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Observations on the Bethe ansatz solutions of the spin-1/2 isotropic anti-ferromagnetic Heisenberg chain

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Abstract

Evidence is presented that the solutions of the Bethe ansatz equations for spin-½ isotropic Heisenberg chains in fixed total spin and momentum sectors are the roots of single variable polynomials with integer (or integer based) coefficients. Such solutions are used as a starting point for investigation of long chain (critical region) properties. In the total spin $S = 0$ sector I conjecture explicit formulae for the Bethe string configuration labelling of all left and right tower excitations in the $k = 1$, SU(2) Wess-Zumino-Witten model.

1. Introduction

This paper presents empirical observations about the states of (even) length L periodic chains of $s = ½$ spins anti-ferromagnetically coupled as defined by the Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{L} \vec{\sigma}_i\, \vec{\sigma}_{i+1}, \qquad \vec{\sigma}_{L+1} = \vec{\sigma}_1 \tag{1}$$

where i labels both the sites and distance along the chain and the components of $\vec{\sigma}_i$ are the Pauli spin matrices. Symmetry dictates that eigenstates of (1) can be labelled by total S and S_z and (quasi) momentum K. Each stretched state ($S_z = S$) is constructed from $N = L/2 - S$ overturned spins from the totally aligned spin configuration. Any $S_z < S$ state can be generated by angular momentum lowering operators but will not be discussed here. Bethe [1] (for an English translation see [2]) showed (1) is soluble by associating with each overturned spin a (quasi) momentum eigenvalue k_n, $-\pi < k_n \leqslant \pi$. These eigenvalues satisfy the Bethe ansatz equations (BAE)

$$\left(\frac{\lambda_n + i}{\lambda_n - i}\right)^L = \prod_{m \neq n}\left(\frac{\lambda_n - \lambda_m + 2i}{\lambda_n - \lambda_m - 2i}\right), \qquad \lambda_n = \cot\left(\frac{k_n}{2}\right), \qquad n, m = 1, 2, \ldots \frac{L}{2} - S. \tag{2}$$

The (scaled) sum of the k_n is the total momentum

$$K = \left(\frac{L}{2\pi}\right)\sum_{n=1}^{N} k_n, \quad N = \frac{L}{2} - S, \tag{3}$$

an integer which, with (symmetric) modulo L understood, satisfies $-L/2 < K \leqslant L/2$. Solutions for negative K, $-L/2 < K < 0$, are obtained from those at positive K by sign reversal of all k_n. The energy of any state that is a solution of the BAE (2) is given by

$$E = \frac{L}{2} - 2\sum_{n=1}^{N}(1 - \cos(k_n)) = \frac{L}{2} - \sum_{n=1}^{N}\frac{4}{1 + \lambda_n^2} \tag{4}$$

and is clearly unaffected by k_n sign reversal.

While some progress has been made in the numerical solution of the BAE (2) (cf Hao *et al* [3]) it remains a difficult challenge. Here I present evidence that there exist important relations satisfied by BAE solutions that can be used as easily implemented checks on existing numerical solutions and/or provide alternative methods of solution. The evidence is most apparent when instead of momenta k or rapidities λ one uses $x = 2\cos(k)$. Consider the case that $K = L/6, L/4$, or $L/3$ (or their negatives) and let $D_K = D_K(L, S)$ be the total number of eigenstates of (1) at the given K, L and S. I find the polynomial

$$P_K(x) = \prod_{i=1}^{ND_K} (x - x_i) = \sum_{i=0}^{ND_K} r_i x^i,\ \ N = \frac{L}{2} - S, \tag{5}$$

formed from the BAE solutions has real, rational coefficients r_i and can be rationalized to form an integer coefficient polynomial $I_K(x)$. One can consider the process in reverse. For any given $I_K(x)$ existing commercial software such as Maple will efficiently find all roots x_i and a finite search algorithm can find the D_K combinations of N momenta $k_i = \pm\arccos(x_i/2)$ that satisfy the BAE. In principle $I_K(x)$ can be found from a single[1] solution $x = x_1$ say, obtained to some minimum accuracy, by an integer relation algorithm such as PSLQ [4] implemented on Maple. More practically, one can combine all the solutions of the BAE that are most easily found with a less accuracy demanding PSLQ to determine $I_K(x)$. Similar considerations apply for $K = 0$ and L/2. Here symmetry allows solution of the BAE to be determined from integer coefficient polynomials $I_K(x)$ of reduced degree whose roots are only the non-trivial x_i.

For all other K the BAE solutions are the roots of polynomials whose coefficients are 'integer based'. What this means is that the K in the interval $0 < K < L/2$ group into blocks K_d with M_d members consisting of those K whose greatest common divisor with L is d. The number of members $M_d = \varphi(L/d)/2$ where $\varphi(n)$ is Euler's function (cf Hardy and Wright [5] section 5.5). If $M_d = 1$ the situation is that described by (5); otherwise the members of K_d have the same D_K and the terms $\cos(2\pi mK/L)$, $m = 0, 1, \ldots, M_d - 1$, are integrally independent. The root polynomial analog of (5) for any member is

$$P_K(x) = \prod_{i=1}^{ND_K} (x - x_i^{(K)}) = \sum_{i=0}^{ND_K} \left(r_{0,i} + 2\sum_{m=1}^{M_d-1} r_{m,i} \cos\left(\frac{2\pi}{L} mK\right)\right) x^i \tag{6}$$

where the coefficients $r_{0,i}$ and $r_{m,i}$ are real, rational and *independent* of K and which can, by rationalization, be converted to integer. Thus although the coefficients $p_i^{(K)}$ in $P_K(x) = \sum_{i=0}^{ND_K} p_i^{(K)} x^i$ are in general irrational they are expressible in terms of rational coefficients by the identity $p_i^{(K)} = r_{0,i} + 2\sum_{m=1}^{M_d-1} r_{m,i} \cos(2\pi mK/L)$ from (6). If $p_i^{(K)}$ is known to sufficient accuracy, the PSLQ algorithm will determine the rationals $r_{0,i}$ and $r_{m,i}$. In other words, if all BAE solutions for one member K are known, the polynomials $P_{K'}(x)$ for all other M_d members follow trivially without reference to the BAE.

All of the polynomial generated BAE solutions have been plausibly identified with Bethe string configurations and, by continuity in L, define the Bethe string content at large L. This is important for discussion of the critical behaviour of (1) which Affleck [6] showed is the $k = 1$, SU(2) Wess-Zumino-Witten (WZW) model. Subsequently Affleck *et al* [7] provided additional analytic and numerical confirmation. An apparent discrepancy in the asymptotic behaviour of the ground state energy has recently been resolved [8], justifying a systematic study of other states in long chains to identify the Bethe string content of the left and right tower excitations in the WZW model in the critical region.

