Spectrum of the biquadratic spin-1 antiferromagnetic chain

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An exact correspondence between the staggered biquadratic spin-1 antiferromagnetic chain and the quantum Hamiltonian limit of the nine-state Potts model is established for finite chains with free ends. For uniform interactions this equivalence is used (via a further exact mapping to a Bethe ansatz soluble *XXZ* model) to calculate exactly the infinite lattice values of the ground-state energy per site and the (nonzero) gap to the lowest-energy excited state. Periodic boundary conditions and the nature of the ground state as a function of bond alternation are also discussed.

Recently, there has been a considerable renewal of interest in the ground-state properties of quantum antiferromagnets. One model of particular interest is the spin-1 bilinear-biquadratic Hamiltonian:

$$H=\sum_i \epsilon_i[J_1\mathbf{S}_i\cdot\mathbf{S}_{i+1}-J_2(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2]\ , \tag{1}$$

where both J_1 and J_2 are positive and

$$\epsilon_i=\begin{cases}1 & \text{if } i \text{ is odd}\\ \lambda & \text{if } i \text{ is even}\ ,\end{cases} \tag{2}$$

controls bond alternation and hence the tendency to dimerization via a possible spin-Peierls transition.[1,2] Key questions involve the determination of the regions of the $(\beta-\lambda)$ plane, $\beta=J_2/J_1$, in which (1) is massless and the elucidation of the associated critical behavior.

For $\lambda=1$ and $J_2=0$, (1) reduces to the spin-1 Heisenberg antiferromagnet, which was predicted by Haldane[3] to be nonintegrable and massive, a conclusion that has been supported by numerical results.[4] For $\lambda=1$, exact solutions are available at two points. At $J_1=J_2$ ($\beta=1$) the model is soluble by the Bethe ansatz.[5,6] At this point the model is found to be massless and conformally invariant; the associated conformal field theory governing the critical behavior being that of the $k=2$ Wess-Zumino-Witten model.[7] This conclusion has been confirmed by series analysis[1] and finite lattice studies.[8,9] An exact solution is also available at $\beta=-\frac{1}{3}$, $\lambda=1$, where the exact ground state is a valence bond state.[10] At this point the model again has a gap. Whether $\beta=1$ is the only massless point on the line $\lambda=1$ remains unclear. In particular, the nature of the ground state for $\lambda=1$, $\beta>1$ remains controversial; Affleck *et al.*[10] predict a massive phase, while series[1] and (less confidently) finite lattice studies[2,11] suggest a massless phase.[12]

In this paper we consider the Hamiltonian (1) with $J_1=0$ and show that in this limit (1) is equivalent to the quantum Hamiltonian version of the nine-state Potts model.[13,14] In addition, we show that an *exact* equivalence exists between eigenstates of (1) with $J_1=0$ and $\lambda=1$ and eigenstates of certain spin-$\frac{1}{2}$ *XXZ* chains thereby clarifying and extending some very intriguing observations made by Parkinson.[15] As a consequence of these equivalences, we are able to calculate the exact values of the ground-state energy per site and the lowest-energy gap in the thermodynamic limit for $\lambda=1$, see (31) and (33) below. This value of the ground-state energy per site confirms that conjectured by Parkinson,[15] while the nonzero gap confirms an earlier conjecture[7] that (1) is massive for $J_1=0$ and $\lambda=1$.

The first step in the derivation of our results is to express the pure biquadratic Hamiltonian

$$H_{bQ}(M,\lambda)=-\sum_{l=1}^{M-1}\epsilon_l(\mathbf{S}_l\cdot\mathbf{S}_{l+1})^2 \tag{3}$$

for a chain of M sites with *free ends* in terms of a set of operators U_l that satisfy a Temperley-Lieb algebra.[16,17] Define

$$U_l=(\mathbf{S}_l\cdot\mathbf{S}_{l+1})^2-1,\quad l=1,2,\ldots,M-1\ , \tag{4}$$

and write

$$H_{bQ}(M,\lambda)=-\sum_{l=1}^{M-1}\epsilon_l U_l-\tfrac{1}{2}M-\lambda(\tfrac{1}{2}M-1)\ . \tag{5}$$

(For convenience, we henceforth assume that M is even.)

