Conformal Invariance and the Spectrum of the XXZ Chain

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Numerical solutions of the Bethe-*Ansatz* equations for the eigenenergies of the XXZ Hamiltonian on very large chains are used to identify, via conformal invariance, the scaling dimensions of various two-dimensional models. With periodic boundary conditions, eight-vertex and Gaussian model operators are found. The scaling dimensions of the Ashkin-Teller and Potts models are obtained by the exact relating of eigenstates of their quantum Hamiltonians to those of the XXZ chain with modified boundary conditions. The irrelevant operators governing the dominant finite-size corrections are also identified.

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Two ideas unify the theory of critical phenomena in two dimensions. These are conformal invariance[1,2] and the notion that there exist general models to which specific models of physical interest can be related by appropriate transformations.[3-5] Examples of such "central theories" are the Coulomb (lattice) gas[3] and the generalized Gaussian model.[4] While analysis[3-6] of these generalized models can yield detailed information on the critical behavior of the related physical models, including critical exponents, the possible universality classes are not predicted by this formalism.[7]

The universality classes of two-dimensional [or equivalently (1+1)-dimensional] theories are constrained, however, by conformal invariance.[2,8] Within conformal theory, these classes are characterized by a single dimensionless number c, the central charge or conformal anomaly of the associated Virasoro algebra, the irreducible representations of which determine the operator algebra describing the critical behavior. If c is less than unity, unitarity restricts[8] c to the values $c=1-6/m(m+1)$, $m=3,4,5....$ For such theories, which include the Ising ($c=\frac{1}{2}$) and three-state Potts ($c=\frac{4}{5}$) models amongst others, the operator algebra is finite; the anomalous dimensions being given by the Kac formula.[9] The limiting value $c=1$ is of particular interest. This class includes the four-state Potts model and models[10] such as the eight-vertex and Askin-Teller models exhibiting continuously varying exponents.

In this Letter, we identify the possible operators of $c=1$ theories from a study of the spectrum of the one-dimensional quantum XXZ model:

$$H_{XXZ}=-\frac{\gamma}{2\pi\sin\gamma}\sum_{i=1}^{L}(\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y+\Delta\sigma_i^z\sigma_{i+1}^z). \tag{1}$$

Here $\sigma^x,\sigma^y,\sigma^z$ are Pauli matrices and $\Delta=-\cos\gamma$, $\gamma\in[0,\pi]$. In the bulk limit, $L\to\infty$, this Hamiltonian is massless with critical exponents varying continuously with Δ.[10] The prefactor in (1) is included to ensure that the resulting equations of motion are conformally invariant.[11] Its precise value can be inferred[12] from the known[13] energy-momentum dispersion relation. The value of the conformal anomaly follows[14] from the behavior of the ground-state energy $E_0(\Delta,L)$ for periodic boundary conditions as $L\to\infty$. Analytical[12] and numerical results[15] yield

$$E_0(\Delta,L)/L=e_\infty-\pi/6L^2+o(L^{-2}), \tag{2}$$

confirming[16] $c=1$.

The major advantage of the XXZ model over other possible Hamiltonians with $c=1$ is that its spectrum on a finite lattice can be calculated by the Bethe *Ansatz*. The Bethe-*Ansatz* solution of the infinite XXZ chain is well known.[10,17] Surprisingly, the method has received relatively little attention as a *numerical* procedure for computation of the spectra of finite chains.[15,18] We have found[19,20] that numerical solution of Bethe-*Ansatz* equations is feasible for quite large lattices up to $L\sim 512$ not only for the ground state[15,18] but also for various excited states. In addition, the method can be extended[20] to yield eigenvalues of (1) subject to the generalized boundary condition

$$\sigma_{L+1}^x\pm i\sigma_{L+1}^y=e^{\pm\varphi}(\sigma_1^x\pm i\sigma_1^y),\quad \sigma_{L+1}^z=\sigma_1^z, \tag{3}$$

where φ is an arbitrary angle. For all φ, H can be block-diagonalized into disjoint sectors labeled by $n=\sum\sigma^z/2$.