In the $S = 0$ sector, the asymptotic $L \to \infty$ energy eigenstates of (1) are expected [7], based on WZW and conformal field theory arguments, to have the form

$$E = -L\left(2\ln(2) - \frac{1}{2}\right) - \frac{\pi^2}{6L} + \frac{\pi^2}{L}\left(\varepsilon + \frac{2s(s+1)}{\ln(L/L_0)} + o\left(\frac{1}{\ln(L)}\right)\right) \tag{7}$$

where ε and -2 s are both non-negative integers and L_0 are non-universal numbers. The spin s in (7) is the spin s_L (s_R) of the independent left (right) excitations in WZW with $\vec{s}_L + \vec{s}_R = \vec{S} = 0$. With the definition $(x)_h = \prod_{n=1}^{h} (1 - x^n)$, the multiplicity of states in (7) at energy ε and relative momentum $\kappa = K - K_c$, $K_c = (L/2 + 2\,s \bmod 2)L/2$, is the coefficient of $e^{\varepsilon} q^k$ in the generator

$$Z(e, q)^{(e/o)} = \sum_{2s=0/1}^{(e/o)} e^{(2s)^2} \left(\sum_{h_L=2s}^{(e/o)} \frac{B_{h_L}^{(2s)}(e^2/q)}{(e^2/q)_{h_L}}\right)\left(\sum_{h_R=2s}^{(e/o)} \frac{B_{h_R}^{(2s)}(e^2 q)}{(e^2 q)_{h_R}}\right) \tag{8}$$

considered as a series expansion in *e*. The notation (e/o) indicates that 2 s and 1-string holes h_L, h_R are either all even or all odd. The essential feature of the generator (8) is its form as a product of independent left and right tower multiplicities. Every term in a tower factor $B_h^{(2s)}(x)/(x)_h$, $h = h_L$ or h_R, can be identified with a Bethe string configuration; the $(x)_h$ denominators account for all possible 1-string excitations obtained by rearrangement of the available 1-string holes *h* while the $B_h^{(2s)}(x)$ are polynomials determined by the remaining (n>1)-strings. General (conjectured) formulas for the $B_h^{(2s)}(x)$ have been confirmed by high order numerical

[1] Provided $I_K(x)$ does not (accidentally) factorize into smaller integer coefficient polynomials. Then a solution is needed for each factor.

calculations to satisfy the WZW tower excitation sum rules

$$x^{s^2}\sum_{\nu=0}^{\infty} B_{2s+2\nu}^{(2s)}(x)/(x)_{2s+2\nu} = (x^{s^2} - x^{(s+1)^2})/(x)_\infty. \tag{9}$$

This brief synopsis of the main results of the paper is expanded in the following sections together with numerous illustrative examples of BAE solutions.

Section 2 is a summary of Bethe's solution for $N = 2$ overturned spins but is here recast in a form that leads directly to (5) and (6). Since the most efficient implementation of the PSLQ algorithm requires the number of unknown constants to be available, section 3 is devoted to deriving formulas for $D_K(L, S)$. At the symmetry points $K = 0$ and $L/2$, states are either non-degenerate or 2-fold degenerate coming from the inversion symmetry $k_n \to -k_n$ that leaves K and E unchanged. Explicit formulas for these symmetry distinct state counts are also derived. Section 4 provides example BAE solutions at $K = 0$ and $L/2$; some of these are directly derivable algebraically from (2) and provide justification for (5) that extends beyond the $N = 2$ overturned spin case. Section 5 reports some general K results for $N = 3$. Here confirmation of (5) and (6) is based entirely on numerical inference but is important because it shows the conjectured structure is not an accidental feature that arises because the BAE have an analytic solution when $N = 2$. Section 6 is devoted to the example $L = 16$, $S = 0$. Results from sections 4, 5 and 6 of the more extensive polynomials and associated state lists are provided as text files L20_nondegen.txt, 3_overturned_spins.txt and L16_singlet.txt respectively in supplementary data. Section 7 describes the basis for the multiplicity generator (8) and the general formulas for the $B_h^{(2s)}(x)$. Conclusions form section 8.

2. Two overturned spins

The BAE (2) for two overturned spins are

$$\left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^L = \frac{\lambda_1 - \lambda_2 + 2i}{\lambda_1 - \lambda_2 - 2i} = \left(\frac{\lambda_2 - i}{\lambda_2 + i}\right)^L \tag{10}$$

and the equality between first and last term implies the roots of unity condition

$$\left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)\left(\frac{\lambda_2 + i}{\lambda_2 - i}\right) = \exp(2\pi i K/L) \Rightarrow k_1 + k_2 = \frac{2\pi}{L}K \tag{11}$$

with the scaling convention (3) for the total momentum. We can also use the first equation in (11) for a second relation,

$$\lambda_2 = \frac{\lambda_1 + T}{\lambda_1 T - 1}, \qquad T = \tan(\pi K/L), \tag{12}$$

and on inserting this into the first equality in (10) obtain

$$\left(\frac{\lambda_1 + i}{\lambda_1 - i}\right)^{L-1} = \frac{(\lambda_1 + i)T - 2}{(\lambda_1 - i)T - 2}, \tag{13}$$

a result that applies equally to λ_2. A useful equivalent to (13) for either λ obtained by cross multiplying and rearranging is

$$(\lambda^2 + 1)((\lambda + i)^{L-2} - (\lambda - i)^{L-2})\sin\left(\frac{\pi K}{L}\right) = 2((\lambda + i)^{L-1} - (\lambda - i)^{L-1})\cos\left(\frac{\pi K}{L}\right). \tag{14}$$

For $K = 0$, the solutions to (14) are given by the roots of unity condition $(\lambda + i)/(\lambda - i) = \exp(2\pi i n/(L - 1))$ or $k_n = 2n\pi/(L - 1)$, $n = -L/2 + 1, -L/2 + 2, \ldots, L/2 - 1$ from which we must exclude $k_n = 0$ as the solution for the $S = L/2$ uniform state. The $S = L/2 - 2$ solutions are the distinct pair combinations satisfying $k_1 + k_2 = 0$. There are $L/2 - 1$ such (non-degenerate) pairs and these exhaust the k_n list for pairs. In summary, the solution lists $\hat{k}_K^S$ and k_K^S of momentum pairs $[k_1, k_2]$ for $K = 0$ are

$$\hat{k}_0^{L/2-2} = \left[\left[\frac{2n\pi}{L-1}, \frac{-2n\pi}{L-1}\right], n = 1, 2, \ldots, \frac{L}{2} - 1\right], \qquad k_0^{L/2-2} = [\text{Null}], \tag{15}$$

adopting the convention of using hatted variables for the non-degenerate states at $K = 0$ and $L/2$. For $K = L/2$, there is one non-degenerate singular solution identified with $\lambda^2 + 1 = 0$. We write the state formally as

$$[\text{Sing}] = [\pi/2 + i\infty, \pi/2 - i\infty] = [-\pi/2 + i\infty, -\pi/2 - i\infty] \tag{16}$$

with finite quantities such as the energy contribution to (4), $\Delta E_{\text{Sing}} = -2$, understood to be the result of a careful limiting procedure. The solutions arising as roots of unity are $k_n = 2n\pi/(L - 2)$, $n = -L/2 + 2$,

