxter R J 1980 *J. Phys. A: Math. Gen.* **13** L61-70
—— 1981 *J. Stat. Phys.* **26** 427-52
—— 1982 *Exactly Solved Models in Statistical Mechanics* (New York: Academic)
Baxter R J and Pearce P A 1982 *J. Phys. A: Math. Gen.* **15** 897-910
—— 1983 *J. Phys. A: Math. Gen.* **16** 2239-55
Belavin A A, Polyakov A M and Zamolodchikov A B 1984 *Nucl. Phys.* B **241** 333-80
Blöte H W J, Cardy J L and Nightingale M P 1986 *Phys. Rev. Lett.* **56** 742-5
Cardy J L 1986 *Nucl. Phys.* B **270** [FS16] 186-204
—— 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (New York: Academic) p 55
den Nijs M P M 1981 *Phys. Rev.* B **23** 6111-25
Friedan D, Qui Z and Shenker S 1984 *Phys. Rev. Lett.* **52** 1575-8
Hamer C J and Barber M N 1981 *J. Phys. A: Math. Gen.* **14** 2009-25
Jimbo M and Miwa T 1985 *Physica* **15D** 335-53
Kadanoff L P and Brown A C 1979 *Ann. Phys., NY* **121** 318-42
Kim D and Pearce P A 1987 *J. Phys. A: Math. Gen.* **20** L451-6
Knops H J F 1980 *Ann. Phys., NY* **128** 448-62

Nienhuis B 1984 *J. Stat. Phys.* **34** 731-61
Pearce P A 1985 *J. Phys. A: Math. Gen.* **18** 3217-26
—— 1987a *J. Phys. A: Math. Gen.* **20** 447-54
—— 1987b *Phys. Rev. Lett.* **58** 1502-4
—— 1987c *J. Phys. A: Math. Gen.* **20** 6463-9
Pearce P A and Baxter R J 1984 *J. Phys. A: Math. Gen.* **17** 2095-108
Pearce P A and Seaton K A 1986 unpublished