Our subsequent analysis and identification of critical operators rely on the predictions[2,21] of conformal invariance concerning the spectrum of a critical quantum Hamiltonian in a finite strip. The key results can be summarized as follows: To each primary operator $\mathcal{O}$, with scaling dimension x and spin s, in the operator algebra there exists a set of states in the quantum Hamiltonian. For a chain with periodic boundary conditions, the energy and momentum of these states are given by

$$E_{n,n'}(L)=E_0(L)+2\pi(x+n+n')L^{-1}+o(L^{-1}),\quad n,n'=0,1,\ldots, \tag{4a}$$

$$P_{n,n'}=2\pi(s+n-n')/L,\quad n,n'=0,1,\ldots, \tag{4b}$$

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respectively. From these relations and our eigenvalue data we are able to estimate with very high precision various anomalous dimensions for any coupling. Typical estimates of several anomalous dimensions are shown for $\gamma=\pi/6$ ($\Delta=-\sqrt{3/2}$) in Table I. Similar accuracy is possible for other values of γ except near $\gamma=0$, where it is necessary to extend the calculations to larger lattices because of the slower convergence with L.

Let us discuss initially our findings for even L and periodic boundary conditions ($\phi=0$). The lowest-energy state in each sector yields, through (4), a set of operators $\mathcal{O}_{n,0}$ with scaling dimensions $x_{n,0}=n^2x_p$ where $x_p=(\pi-\gamma)/2\pi$. The operators $\mathcal{O}_{1,0}$ and $\mathcal{O}_{2,0}$ correspond to the polarization and energy operators of the eight-vertex model.[5] This identification of $\mathcal{O}_{1,0}$ confirms that made from an analytical treatment[12] of the Bethe-*Ansatz* equations. We have also obtained the lower levels in the conformal blocks associated with these operators, in accord with (4). Stringlike solutions of the Bethe-*Ansatz* equations yield excited states corresponding to further operators $\mathcal{O}_{n,m}$ with dimensions

$$x_{n,m}=n^2x_p+m^2/4x_p,\quad n,m=0,1,2,\ldots. \tag{5}$$

These operators are the analogs of the Gaussian-model operators[4,5] composed of a spin-wave excitation of index n and a "vortex" excitation of vorticity m. Hence, we can identify the operator $\mathcal{O}_{0,1}$ as the crossover operator of the eight-vertex model or equivalently the energy operator of the Ashkin-Teller model. The operator $\mathcal{O}_{0,2}$ is irrelevant for $\gamma>0$ but becomes marginal at $\gamma=0$. As we shall see, this operator is the main determinant of finite-size corrections for both the XXZ and Ashkin-Teller models as well as for the logarithmic corrections that appear in the four-state Potts model. Finally, the spectrum contains a state which gives $x=2$ for all γ. The associated operator is thus marginal corresponding to the four-spin coupling of the eight-vertex model. Its presence in $c=1$ theories results in the appearance of a line of critical points, the operator itself governing motion along the critical line.[4-6]

The identification of $\mathcal{O}_{0,1}$ as the Ashkin-Teller energy operator can be confirmed directly since it is possible to derive[20] the eigenvalues of the critical quantum Ashkin-Teller model[22] with four-spin coupling λ on an M-site chain exactly from those of a $2M$-site XXZ chain with $\Delta=-\lambda$ subject to (3) for particular values of ϕ. High-precision estimates of the anomalous dimensions of the Ashkin-Teller model then follow from (4). In addition to identifying $x_{0,1}$, we find[20] that the difference in ground-state energy for $\varphi=\pi$ and $\varphi=0$ gives the mass-gap amplitude corresponding to the Ashkin-Teller polarization operator with dimension $x_{0,1/2}$, the indices in (5) being extended to fractional values. Similarly, we are able to locate all of the parafermions present in the Ashkin-Teller model. Our numerical results suggest that the dimension of the spin-$\frac{1}{4}$ parafermion is $x_{1,1/4}$, which clarifies previous results.[23]