Denote the eigenstates of S_l^z and S_{l+1}^z by $|m_1m_2\rangle$, $m_1=\pm,0$, $m_2=\pm,0$, and order them

$$|++\rangle,\ |+0\rangle,\ |0+\rangle,\ |+-\rangle,\ |00\rangle,$$
$$|-+\rangle,\ |0-\rangle,\ |-0\rangle,\ |--\rangle\ .$$

A simple computation shows that $U_l|m_1m_2\rangle=0$ unless $m_1+m_2=0$. Hence, in this representation, U_l takes the

simple form[15]

$$U_l=\begin{bmatrix}0&0&0\\0&\mathbf{V}&0\\0&0&0\end{bmatrix}, \tag{6}$$

where $\mathbf{0}$ is the 3×3 zero matrix and

$$V=\begin{bmatrix}1&-1&1\\-1&1&-1\\1&-1&1\end{bmatrix}. \tag{7}$$

It is now straightforward algebra to show that

$$U_l^2=3U_l\ , \tag{8}$$

$$U_lU_{l\pm1}U_l=U_l\ , \tag{9}$$

$$[U_l,U_{l'}]=0,\quad |l-l'|>1\ . \tag{10}$$

The first of these relations was noted in passing by Parkinson.[15] Together they establish that the operators U_l satisfy the same Temperley-Lieb algebra that arises in the nine-state Potts model.[17,18]

To explicitly recover the quantum Hamiltonian of the Potts model, we introduce an alternative representation[19,20] of the U's:

$$U_{2l-1}=\tfrac{1}{3}\sum_{k=0}^{8}\Omega_l^k,\quad l=1,2,\ldots,L\ , \tag{11}$$

$$U_{2l}=\tfrac{1}{3}\sum_{k=0}^{8}R_l^kR_{l+1}^{9-k},\quad l=1,2,\ldots,L-1\ , \tag{12}$$

where $L=M/2$. The operators Ω_l and R_l at site l obey a $Z(9)$ algebra

$$\Omega_lR_l=\omega^{-1}R_l\Omega_l\ , \tag{13}$$

$$\Omega_lR_l^\dagger=\omega R_l^\dagger\Omega_l\ , \tag{14}$$

$$\Omega_l^9=R_l^9=1\ , \tag{15}$$

with $\omega=e^{2\pi i/9}$. Hence, we can write

$$3H_{bQ}(2L,\lambda)=H_{P_9}(L,\lambda)-4L-4\lambda(L-1)\ , \tag{16}$$

where

$$H_{P_9}(L,\lambda)=-\sum_{l=1}^{L}\sum_{k=1}^{8}\Omega_l^k-\lambda\sum_{l=1}^{L-1}\sum_{k=1}^{8}R_l^kR_{l+1}^{9-k} \tag{17}$$

is the $(1+1)$-dimensional quantum Hamiltonian of the nine-state Potts model[21,22] on a chain of L sites with, again, free ends. The coupling parameter λ is the analogue of temperature in the conventional statistical mechanical formulation of the Potts model. The transition point of the Potts model corresponds to $\lambda=\lambda_c=1$ with $\lambda>1$ corresponding to the ordered phase ($T<T_c$).