$-L/2+3, \ldots, L/2-1$ from which we exclude $k_n = \pi$ as the solution for the $S = L/2 - 1$ spin-wave. The $S = L/2 - 2$ solutions are the distinct k_n pairs which sum to π (modulo 2π). One such set is $k_1 = 2n\pi/(L-2)$, $k_2 = (L-2-2n)\pi/(L-2), 0 < n < \lfloor L/4 \rfloor$. The negatives, $-k_1, -k_2$ are also solutions and exhaust the possibilities. Since reversing the signs of all k_n leaves the energy unchanged as well as the sum $k_1 + k_2 = \pi$ (modulo 2π), each state is doubly degenerate. In summary, for $K = L/2$,

$$\hat{k}_{L/2}^{L/2-2} = [[\text{Sing}]], \quad k_{L/2}^{L/2-2} = \left[\left[\frac{2n\pi}{L-2}, \frac{(L-2-2n)\pi}{L-2}\right], n = 1, 2, \ldots, \lfloor L/4 \rfloor - 1\right] \tag{17}$$

where it is understood that we list only the positive half of the degenerate states.

For $0 < K < L/2$ we first express (14) in alternative forms. By dividing through by $(\lambda^2+1)^{L/2}$ we get the equivalent

$$\sin\left(\frac{k}{2}(L-2)\right)\sin\left(\frac{\pi K}{L}\right) = 2\sin\left(\frac{k}{2}\right)\sin\left(\frac{k}{2}(L-1)\right)\cos\left(\frac{\pi K}{L}\right) \tag{18}$$

which is useful for contributing to the discussion by Bethe [1] and Essler *et al* [9] of a possible complex pair $k = \pi K/L \pm i y_K$ solution for $K > 1$. On substituting either k into (18) we find after some algebra that y_K must satisfy

$$\cos(\pi K/L) = \begin{cases} \sinh(y_K(L-2)/2)/\sinh(y_K L/2), & K\ odd, \\ \cosh(y_K(L-2)/2)/\cosh(y_K L/2), & K\ even. \end{cases} \tag{19}$$

The left hand side of (19) differs from unity by $O(1/L^2)$ for large L whereas the right hand side for odd K never exceeds $1 - 2/L$. Thus we recover the known result that for fixed odd $K > 1$ there is always some critical length L_c satisfying $\cos(\pi K/L_c) = 1-2/L_c$ beyond which the complex solution transforms via $y_K \to i y_K$ to two real solutions. The (19) for even K always has a solution but is interesting in that the associated λ pair has imaginary parts $\Im(\lambda) \approx \pm 2L^{1/2}/(\pi K)$ for fixed K and $L \to \infty$ that do not approach the ideal 2-string values ± 1 [10].

A second alternative forms the basis for the polynomials (5) and (6). Squaring both sides of (14) yields an equation explicitly dependent on λ^2 only which we write as $\lambda^2 = (2+x)/(2-x), x = 2\cos(k)$. After rearranging and multiplying through by the denominator factor $(2-x)^{L-1}$ and a convenient normalization we arrive at an equation for k given by

$$C_K(x) = A + B - (A - B)\cos\left(\frac{2\pi K}{L}\right) = 0, \quad k_n = \pm\arccos(x_n/2), \tag{20}$$

where the x_n are the roots of $C_K(x)$. In the process of squaring (14) we have lost k_n sign information but this can be recovered by a finite m, n and sign search process in which we demand the correct signs in (20) are those for which $k_m + k_n = 2\pi K/L$. The A and B in (20) are polynomials in $x = 2\cos(k)$ of degree $L-3$ and $L-1$ respectively; explicitly,

$$\begin{aligned} A &= \frac{x+2}{4^{L-3}}\left(\sum_{n=1}^{L/2-1}\binom{L-2}{2n-1}(x+2)^{L/2-1-n}(x-2)^{n-1}\right)^2 \\ &= (x+2)\left(\sum_{m=0}^{\lfloor L/4\rfloor-1}(-1)^m\binom{L/2-2-m}{m}x^{L/2-2-2m}\right)^2, \\ B &= \frac{x-2}{4^{L-2}}\left(\sum_{n=1}^{L/2}\binom{L-1}{2n-1}(x+2)^{L/2-n}(x-2)^{n-1}\right)^2 \\ &= (x-2)\left(\sum_{m=0}^{\lfloor (L-2)/4\rfloor}(-1)^m\binom{L/2-1-m}{m}x^{L/2-2-2m}\left(x+\frac{L/2-1-2m}{L/2-1-m}\right)\right)^2. \end{aligned} \tag{21}$$

To reduce $C_K(x)$ to the polynomial $P_K^S(x)$ whose only roots are those for $S = L/2\text{–}2$ we must divide out the factor $x - 2\cos(2\pi K/L)$ for the $S = L/2\text{–}1$ spin-wave. If K is odd we must also divide out two spurious root factors $(x - 2\cos(\pi K/L))(x + 2\cos(\pi K/L))$; the first ($k = \pi K/L$) is easily shown to be a solution of (18) but has no pair partner for a BAE solution because the second ($k = \pi - \pi K/L$) leads to left and right hand sides of (18) having opposite sign. In summary,

$$P_K^{L/2-2}(x) = \begin{Bmatrix} C_K(x)/\begin{pmatrix} x^3 - 2c_{1K}x^2 - (2+2c_{1K})x \\ +2 + 4c_{1K} + 2c_{2K} \end{pmatrix}, & K\ odd \\ C_K(x)/(x - 2c_{1K}), & K\ even \end{Bmatrix}, \quad c_{nK} = \cos\left(\frac{2\pi n K}{L}\right), \tag{22}$$

where the roots x_n of $P_K^{L/2-2}$ combine into $L/2 - 2(L/2-1)$ BAE solution pairs for K odd(even). For every BAE solution of (22) one automatically has also a BAE solution for $-K$ obtained by simply reversing all k_n signs.