To obtain the order and disorder operators of the Ashkin-Teller model it is necessary to apply the boundary condition, $\sigma_{L+1}^x=\sigma_1^x$, $\sigma_{L+1}^y=-\sigma_1^y$, $\sigma_{L+1}^z=\sigma_1^z$, to the XXZ chain. The "magnetic" [$Z(2)$-charged] sector of the Ashkin-Teller model is then located in the ground-state sector of the XXZ model. While the Bethe-*Ansatz* is no longer applicable, the required eigenvalues can be computed easily by the Lanczos method for chains up to $L=20$. Extrapolation of the resulting gaps gives, for all γ, the values $\frac{1}{8}$ and $\frac{5}{8}$ for the dimensions of the magnetic order and spin-$\frac{1}{2}$ parafermion operators of the Ashkin-Teller model, respectively.

The generalized boundary conditions (3) are also of interest because they connect the XXZ model to the q-state Potts model. Specifically, the eigenvalues in the ground-state sector of the quantum Hamiltonian[24] of the critical q-state Potts model on a lattice of M sites can be related[20] exactly to eigenvalues of a $2M$-site XXZ chain with $\Delta=-\cos\gamma=-\frac{1}{2}\sqrt{q}$ and $\varphi=2\gamma$. For $\varphi\neq0$, (2) is no longer valid. The coefficient of the L^{-2} term becomes $-\pi c(\varphi)/6$, where our results strongly suggest that $c(\varphi)=1-12x_{0,\varphi/2\pi}$. Setting $\varphi=2\gamma$ reproduces the value of the conformal anomaly of the Potts model,[14,25] namely, $c(q)=1-6\gamma^2/\pi(\pi-\gamma)$. New higher-energy states also appear in the XXZ spectrum corresponding to (new) Potts operators. In particular, the Potts energy operator (dimension x_ε) is associated with a string state in the ground-state sector of the XXZ model. Similarly, the eigenstates of the Potts Hamiltonian associated with the

TABLE I. Finite-lattice estimates of anomalous dimensions of the XXZ chain for $\gamma=\pi/6$, $x_p=\frac{5}{12}$, $x_{n,m}=n^2x_p+m^2/4x_p$.

L \ (n,m)	$(0,\frac{1}{2})$	$(1,0)$	$(1,\frac{1}{4})$	$(0,1)$	Marginal
8	0.155 19	0.397 93	0.436 06	0.4791	1.5699
16	0.152 17	0.405 94	0.444 60	0.5074	1.7522
32	0.151 04	0.410 63	0.448 97	0.5289	1.8538
64	0.150 55	0.413 27	0.451 28	0.5453	1.9126
128	0.150 30	0.414 74	0.452 54	0.5579	1.9477
256	0.150 17	0.415 57	0.453 24	0.5677	1.9690
$x_{n,m}$	0.15	0.416	0.454 16	0.6	2.0

order and spin-$1/q$ parafermion operators (dimensions x_σ and $x_{\rm pf}$) can be obtained from the XXZ Hamiltonian by application of (3) with $\phi=\pi$ and $\phi=2\pi/q$, respectively. As a result, we are able to compute eigenenergies of the Potts Hamiltonian on very large lattices for any q. In contrast, conventional finite lattice calculations[24] are restricted to $M\le 10$. Table II lists the resulting estimates of x_ε, x_σ, and $x_{\rm pf}$ for $q=4$. Cardy[26] has recently shown that these estimates should converge as $1/\ln M$. Allowing for such a convergence rate yields the "extrapolated" values quoted in Table II. These are in excellent agreement with the expected results. More generally, for arbitrary $q=4\cos^2\gamma$, our numerical estimates[20] are in full agreement with the expressions

$$x_\varepsilon=(\pi+2\gamma)/2(\pi-\gamma),$$

$$x_\sigma=(\pi^2-4\gamma^2)/8\pi(\pi-\gamma),$$

$$x_{\rm pf}=(\pi-\gamma)/2\pi+(\pi^2-q^2\gamma^2)(\pi-\gamma),$$

thereby confirming predictions from Coulomb-gas calculations[27] and the identifications made by Dotsenko.[25]