Unfortunately, the Potts Hamiltonian (17) cannot be diagonalized exactly. However, introducing the representation[16,17] of the Temperley-Lieb operators in terms of Pauli spin operators:

$$U_l=\tfrac{1}{2}(\sigma_l^x\sigma_{l+1}^x+\sigma_l^y\sigma_{l+1}^y)+\tfrac{1}{2}\cosh\theta(1-\sigma_l^z\sigma_{l+1}^z)+\tfrac{1}{2}\sinh\theta(\sigma_{l+1}^z-\sigma_l^z)\ , \tag{18}$$

where $\cosh\theta=\sqrt{q}\,/2=\frac{3}{2}$, allows H_{P_9} (and hence H_{bQ}) to be related to a staggered XXZ model.[20,22] For $\lambda=1$, the staggering vanishes and we find

$$H_{bQ}(M,\lambda=1)=H_{XXZ}(M)-\tfrac{7}{4}(M-1)\ , \tag{19}$$

where

$$H_{XXZ}(M)=-\tfrac{1}{2}\sum_{l=1}^{M-1}(\sigma_l^x\sigma_{l+1}^x+\sigma_l^y\sigma_{l+1}^y+\Delta\sigma_l^z\sigma_{l+1}^z)+\tfrac{1}{2}p(\sigma_1^z-\sigma_M^z) \tag{20}$$

is the Hamiltonian of an XXZ model on a chain of M sites with fields $\frac{1}{2}p$ and $-\frac{1}{2}p$ applied to the two free ends. In our present case

$$\Delta=-\tfrac{3}{2} \tag{21}$$

and

$$p=\tfrac{1}{2}\sqrt{5}\ .$$

The XXZ Hamiltonian (20) is solvable by the Bethe ansatz.[23,24] Since the total spin $\sum\sigma^z$ commutes with H_{XXZ}, we can label the sectors of H_{XXZ} by $n=\frac{1}{2}M-\frac{1}{2}\sum\sigma^z$, where for M even n is an integer. The eigenvalues of H_{XXZ} in sector n are then given by[23]

$$E=\tfrac{3}{4}(M-1)-\sum_{j=1}^{n}(3+z_j+z_j^{-1})\ , \tag{22}$$

where the z_j are solutions of the Bethe ansatz equations

$$z_j^{2M}=\prod_{\substack{k=1\\k\neq j}}^{n}\frac{S(z_k,z_j)S(z_k^{-1},z_j)}{S(z_j,z_k)S(z_j,z_k^{-1})}\ ,\quad j=1,2,\ldots,n \tag{23}$$

with

$$S(z,z')=1+3z'+zz'\ . \tag{24}$$

The lowest-energy state in sector n is characterized by n zeros distributed around the upper half of the unit circle. In particular, the ground state corresponds to the choice $n=\frac{1}{2}M$.

Equations (16) and (19) are exact operator equivalencies: apart from additive and multiplicative constants $H_{bQ}(2L,\lambda=1)$, $H_{P_9}(L,\lambda=1)$, and $H_{XXZ}(2L)$ are simply the sum $\sum U_l$ of the Temperley-Lieb operators. The possible eigenvalues of this sum, and hence the three Hamiltonians, are determined by the algebra (8)–(10). However, degeneracies are not determined by the algebra but by the dimension of the specific representation chosen for the Temperley-Lieb operators.[17] This is not a problem for H_{P_9} on L sites and H_{bQ} on $M=2L$ sites (both with free ends) since both Hamiltonians are represented by $3^{2L}\times3^{2L}$ matrices. Hence, all eigenvalues of $H_{P_9}(L,\lambda)$ should also be eigenvalues of $H_{bQ}(2L,\lambda)$ and all eigenvalues should occur with the same degeneracies in both cases.[25] On the other hand, since $H_{XXZ}(2L)$ is only of dimension 2^{2L} eigenvalues of $H_{bQ}(2L)$ will appear in the spectrum of H_{XXZ} with, in general, smaller multiplicities. Indeed, it is possible for eigenvalues of H_{bQ} not to occur

at all in the spectrum of H_{XXZ}, although our numerical diagonalizations for small L suggest that this does not occur.