A summary list of the number of solutions $\hat{\nu}_K$ which is the non-degenerate part of $D_K(L, S)$ for $K = 0$ and $L/2$, ν_K which is one-half of the remaining degenerate part and $\nu_K = D_K(L, S)$ for $0 < K < L/2$ is

$$[\hat{\nu}_0, \nu_0, \nu_K(0 < K < L/2), \nu_{L/2}, \hat{\nu}_{L/2}] = [L/2 - 1, 0, L/2 - 2, L/2 - 1, \ldots, \lfloor L/4 \rfloor - 1, 1] \tag{23}$$

where the ellipsis indicates a repetition of the alternating sequence $L/2 - i, i = 2, 1, 2, \ldots$ to a total of $L/2 - 1$ terms. The total number of states from (23) is

$$\hat{\nu}_0 + 2\left\{\sum_{K=0}^{L/2} \nu_K\right\} + \hat{\nu}_{L/2} = \frac{L(L-3)}{2} \tag{24}$$

in agreement with the expected binomial difference $\binom{L}{N} - \binom{L}{N-1}$ for $N = 2$ overturned spins.

For $K = L/6, L/4$ or $L/3$ all cosine terms in (22) are rational so that (22) simplifies by elementary division to a polynomial with rational coefficients. As example, for $L = 12, S = 4$ and $K = 2, 3$ and 4 we find the rationalized polynomials $P_K^4(x) = \sum_{i=0}^{2\nu_K} I_{K,i}^4 x^i$ where the integer lists $[I_{K,i}^4,\ i = 0..2\nu_K]$ are

$$\begin{aligned}
I_2^4 &= [4, 36, 48, -111, -133, 87, 99, -27, -29, 3, 3],\\
I_3^4 &= [5, 6, -22, -8, 22, 2, -8, 0, 1],\\
I_4^4 &= [4, -12, -24, 61, 5, -49, 13, 13, -7, -1, 1].
\end{aligned} \tag{25}$$

In general let the roots x_i of the polynomials $P_K^{L/2-2}(x)$ be arranged in lists of non-decreasing $\Re(x_i)$ order. Then the corresponding BAE solutions, which are the momentum pairs $[k_m, k_n]$ satisfying $k_m + k_n = 2\pi K/L$, are compactly given in lists $k_K^{L/2-2} = [[n_1, n_2], [n_3, n_4], \ldots]$ where $|n_i|$ are position pointers to the root lists and

$$k_{n_i} = \frac{n_i}{|n_i|}\arccos(x_{|n_i|}/2). \tag{26}$$

For the example leading to the polynomials (25), the associated state lists when energy ordered are

$$\begin{aligned}
k_2^4 &= [[-1, -3], [2, -5], [4, -7], [6, -8], [9, 10]],\\
k_3^4 &= [[-1, -4], [2, -5], [3, -8], [6, 7]],\\
k_4^4 &= [[-3, -4], [-1, -6], [2, -10], [5, 9], [7, 8]].
\end{aligned} \tag{27}$$

For general K in $0 < K < L/2$ excluding $K = L/6, L/4$ and $L/3$ treated above, elementary algebraic division in (22) will lead to products of cosines that can always be eliminated by use of $2\cos(a)\cos(b) = \cos(a + b) + \cos(a - b)$. The resulting polynomial $P_K^{L/2-2}$ has coefficients that are sums of (possibly many redundant) c_{nK}. By using various trigonometric identities it is possible to reduce the number of c_{nK} in the coefficient of any x^i to a minimum number of integrally independent terms. As a first step in this reduction, inversion and shifts

$$c_{nK} = (-1)^K c_{\left(\frac{L}{2}-n\right)K} = (-1)^K c_{\left(n-\frac{L}{2}\right)K} = c_{(L-n)K} = \cdots \tag{28}$$

allow replacement of any c_{nK} by c_{mK} with $0 \leqslant m \leqslant \lfloor L/4 \rfloor$ provided we treat separately even and odd K so that the replacement rule (28) with its $(-1)^K$ factors is the same for all K in either category. Such separation with distinct rules for different groups but the same rules for every K within a group dictates that the general grouping is defined by blocks K_d where d is the greatest common divisor of K and L. The number of members M_d in block K_d is $\varphi(L/d)/2$ where $\varphi(n)$ is Euler's function and the division by 2 arises from our restriction $0 < K < L/2$. Any K_d with one element will be one of $L/6, L/4$ or $L/3$ which was considered in the preceding paragraph.

Before dealing with the general c_{mK} reduction to an integrally independent set consider the $L = 12, S = 4$ example again. The distinct blocks are $K_1 = 1, 5$ and $K_2 = 2, K_3 = 3, K_4 = 4$ so that only K_1 remains to be treated[2]. The c_{mK} left after reduction by (28) are $1, c_{1K}, c_{2K}$ and c_{3K} but for $K = K_1 = 1$ or 5, $c_{2K_1} = 1/2$ and $c_{3K_1} = 0$ leaving only the integrally independent 1 and c_{1K_1} in which to express the result of the division (22). The explicit result for the rationalized P_K^4 from (22) is

$$P_K^4(x) = \sum_{i=0}^{2\nu_K}(I_{1,i}^4 + 2I_{5,i}^4\cos(\pi K/6))x^i,\ \ K = 1, 5 \tag{29}$$

where $\nu_1 = \nu_5 = 4$ and

$$\begin{aligned}
I_1^4 &= [-8, 0, 16, 8, -1, -11, -7, 3, 2],\\
I_5^4 &= [4, -4, -12, 11, 10, -9, -5, 2, 1].
\end{aligned} \tag{30}$$

This differs from (6) only in notation; in any specific case it is preferable to replace generic labels by the distinct K_d values, e.g. $\{r_0,r_1\} \to \{I_1,I_5\}$ here. From the roots of $P_K^4(x)$ we can construct the BAE states

[2] I use K_d as a label both for a single element and the set of elements $\{K_d\}$; the context determines what is meant.

$$k_1^4 = [[1, -2], [3, -4], [5, -6], [7, -8]],$$
$$k_5^4 = [[-2, -4], [-1, -8], [3, 7], [5, 6]] \tag{31}$$

exactly as was done in arriving at (27) including energy ordering.