We have also investigated numerically the corrections to (4a). These corrections arise[21] since a lattice Hamiltonian such as (1) deviates from the conformally invariant Hamiltonian H^* of the continuum theory by terms involving irrelevant operators, i.e.,

$$H=H^*+\sum_{j=1}^{n} a_j\mathcal{O}_j+\ldots, \tag{6}$$

where a_j are coupling constants. Among these operators are those associated with the conformal block of the identity operator $\mathcal{O}_I$, the leading operator of which has dimension $x_I=4$. For the periodic case ($\varphi=0$), our numerical results indicate that the dominant correction terms in (4a) can be accounted for by considering in addition to $\mathcal{O}_I$ the operator $\mathcal{O}_{0,2}$, with scaling dimension $\bar{x}\equiv x_{0,2}=2\pi/(\pi-\gamma)$. It is, however, necessary to go beyond the first-order perturbation calculation of the corrections performed by Cardy.[21] More generally, we obtain[20] for the eigenenergy, $E_{n,m}$, associated with dimension $x_{n,m}$, the expansion

$$\frac{E_{n,m}}{L}\approx e_\infty+2\pi L^{-2}\left(x_{n,m}-\frac{1}{12}+\sum_{\substack{k=0\\(k,l)\neq(0,0)}}^{\infty}\sum_{l=0}^{\infty}\alpha_{k,l}L^{-k(\bar{x}-2)-2l}\right), \tag{7}$$

where e_∞ is the ground-state energy per particle of the infinite lattice and the periodic ground state corresponds to $(n,m)=(0,0)$ and $x_{0,0}=0$. The coefficients $\alpha_{k,l}$ depend[20,21] on the couplings a_i and the operator-product expansion coefficients $c_{i,j,k}$. In particular, $\alpha_{1,0}$ depends linearly on $c_{n,m;n,m;0,2}$. In the Gaussian model,[4] this coefficient vanishes unless $(n,m)=(0,1)$. It appears that this selection rule remains true for the XXZ chain. Specifically, we find that the corrections to the amplitude corresponding to the energy operator of the Ashkin-Teller model, the operator $\mathcal{O}_{0,1}$ in the XXZ model, are of the form $L^{-2}(b_0L^{-2\gamma/(\pi-\gamma)}+b_1L^{-2})$ while for all the other operators leading corrections are $L^{-2}(b_0\times L^{-4\gamma/(\pi-\gamma)}+b_1L^{-2})$. In this case the dominant correction term switches at $\gamma=\pi/3$ which accounts for the behavior found by Hamer.[12] At $\gamma=\pi/3$, the leading correction is $O((\ln L)/L^4)$. It is also interesting to observe that as $\gamma\to 0$, $x_{0,2}\to 2$ and more powers in (7) corresponding to higher values of k become important. This gives a simple visualization of the reason for the poor convergence rate observed in finite lattice calculations around the four-state Potts point ($\gamma=0$). Strictly at $\gamma=0$ the number of equally important corrections tends to infinity and the original couping constants in (6) renormalize giving rise to the logarithmic corrections.[26]

We have analyzed the correction terms for the generalized boundary conditions. In particular, for the Potts model with $q>2$, the leading corrections for the energy and order-parameter amplitudes are of order $L^{-(2-x')}$,

TABLE II. Estimates of anomalous dimensions of the four-state Potts model.

M	x_ε	x_σ	$x_{\rm pf}$
4	0.771 229	0.143 407	0.459 772
8	0.722 621	0.139 056	0.474 226
16	0.684 992	0.136 751	0.483 573
32	0.657 247	0.135 233	0.490 105
64	0.636 473	0.134 106	0.494 965
128	0.620 490	0.133 217	0.498 747
256	0.607 858	0.132 493	0.501 786
512	0.597 638		
Extrapolated	0.501 ± 0.002	0.126 ± 0.002	0.529 ± 0.003
Exact	0.5	0.125	0.531 25

where $x'=2(\pi+\gamma)/(\pi-\gamma)$. This value is precisely that of the second thermal exponent of the Potts model.[25,28]

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