The finite lattice spectra of the q-state Potts Hamiltonians with $q>4$ are fairly well understood.[26,27] We can use this information to elucidate the ground state and spectrum of the biquadratic Hamiltonian. It is convenient to divide the state space of H_{P_9} into sectors labeled by the eigenvalues of

$$\prod_{l=1}^{L}\Omega_l=\omega^{\hat{q}},\quad \hat{q}=0,1,\ldots 8\ . \tag{25}$$

and to similarly block diagonalize H_{bQ} and H_{XXZ} into sectors labeled by $S_T^z=\sum S^z$ and $\sigma_T^z=\sum\sigma^z$, respectively.

In the thermodynamic limit the nine-state Potts model exhibits a first-order transition.[28] In the Hamiltonian formulation this transition occurs at $\lambda=1$. For $\lambda>1$ (corresponding to $T<T_c$) the ground state of H_{P_9} in the thermodynamic limit should be ninefold degenerate. This degeneracy is partially removed for finite L with the sectors $\hat{q}=1,\ldots 8$ remaining degenerate by the Potts symmetry by a nonzero gap

$$F(\lambda,L)=E_1(\lambda,L)-E_0(\lambda,L) \tag{26}$$

opening between $E_0(\lambda,L)$, the ground state in the sector $\hat{q}=0$, and $E_1(\lambda,L)$, the lowest-energy state in any sector $\hat{q}\neq 0$. A simple perturbation argument, similar to that in Barber and Cates,[29] establishes that

$$F(\lambda,L)=O(\lambda^{-L}),\quad L\to\infty,\quad \lambda>1\ . \tag{27}$$

On the other hand, for $\lambda<1$, the thermodynamic limit of the ground state of H_{P_9} is a singlet and we have[30]

$$\lim_{L\to\infty}F(\lambda,L)=F_\infty(\lambda)>0,\quad \lambda<1\ . \tag{28}$$

The existence of the first-order transition implies

$$\lim_{\lambda\to 1^-}F_\infty(\lambda)=F_\infty(1)\neq 0\ . \tag{29}$$

While we know of no rigorous proof, the limit $\lambda\to 1^-, L\to\infty$ is believed (e.g., on the basis of finite-size scaling) to be uniform and that

$$\lim_{L\to\infty}F(1,L)=F_\infty(1)\ . \tag{30}$$

In the thermodynamic limit the first-order nature of the transition is also heralded[26,27] by the crossing of two states in the $\hat{\mathbf{q}}=0$ sector at $\lambda=1$. This crossing gives rise to a jump discontinuity in the first derivative of the ground-state energy with respect to λ and hence a latent heat. On a finite lattice these two states hybridize to give a finite gap

$$F_0(\lambda,L)=E_2(\lambda,L)-E_0(\lambda,L)\ ,$$

which is greater than zero for all λ. However, in distinction to $F(1,L)$, $F_0(1,L)\to 0$ as $L\to\infty$.

Since for finite L, both $H_{P_9}(L,\lambda)$ and $H_{bQ}(2L,\lambda)$ have matrix representations of the same dimension we can translate these conclusions on the behavior of the spectrum of $H_{P_9}(L,\lambda)$ directly to that of $H_{bQ}(2L,\lambda)$. The only subtlety concerns the assignment of the Potts eigenstates to the correct total spin sectors of H_{bQ}. Denote the Potts states of energies E_0 and E_2 in the ground-state sector by $|0;L\rangle$ and $|2;L\rangle$, respectively, and the eight degenerate states of energy E_1 by $|1,j;L\rangle$, $j=1,\ldots,8$. Comparison of the actual spectra for small values of L reveals that the ground state of $H_{bQ}(2L,\lambda)$ is $|0;L\rangle$, the ground state having $S_T^z=0$, while the eight degenerate states $|1,j;L\rangle$ occur in the sectors $S_T^z=0,\pm 1$ and ± 2 with degeneracies 2, 2, 2, 1, and 1, respectively. Finally, $|2;L\rangle$ is a singlet in the $S_T^z=0$ sector but for small L this state lies well above the states $|1;L\rangle$ and only approaches the ground state for relatively long chains. Turning to the spectrum of $H_{XXZ}(2L)$ we find that $E_0(\lambda=1,L)$ and $E_1(\lambda=1,L)$ are related to the lowest energies in the sectors $\sigma_T^z=0(n=L)$ and $\sigma_T^z=2(n=L-1)$, respectively, while $E_2(\lambda=1,L)$ is similarly related to the energy of a two-string state in the ground-state $(n=L)$ sector. Consequently, $E_0(\lambda=1,L)$, $E_1(\lambda=1,L)$, and $E_2(\lambda=1,L)$ can all be found by solving the Bethe ansatz equations (23) with $M=2L$ rather than by direct diagonalization of the Hamiltonian. For E_0 and E_1 this solution is numerically feasible[31] for M up to 256. Table I lists the resulting values of the ground-state energy per site, e_g of $H_{bQ}(M,\lambda=1)$ and the associated gap