Some general results for the reduction of the number of c_{mK} below the $\lfloor L/4 \rfloor + 1$ left following use of (28) have been obtained and I begin by illustrating this for block K_1. The number of elements in K_1 cannot exceed the $\lfloor L/4 \rfloor$ reached when block K_1 contains all odd K in the interval $0 < K < L/2$ so that one replacement beyond (28) will always be required. This can be taken to be

$$c_{MK_1} = \begin{cases} 0, & L = 4M \\ (-1)^{M-1}\left(\frac{1}{2} + \sum_{m=1}^{M-1}(-1)^m c_{mK_1}\right), & L = 4M + 2 \end{cases} \tag{32}$$

where the $L = 4M$ case is the trivial $\cos(\pi n/2) = 0$ for n odd (e.g. $c_{3K_1} = 0$ in the $L = 12$ example above). The result in (32) for $L = 4M + 2$ follows from the roots of unity condition $\sum_{n=1}^{N} \cos((2n - 1)\pi/(2N + 1)) = 1/2$ together with (28). No identities beyond (28) and (32) are needed if $L/2 = p$, p prime >2, or $L/2 = 2^{\ell}$. If L has odd divisors >1 some of the odd K in the interval $0 < K < L/2$ will be excluded in the construction of K_1. We will then need as many new identities as there have been exclusions. One set of identities follows trivially from (32) – whenever L is a multiple of some $4M + 2$, $M > 0$, then

$$c_{fMK_1} = (-1)^{M-1}\left(\frac{1}{2} + \sum_{m=1}^{M-1}(-1)^m c_{fmK_1}\right), \quad L = f(4M + 2), \tag{33}$$

which with $f > 1$ supplements (32). An example is $f = 2$, $M = 1$ giving $c_{2K_1} = 1/2$ used in the $L = 12$ discussion leading to (29). Other identities follow from (33) which we get by first rewriting (33) as $1 + \sum_{m=1}^{M}(-1)^m 2c_{fmK_1} = 0$. On multiplying this by c_{iK_1} and again using the identity $2\cos(a)\cos(b) = \cos(a + b) + \cos(a - b)$ we obtain

$$c_{iK_1} + \sum_{m=1}^{M}(-1)^m(c_{(fm+i)K_1} + c_{(fm-i)K_1}) = 0, \quad L = f(4M + 2). \tag{34}$$

An example replacement using (34) is at $L = 24$ ($f = 4$, $M = 1$) where $K_1 = 1, 5, 7, 11$ and with $i = 1$, $c_{5K_1} = c_{1K_1} - c_{3K_1}$. Together with $c_{4K_1} = 1/2$ from (33) and $c_{6K_1} = 0$ from (32) we are left with the required four integrally independent 1, c_{1K_1}, c_{2K_1} and c_{3K_1} coefficients.

Every block K_d has its own set of rules analogous to (32)–(34). For example for K_2,

$$c_{MK_2} = \begin{cases} -1, & L = 4M \\ -\frac{1}{2} - \sum_{m=1}^{M-1} c_{mK_2}, & L = 4M + 2 \end{cases} \tag{35}$$

replaces (32) and there are corresponding replacements for (33) and (34). For any given L and divisor d, at most two c_{mK_d} relations are needed to complete the division (22) provided these are used in replacements at each step of the division process so as to always limit the maximum m in c_{mK_d} to a fixed number. Furthermore, the effort to derive the required relations from formulas such as (32)–(34) can be avoided by using a PSLQ determination instead. Specifically, for any L and d we know the number of K_d elements is $M_d = \varphi(L/d)/2$ and the empirical evidence, based on PSLQ analysis, is that $c_{mK_d} = \cos(2\pi m K_d/L)$, $m = 0, 1, \ldots, M_d - 1$, are integrally independent and can be used as a basis in which to express any c_{mK_d}, $m \geqslant M_d$, as a sum with rational coefficients. The PSLQ algorithm, with any K_d as numerical input, will provide an analytical expression for $c_{M_d K_d}$ that suffices for d even and in addition $c_{(M_d+1)K_d}$ that is required for d odd. This procedure has been confirmed for all even L to 100.

This completes the $N = 2$ overturned spin analysis that forms the basis for (5) and (6). Many examples have shown the structure of (5) and (6), as defined by the blocks K_d with M_d members, remains unchanged for any $N \leqslant L/2$ overturned spins. The N dependence lies entirely in the degree of the integer polynomials which relates directly to the number of states $D_K(L, S)$ determined in the next section.

3. State counting

To determine the number D(N, L, K) of states of total momentum K for N overturned spins in a length L periodic chain start with the observation that the binomial $\binom{L}{N}$ is the total number of configurations ψ for fixed N and L and these can be separated into exclusive classes ψ_d where d is a common divisor of L and N. The distinguishing feature of class ψ_d is that for configurations $T_n\psi_d$ (translations by $n = 1, 2, \ldots$ from ψ_d) the first occurrence of $T_n\psi_d = \psi_d$ is at $n = L/d$. Such configurations are formed from d repetitions of N/d overturned spins on segments of length L/d.

The configurations in ψ_d can be grouped into D_d blocks, each block containing L/d translation related configurations $T_{n-1}\psi$, $n = 1, \ldots, L/d$, which provide a basis for forming, by superposition, D_d states for each total K which is necessarily restricted to multiples of d. Adding together the state counts (L/d) D_d of every class ψ_d gives the total $\begin{pmatrix} L \\ N \end{pmatrix}$; this is the sum rule

$$\begin{pmatrix} L \\ N \end{pmatrix} = \sum_{d|(N,L)} \frac{L}{d} D_d. \tag{36}$$

The notation used in (36) and the following is that (M, M′) is the greatest common divisor of a pair M, M′ while m|M denotes m is a divisor, including 1 and M, of M and $\Sigma_{m|M}$ means sum over m subject to the constraint m|M. More generally, the total number of periodic configurations of period L/d is $\begin{pmatrix} L/d \\ N/d \end{pmatrix}$ and contributing to this total are the classes $\psi_{(N,L)/d'}$ for d′|(N, L)/d. The corresponding sum rule is

$$\begin{pmatrix} L/d \\ N/d \end{pmatrix} = \sum_{d'|(N,L)/d} \frac{d'L}{(N,\,L)} D_{(N,L)/d'},\quad d|(N,\,L), \tag{37}$$

with (36) being the special case d = 1. The number of equations (37) are the number σ_0 of divisors d of (N, L) and these uniquely determine the σ_0 unknown D_d. The number of states D(N, L, K) then follows as

$$D(N,\,L,\,K) = \sum_{d|(N,L)} \Delta_{d,K} D_d \tag{38}$$

where $\Delta_{d,K} = 1$ if d|K and 0 otherwise; this incorporates the fact that K for states in class ψ_d are restricted to multiples of d. By periodicity, K can only take on L distinct values giving $\sum_K \Delta_{d,K} = L/d$ and so we confirm $\sum_K D(N,\,L,\,K) = \begin{pmatrix} L \\ N \end{pmatrix}$ from (38) together with (36).

An explicit formula for D_d is obtained as follows. Define f(d′) as the expression in the sums (37) and replace that equation list by the equivalent

$$\begin{pmatrix} dL/(N,\,L) \\ dN/(N,\,L) \end{pmatrix} = g(d) = \sum_{d'|d} f(d'),\quad d|(N,\,L), \tag{39}$$

formed by the substitution d → (N, L)/d which runs over the same values. The Möbius inversion formula (cf Hardy and Wright [5] section 16.4) applied to (39) gives

$$\frac{dL}{(N,\,L)} D_{(N,L)/d} = f(d) = \sum_{d'|d} \mu(d') g\left(\frac{d}{d'}\right),\quad d|(N,\,L), \tag{40}$$

where μ is the Möbius function. An equivalent of (40) is obtained by the substitution d → (N, L)/d again and when the resulting D_d is substituted into (38) we get the explicit state count

$$D(N,\,L,\,K) = \sum_{d|(N,L)} \Delta_{d,K} \frac{d}{L} \sum_{d'|(N,L)/d} \mu(d') \begin{pmatrix} L/(dd') \\ N/(dd') \end{pmatrix},\quad 0 < N < L. \tag{41}$$

For N = 0 or L, $D(N, L, K) = \delta_{0K}$, the fully aligned states. The number of states $D_K(L, S)$ at fixed $S = S_z$ is given by the well known subtraction

$$D_K(L,\,S) = D(L/2 - S,\,L,\,K) - D(L/2 - S - 1,\,L,\,K),\quad S < L/2, \tag{42}$$

supplemented by $D_K(L, L/2) = \delta_{0K}$.

As an example consider L = 12. We get from D(N, L, K) in (41) that D(1, 12, K) = 1, D(2, 12, K) = $5 + \Delta_{2,K}$, D(3, 12, K) = $18 + \Delta_{3,K}$, D(4, 12, K) = $40 + 2\Delta_{2,K} + \Delta_{4,K}$, D(5, 12, K) = 66, D(6, 12, K) = $75 + 3\Delta_{2,K} + \Delta_{3,K} + \Delta_{6,K}$ while a subtraction (42) gives $D_K(12, 0) = 9 + 3\Delta_{2,K} + \Delta_{3,K} + \Delta_{6,K}$. The values $D_0(12, 0) = 14$ and those for other L using (41) and (42) agree with the sums D(SP01) + D(SP02) given by Fabricius *et al* [11] in their Table II. On the other hand D(6, 12, 0) = 80 calculated here differs from their $D(S_z{=}0, K = 0) = 44$. More detailed comparison shows that $D(S_z = 0, K = 0)$ in [11] incorrectly includes only even S contributions. That the state counts (41) are correct has been confirmed by many additional checks including comparison to a generalization of Bethe's [1] state counting to which I now turn.

A string configuration for a state of total spin S and $S_z = S$ on a chain of even length L with periodic boundary conditions is specified by the list $(p_1, p_2, p_3, \ldots)$ where the p_n are the number of n-strings in the configuration. Each n-string is associated with n overturned spins and this yields the constraint

$N = \sum np_n = L/2 - S$ on the total number of overturned spins N. The Bethe formula for the number of states with this configuration, denoted below as $\{p_n\}$, is the product

$$D(L, S, \{p_n\}) = \prod_n \binom{p_n + h_n}{p_n} = \prod_n \binom{p_n + h_n}{h_n}, \quad h_n = 2S + 2\sum_{m>n}(m - n)p_m \tag{43}$$

with each binomial factor the number of ways p_n 'particles' (i.e. strings) and h_n 'holes' can be arranged in $p_n + h_n$ integer slots. An important observation from (43) is that h_n depends only on p_m, $m > n$ and in particular $h_1 = 2S + 2\sum(n - 1)p_n$ is fixed by the n-string content for $n \geqslant 2$. Since the constraint $N = \sum np_n = L/2 - S$ also fixes $p_1 = N - \sum_{n>1}(np_n)$, any configuration can equally be specified by just the list $(p_2, p_3, \ldots)$. Bethe also introduced $P = \sum p_n$ for the total number of 'particles' which yields the alternative expressions $h_1 = 2S + 2\sum(n - 1)p_n = 2S + 2N - 2P = L - 2P$, results that will be of use later (cf (54)).

Bethe shows that $D(L, S, \{p_n\})$ summed over all $\{p_n\}$ that are the unrestricted partitions of N, gives the correct total number of states for N overturned spins but does not explicitly remark on the number of states at fixed total (scaled) momentum $K = (L/2\pi)\sum k_i$. However, implicit in (43) is the observation that a shift of any 'particle' or 'hole' to an adjacent slot leads to the same change $|\Delta K| = 1$. Consequently it is possible to define a generator $Z(L, S, \{p_n\})_q$ which is a polynomial invariant under the interchange $q \leftrightarrow 1/q$ with the coefficient of q^κ being the number of states at $K = \kappa$ relative to a central value $K = K_c$. This generator has the form of $D(L, S, \{p_n\})$ in (43) but with every binomial $\binom{p + h}{p}$ replaced by the Gaussian binomial modified by a prefactor $q^{-ph/2}$ for $q \leftrightarrow 1/q$ invariance. Explicitly,

$$\binom{p + h}{p} \to \begin{bmatrix} p + h \\ p \end{bmatrix}_q = q^{-ph/2}\prod_{k=1}^{h}\frac{(1 - q^{p+k})}{(1 - q^k)} = q^{-ph/2}\prod_{k=1}^{p}\frac{(1 - q^{h+k})}{(1 - q^k)} = \begin{bmatrix} p + h \\ h \end{bmatrix}_q. \tag{44}$$

The justification for this prescription relies first on Pólya's [12] observation that the coefficient of q^A in the expansion of $\prod_{k=1}^{p}(1 - q^{h+k})/(1 - q^k)$ is the number of $p + h$ step walks between (0, 0) and (h, p) that enclose area A between the walk, the x-axis and the line $x = h$. Second, there is a one to one correspondence between Pólya walks and configurations of p particles and h holes and, to within an additive constant, $K = A$. To show this adopt the reference configuration corresponding to the zero area Pólya walk to be that of all particles to the left of all holes with the holes labelled $1, 2, \ldots, h$ in sequence starting with hole 1 as the rightmost hole. A general configuration will have n_i particles to the right of hole i with $0 \leqslant n_1 \leqslant n_2 \leqslant \ldots \leqslant n_h \leqslant p$. If this configuration is represented as a histogram of n_i versus i inscribed in an $h \times p$ rectangle it will be seen to be one of Pólya's walks with $A = \sum_i n_i$. Furthermore every particle to the right of a hole is the result of an adjacent particle hole interchange and a unit increase in momentum implying $\sum_i n_i = K$ and hence $A = K$ relative to the reference configuration momentum.