$$\Lambda_{bQ}=\tfrac{1}{3}[E_1(\lambda=1,\tfrac{1}{2}M)-E_0(\lambda=1,\tfrac{1}{2}M)]$$

as functions of M. Estimates of the limiting values of e_g and Λ_{bQ} in the limit $M\to\infty$ are also given in the last line of Table I, these being obtained by standard acceleration techniques.[32] Unfortunately, the solution corresponding to the state associated with energy E_2 is more difficult to determine numerically because of ill-conditioning problems. Consequently, we have not been able to track this state for as large lattices. However, as we discuss later, it is possible to do so for periodic boundary conditions thereby confirming that the gap $F_0(1,L)$ does close as $L\to\infty$.

The thermodynamic limit of the ground-state energy of $H_{XXZ}(M)$ is known exactly.[33,34] From this result and (19) we obtain the exact value

$$e_g=-1-\frac{\sqrt{5}}{2}\left[1+4\sum_{n=1}^{\infty}(1+x^n)^{-1}\right]\ , \tag{31}$$

TABLE I. Numerical estimates of e_g and Λ_{bQ} for $H_{bQ}(M,\lambda=1)$.

M	e_g	Λ_{bQ}
4	−2.390 388	2.147 339
8	−2.591 376	1.410 916
16	−2.693 622	0.886 786
32	−2.745 162	0.555 720
64	−2.771 005	0.362 166
128	−2.783 934	0.256 914
256	−2.790 399	0.205 372
extrap.	−2.796 88±0.000 02	0.175±0.003

where

$$x=\tfrac{1}{2}(7+3\sqrt{5})\ . \tag{32}$$

The result (31) is precisely that conjectured recently by Parkinson.[15] Numerically, $e_g=-2.796\,863\ldots$, which confirms the limit estimated in Table I.

Similarly, we can calculate the value of the lowest-lying gap in $H_{bQ}(M,\lambda=1)$ in the limit $M\to\infty$ from the XXZ results of des Cloizeaux and Gaudin.[35] Explicitly, we find that

$$\Lambda_{bQ}=\tfrac{1}{3}F_\infty(1)=\sqrt{5}\prod_{n=1}^{\infty}\left[\frac{1-t^n}{1+t^n}\right]^2, \tag{33}$$

where $t=\sqrt{x}=(3+\sqrt{5})/2$. Evaluating this expression numerically yields

$$\Lambda_{bQ}=0.173\,178\ldots\ , \tag{34}$$

which again confirms the numerical estimate in Table I. Note that this is actually a rather more significant confirmation than the agreement of the results for e_g since it is not *a priori* obvious that a finite lattice calculation with free-end boundary conditions will display the same gaps as one with periodic boundary conditions.

A possible connection between eigenstates of $H_{bQ}(M,\lambda=1)$ and the XXZ Hamiltonian has been suggested previously by Parkinson.[15] However, Parkinson's considerations were based on the biquadratic model with *periodic boundary conditions* rather than free ends. Specifically, Parkinson observed that eigenenergies of states with nonzero spin S_T^z of $H_{bQ}(M,\lambda=1)$ with periodic boundary conditions also occurred in the M-site periodic XXZ chain with again $\Delta=-\frac{1}{2}$. However, this equivalence did not extend to states with $S_T^z=0$, although in the thermodynamic limit both Hamiltonians appeared to have the same ground-state energy per site.