It is observed empirically that the central (symmetric) K_c is either 0 or $L/2$ (mod L), depending on whether $P = \sum p_n$, is even or odd respectively. On incorporating this result we get as our generalization of the Bethe formula (43) the q-generator

$$Z(L, S, \{p_n\})_q = q^{(P \bmod 2)L/2}\prod_n \begin{bmatrix} p_n + h_n \\ p_n \end{bmatrix}_q, \quad h_n = 2S + 2\sum_{m>n}(m - n)p_m \tag{45}$$

with $[]_q$ for each n given by (44). The coefficient of q^K in (45) is the contribution of the particle configuration $\{p_n\}$ to the number of states at momentum K. Shifts of K by multiples of L are understood to bring K into the first Brillouin zone $-L/2 < K \leqslant L/2$. The relation to the total number of states (42) is

$$\sum_{\{p_n\}} Z(L, S, \{p_n\})_q = \sum_{K=-\frac{L}{2}+1}^{K=\frac{L}{2}} D_K(L, S)q^K \tag{46}$$

where the left hand side sum is understood to be over all partitions of $N = L/2 - S$.

Consider as example $L = 12, S = 0$. Separate the partitions p(6) into even and odd P; then, in a truncated notation and $\{p_n\}$ written as product $\prod n^{p_n}$,

$$
\begin{aligned}
Z_{even} &= \sum_{\{p_n\},P\ even} Z(L=12,\ S=0,\ \{p_n\})_q\\
&= Z(1^6)+Z(1^2 2^2)+Z(1^3 3^1)+Z(3^2)+Z(2^1 4^1)+Z(1^1 5^1)\\
&= 1+\frac{(1-q^5)(1-q^6)}{q^4(1-q)(1-q^2)}+\frac{(1-q^5)(1-q^6)(1-q^7)}{q^6(1-q)(1-q^2)(1-q^3)}+1+\frac{(1-q^5)}{q^2(1-q)}+\frac{(1-q^9)}{q^4(1-q)}\\
&= q^{-6}+q^{-5}+4q^{-4}+5q^{-3}+8q^{-2}+8q^{-1}+12+8q+8q^2+5q^3+4q^4+q^5+q^6,\\
Z_{odd} &= \sum_{\{p_n\},P\ odd} Z(L=12,\ S=0,\ \{p_n\})_q\\
&= Z(1^4 2^1)+Z(2^3)+Z(1^1 2^1 3^1)+Z(1^2 4^1)+Z(6^1)\\
&= q^6\left(\frac{(1-q^5)(1-q^6)}{q^4(1-q)(1-q^2)}+1+\frac{(1-q^7)(1-q^3)}{q^4(1-q)^2}+\frac{(1-q^7)(1-q^8)}{q^6(1-q)(1-q^2)}+1\right)\\
&= q^6 Z_{even}
\end{aligned}
\tag{47}
$$

The sum mapped to the first Brillouin zone is

$$
\begin{aligned}
&Z(L=12,\ S=0)_q=\sum_{\{p_n\}}Z(12,\ 0,\ \{p_n\})_q=Z_{even}+Z_{odd}\\
&=9q^{-5}+12q^{-4}+10q^{-3}+12q^{-2}+9q^{-1}+14+9q+12q^2+10q^3+12q^4+9q^5+14q^6
\end{aligned}
\tag{48}
$$

which agrees with $D_K(12, 0) = 9 + 3\Delta_{2,K} + \Delta_{3,K} + \Delta_{6,K}$ noted in the paragraph following (42). Neither method of calculation distinguishes between degenerate and non-degenerate states at the symmetry points $K = 0$ and $K = L/2$. For that I turn to another generalization of Bethe's method.

Some of the states at $K = K_c$ arise from terms in which, in every binomial factor in (43), the particles and holes are symmetrically distributed. If the number of overturned spins is odd one of the associated Bethe wave-vectors will be π but except for this isolated case the Bethe wave-vectors k_i will occur in symmetric pairs[3] $(k_i, -k_i)$ and describe the non-degenerate states at $K = 0$ or $K = L/2$. To obtain the number of these states note that the number of holes h_n is always even in each binomial distribution and exactly half of the holes, $h_n/2$, must occupy, say the right, half of the available slots, $\lfloor p_n/2\rfloor + h_n/2$. The occupancy of the left half is fixed by the required symmetry so that the symmetric (non-degenerate) state count is just the new binomial product

$$
D^{sym}(L,\ S,\ \{p_n\})=\prod_n\binom{\lfloor p_n/2\rfloor+h_n/2}{h_n/2},\ h_n=2S+2\sum_{m>n}(m-n)p_m,
\tag{49}
$$

that replaces (43). From (49) one can derive an explicit formula for the total number of symmetric states that parallels Bethe's derivation of the total number of states. Begin by defining a constrained sum

$$
D^{sym}(L,\ S,\ P)=\sum{}'D^{sym}(L,\ S,\ \{p_n\})
\tag{50}
$$

in which the number of 'particles' $\sum p_n = P, 1 \leqslant P \leqslant N$, in addition to the number of overturned spins $N = \sum np_n = L/2 - S$, is fixed. By comparing with a large number of examples I conclude

$$
D^{sym}(L,\ S,\ P)=\binom{\lfloor (L/2+(-1)^N S)/2\rfloor}{\lfloor P/2\rfloor}\binom{\lfloor (L/2-(-1)^N S-1)/2\rfloor}{\lfloor (P-1)/2\rfloor}.
\tag{51}
$$

Bethe has proved the analogous formula $D(L, S, P)$ for the constrained total number of states by induction after first showing it satisfies the recursion

$$
\begin{aligned}
D(L,\ S,\ P)&=\frac{2S+1}{L/2+S+1}\binom{L/2+S+1}{P}\binom{L/2-S-1}{P-1}\\
&=\sum_{p_1=0}^{P-1}\binom{p_1+h_1}{h_1}D(L-2P,\ S,\ P-p_1)\,.
\end{aligned}
\tag{52}
$$

The corresponding recursion here follows by replacing the binomial in the second equality in (52), which is the $n = 1$ factor in (43), by the $n = 1$ factor in (49) thus giving

$$
D^{Sym}(L,\ S,\ P)=\sum_{p_1=0}^{P-1}\binom{\lfloor p_1/2\rfloor+h_1/2}{h_1/2}D^{Sym}(L-2P,\ S,\ P-p_1)\,.
\tag{53}
$$

To show (51) satisfies (53) the four cases in which N and P are separately even or odd must be considered. For the even-even case set $N = 2R$, $R = 1, 2, \ldots$ and $P = 2Q$, $Q = 1, 2, \ldots, R$; then (53) reduces to

[3] In this context we must treat $(\pi/2 + i\infty, \pi/2 - i\infty)$ as a symmetric pair also. The associated spins are always nearest neighbours so the only wave-vector describing the pair is the sum wave-vector π which is also $-\pi$ (mod 2π).