The relation of the Potts Hamiltonian with periodic boundary conditions to the XXZ chain is also more complicated than with free ends.[20] In this case the ground-state sector of the periodic Potts Hamiltonian on L sites corresponds to the spin-zero sector of an XXZ model on $2L$ sites with a defect seam or *twisted* boundary conditions.[20,36] For the nine-state Potts model, the operator equivalence is

$$H_{P_9}^0(L,\lambda=1)=-\tfrac{5}{2}L+3H_{XXZ}(2L;\theta)\ . \tag{35}$$

Here $H_{P_9}^0(L,\lambda)$ is given by (17) with the second sum extended to L and periodic boundary conditions applied, i.e., $R_L+1=R_1$, while

$$H_{XXZ}(M;\theta)=-\tfrac{1}{2}\sum_{l=1}^{M}(\sigma_l^x\sigma_{l+1}^x+\sigma_l^y\sigma_{l+1}^y-\tfrac{3}{2}\sigma_l^z\sigma_{l+1}^z) \tag{36}$$

subject to the "twisted" boundary conditions

$$\sigma_{M+1}^z=\sigma_1^z,\quad \sigma_{M+1}^x\pm i\sigma_{M+1}^y=e^{\mp 2\theta}(\sigma_1^x\pm\sigma_1^y)\ , \tag{37}$$

where $e^{2\theta}=x$.

Since the total spin $\sum\sigma^z$ remains a good quantum number, $H_{XXZ}(M;\theta)$ can still be diagonalized by the Bethe ansatz.[20] The eigenvalues in sector n are given by

$$E=\tfrac{3}{4}M-\sum_{j=1}^{n}(3+z_j+z_j^{-1})\ , \tag{38}$$

where the z_j now satisfy

$$z_j^M=(-1)^{n-1}e^{-2\theta}\prod_{k=1}^{n}\frac{S(z_k,z_j)}{S(z_j,z_k)},\quad j=1,\ldots,n \tag{39}$$

with the function $S(z,z')$ defined in (24).

In view of the equivalences (35) and (16), it is tempting to conjecture that the ground-state sector ($S_T^z=0$) of the periodic biquadratic Hamiltonian

$$H_{bQ}^0(2L,\lambda)=-\lambda\sum_{i=1}^{L}(\mathbf{S}_{2i}\cdot\mathbf{S}_{2i+1})^2-\sum_{i=1}^{L}(\mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i})^2 \tag{40}$$

with $\mathbf{S}_{2L+1}=\mathbf{S}_1$ is similarily related for $\lambda=1$ to the ground-state sector of $H_{XXZ}(M;\theta)$ by the operator equivalence

$$H_{bQ}^0(M,\lambda=1)=H_{XXZ}(M;\theta)-\tfrac{7}{4}M\ . \tag{41}$$

While we are unable to establish this equivalence rigorously we have tested it numerically for small lattices and found excellent agreement up to multiplicities between the two spectra.

In the limit $M\to\infty$, the boundary conditions do not affect the value of the ground-state energy per spin and we recover (31). The gap is somewhat more subtle because the XXZ equivalence involves eigenstates defined with *different* boundary conditions. Explicitly, we have

$$\Lambda_{bQ}=\lim_{M\to\infty}[E_{XXZ}^1(M,\theta=0)-E_{XXZ}^0(M,\theta)]\ , \tag{42}$$

where $E_{XXZ}^0(M,\theta)$ is the ground-state energy of (36) subject to the boundary conditions (37) and $E_{XXZ}^1(M,\theta=0)$ is the lowest energy in the sector $\sum\sigma^z=1$ of (36) with $\theta=0$ in (37); i.e., periodic boundary conditions. We can write (42) as

$$\Lambda_{bQ}=\Lambda_{XXZ}+\lim_{M\to\infty}\Delta E_{XXZ}^0(\theta)\ , \tag{43}$$

where

$$\Lambda_{XXZ}=\lim_{M\to\infty}[E_{XXZ}^1(M,\theta=0)-E_{XXZ}^0(M,\theta=0)] \tag{44}$$

is precisely the XXZ gap calculated by des Cloizeaux and Gaudin[35] and

$$\Delta E_{XXZ}^0(\theta)=E_{XXZ}^0(2L,\theta)-E_{XXZ}^0(2L,\theta=0) \tag{45}$$

is the shift in the ground-state energy due to the modification in the boundary conditions. Numerically, this shift appears to go to zero very rapidly but for technical reasons we have not been able to establish this analytically from the Bethe ansatz equations.[37]

The solution of the Bethe ansatz equations (39) corresponding to the ground state of $H_{bQ}^0(M,\lambda=1)$ is characterized by $n=\frac{1}{2}M$ zeroes satisfying $\prod_{j=1}^{n}z_j=e^{-\theta}$. For

large M, a second spin-zero state approaches the ground state. This state is a one-string solution of (39) with one zero at $z_1=-e^{-\theta}$ and the remaining $n-1$ zeroes satisfying $\prod_{j=2}^{n} z_j=1$. These zeroes lie on the unit circle and are distributed symmetrically about the real axis. The energy of this state agrees precisely with the ($k=\pi$) state detected by Parkinson[15] in direct finite lattice calculations on $H_{bQ}^{0}(M,\lambda=1)$ with $M\leq 14$.

The equivalence of H_{bQ} and H_{P_9} has one rather surprising implication: the ground state of H_{bQ} for $\lambda>1$ (which corresponds to $T<T_c$ in the Potts model) is asymptotically ninefold degenerate. This is, however, an artifact of the free-end boundary conditions and does not pertain to H_{bQ} with periodic boundary conditions or presumably in the thermodynamic limit. This is most easily seen if we consider H_{bQ} for $\lambda\gg 1$. In this limit, the ground-state energy of $H_{bQ}(\lambda,2L)$ asymptotes to $-3\lambda L$: the ground state being formed by placing each spin pair $\mathbf{S}_{2i}\cdot\mathbf{S}_{2i+1}$, $i=1,2,\ldots,L$, in the singlet state

$$(|+-\rangle-2|00\rangle+|-+\rangle)/\sqrt{3}\ .$$

The end spins $\mathbf{S}_1$ and $\mathbf{S}_{2L}$ are, however, not included in any dimer and to leading order in $1/\lambda$ become decoupled. The ninefold degeneracy of the ground state for $\lambda\rightarrow\infty$ is then just a trivial consequence of the three possible values that each end spin can take. Three of these states, ($S_1^z=+,S_{2L}^z=-$), ($S_1^z=-,S_{2L}^z=+$), and ($S_1^z=0$, $S_{2L}^z=0$), lie in the $S_T^z=0$ sector of H_{bQ}. The addition of a coupling $-\lambda\mathbf{S}_{2L}\cdot\mathbf{S}_1$ between $\mathbf{S}_1$ and $\mathbf{S}_{2L}$ as occurs with periodic boundary conditions breaks this degeneracy and results in (for $\lambda>0$) a singlet ground state. A similar situation occurs in the spin-1 Hamiltonian discussed by Affleck *et al.*[10] In that case, a rigorous proof can be given of the uniqueness of the ground state in the thermodynamic limit.[10] It seems plausible that this is also true for the biquadratic Hamiltonian with $\lambda\neq 1$ although we have as yet no proof.

One other piece of useful information concerning the ground-state energy per site, $e_g(\lambda)$, of $H_{bQ}(\lambda)$ in the thermodynamic limit can be deduced from the equivalence to the nine-state Potts model. We observe from (40) that

$$e_g(\lambda)=\lambda e_g(1/\lambda)\ , \tag{46}$$

which corresponds to the duality relation in the Potts model.[21] Now from (16)

$$e_g(\lambda)=\tfrac{1}{6}e_{\mathrm{Potts}}(\lambda)-\tfrac{2}{3}(1+\lambda)\ , \tag{47}$$

where $e_{\mathrm{Potts}}(\lambda)$ is the ground-state energy per site of the nine-state Potts Hamiltonian in the thermodynamic limit. This energy is known to have a discontinuous first derivative at $\lambda=1$ corresponding to the latent heat.[22] Hence, we have that

$$e_g(\lambda)=e_g(1)+A_{\pm}|1-\lambda|+O[(1-\lambda)^2]\ , \tag{48}$$

where $e_g(1)$ is given by (31) and

$$A_{\pm}=\pm\tfrac{1}{2}[e_g(1)\mp L_h] \tag{49}$$

with L_h equal to one-third of the latent heat of the nine-state Potts model. This has been calculated by Hamer[27] from the results of Baxter.[28] From Hamer's result we obtain

$$L_h=\sqrt{5}\prod_{n=1}^{\infty}\left[\frac{x^n-1}{x^n+1}\right]^2\ , \tag{50}$$

where x is given by (32). Evaluating this expression numerically gives

$$A_+=-1.9606\ldots$$

and

$$A_-=0.8362\ldots\ . \tag{51}$$

An attempt to extract the variation of $e_g(\lambda)$ near $\lambda=1$ from finite lattice calculations has been reported by Sólyom[2,38] who concluded that

$$e_g(\lambda)-e_g(1)\sim|1-\lambda|^{2\nu} \tag{52}$$

with $\nu\sim 0.5$. While this estimate of ν is not inconsistent with a linear dependence on $|1-\lambda|$, Sólyom does not appear to have contemplated a jump discontinuity in $e_g'(\lambda)$ at $\lambda=1$ and his subsequent inference that the spectrum at $\lambda=1$ is gapless is incorrect. Instead $\lambda=1$ is a point at which two spontaneously dimerized states exchange stability. These states can be distinguished by the value of the *dimerization order parameter*[1]

$$D(\lambda)=\lim_{M\rightarrow\infty}\sum(-)^i\langle\mathbf{S}_i\cdot\mathbf{S}_{i+1}\rangle/M\ ,$$

where the angular brackets denote a ground-state expectation value. Unique ground states exist for $\lambda>1$ and $\lambda<1$ with $D>0$ and $D<0$, respectively. Unfortunately, it does not seem possible to compute the limiting values $D(1^{\pm})$ from the Potts and/or XXZ equivalences.

In conclusion, we have mapped the spin-1 bilinear-biquadratic Hamiltonian (1) for $J_1=0$ onto the quantum Hamiltonian of the nine-state Potts model. As a consequence of this mapping we conclude that the isotropic (i.e., $\lambda=1$) pure biquadratic Hamiltonian has a twofold degenerate ground state with a finite gap of approximately $0.17J_2$ to the next excited state. This gap is less than half the value ($\sim 0.41J_1$) that has been estimated[39] for the Haldane gap in the pure Heisenberg model ($J_2=0$). While our analysis cannot be extended in any obvious way to $J_1\neq 0$, it seems plausible that the picture we discussed of the ground state of H_{bQ} as a function of λ also holds for $1<\beta<\infty$ with, in particular for $\lambda=1$, a finite gap that decreases to zero as β approaches unity. If this is the case, it could explain why series and finite lattice analyses have tended to conclude that the line $\lambda=1$, $\beta>1$ is massless. It would be worthwhile to repeat some of these analyses in the light of the exact results reported in this paper.

Note added in proof. After completing this work we received a report from A. Klümper (unpublished) confirming our result (34) by a direct calculation on a corresponding vertex model.

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