$$\binom{R+S}{Q}\binom{R-1}{Q-1} = \sum_q \binom{q+2(R-Q)+S}{2(R-Q)+S}\binom{R-Q-1}{Q-q-1}\left\{\binom{R-Q+S}{Q-q} + \binom{R-Q+S}{Q-q-1}\right\} \tag{54}$$

where the two terms in braces arise from the even $p_1 = 2q$ and odd $p_1 = 2q + 1$ terms in the original p_1 sum in (53). These can be combined into a single binomial and if we define R-Q = A, Q-q-1 = k the right hand side of (54) can be written

$$\sum_{k=0}^{A-1}\binom{R+A+S-1-k}{2A+S}\binom{A-1}{k}\binom{A+S+1}{k+1}$$
$$= (A+S+1)\binom{R+A+S-1}{2A+S}{}_3F_2\left(\begin{matrix}1-R+A,\ -A-S,\ 1-A\\ 2,\ 1-R-A-S\end{matrix};1\right) \tag{55}$$

with the equality verified by direct comparison of terms in the sum with terms in the hypergeometric function. The latter is Saalschützian (cf Erdélyi *et al* [13] section 4.4) and satisfies ${}_3F_2\left(\begin{matrix}a,\ b,\ -n\\ c,\ 1+a+b-c-n\end{matrix};1\right) = \frac{(c-a)_n(c-b)_n}{(c)_n(c-a-b)_n}$ where $(x)_n = \Gamma(x+n)/\Gamma(x)$ is Pochhammer's symbol. With this result one finds (55) is

$$(A+S+1)\frac{(R+A+S-1)!}{(2A+S)!(R-A-1)!}\frac{(R-1)!}{(R-A)!}\frac{(2A+S)!}{(A+S+1)!}\frac{1}{A!}\frac{(R+S)!}{(R+A+S-1)!}$$
$$= \binom{R+S}{R-A}\binom{R-1}{R-A-1} \tag{56}$$

which, since R − A = Q, then confirms (54) is correct. A similar analysis for the remaining N and P even/odd cases verifies that (51) satisfies the recursion (53) in general. Furthermore, the special values $Z^{Sym}(L, S, 1) = 1$ and $Z^{Sym}(L, S, 2) = \lfloor (L/2 + (-1)^N S)/2 \rfloor$ from (51), which are easily shown to agree with the definition (50), serve as the initial conditions to complete the inductive proof of (51) for P > 2.

Now only a sum over P in (51) remains to obtain the total number of symmetric (non-degenerate) states. In compliance with the discussion on whether the center of symmetry K_c is 0 or L/2, we have

$$D^{sym}_{K=0}(L, S) = \sum_{Peven} D^{sym}(L, S, P) = \binom{L/2-1}{\lfloor (L/2+S-(-1)^{L/2-S})/2 \rfloor},$$
$$D^{sym}_{K=\frac{L}{2}}(L, S) = \sum_{Podd} D^{sym}(L, S, P) = \binom{L/2-1}{\lfloor (L/2+S)/2 \rfloor} \tag{57}$$

where the final equalities follow using Vandermonde's identity $\sum_{m=0}^{n}\binom{a}{m}\binom{b}{n-m} = \binom{a+b}{n}$ for the sums. Explicit calculation of Bethe states has confirmed (57) in many cases, including all S ⩽ L/2 and even L ⩽ 12. All other states at K = 0 and L/2, necessarily including those translated from outside the first Brillouin zone, are doubly-degenerate states related by the reflection symmetry $k_i \to -k_i$. The state counts (57) take a particularly simple form when related directly to the wave-vector lists that occur. These are of the form $[^*, (k_1, -k_1), (k_2, -k_2),\ldots,(k_n, -k_n)]$ where * are special values comprising four cases of $N^* = 0$ to 3 wave-vectors — null; π; $\pi/2 + i\infty, \pi/2 - i\infty$; $\pi/2 + i\infty, \pi/2 - i\infty, \pi$ — with associated $K^* = 0$, L/2, L/2, 0 respectively. The state counts (57) now take the form

$$D^{sym}_K(L, S) = \binom{L/2-1}{n},\ S = L/2 - N^* - 2n,\ K = \begin{cases} 0, & N^* = 0, 3\\ L/2, & N^* = 1, 2\end{cases}. \tag{58}$$

The results in (58) confirm those for $N^* = 3$ for L ≡ 2 mod 4 and $N^* = 2$ for even L in [14] (their equations (29) and (30)). These authors do not give general results for the remaining case $N^* = 3$ for L ≡ 0 mod 4 but their specific count of 4 for L = 12 with 5 overturned spins is in error — disagreeing with the count of 5 from (58), the explicit (61) arrived at by an independent calculation below, and the results reported in [15].

4. Non-degenerate states at K = 0 and L/2

The simplest extension of BAE solutions to more than 2 overturned spins is for states of symmetrically distributed particles and holes discussed in the preceding section. These are the non-degenerate states at K = 0 and L/2 and I begin with a few examples of states contributing to counts (58). The result of fixing the N^* special wave-vectors is a reduced set of BAE for the remaining n independent rapidities $\lambda_j = \cot(k_j/2)$[4]. These equations are

[4] The defining equations for the N^* special rapidities are trivially satisfied but in the pair $\lambda = \pm i$ case a careful limiting procedure such as that described in [16] must be used to determine their energy contribution $\Delta E_{sing} = -2$.

$$\left(\frac{\lambda_j + i}{\lambda_j - i}\right)^{L-1} = F_j \begin{cases} 1, & N^* = 0 \\ \dfrac{\lambda_j + 2i}{\lambda_j - 2i}, & N^* = 1 \end{cases}, \left(\frac{\lambda_j + i}{\lambda_j - i}\right)^{L-2} = F_j \frac{\lambda_j + 3i}{\lambda_j - 3i} \begin{cases} 1, & N^* = 2 \\ \dfrac{\lambda_j + 2i}{\lambda_j - 2i}, & N^* = 3 \end{cases} \tag{59}$$

where

$$F_j = \prod_{m \neq j} \frac{(\lambda_j + 2i)^2 - \lambda_m{}^2}{(\lambda_j - 2i)^2 - \lambda_m{}^2}, \ j, m = 1, 2, \ldots, n. \tag{60}$$

Simplifying (59) for n $= 1$, in which case F $= 1$, leads trivially to $\lambda^{N^* mod\ 2} P^{N^*}_{L/2-1}(\lambda^2) = 0$ where $P^{N^*}_m$ is a polynomial of degree m but different for every N*. The possible root $\lambda = 0$ (k $= \pi$) has no independent partner at –k and is to be discarded. The L/2–1 roots of $P^{N^*}_{L/2-1}$ exhaust the state counts (58). Consider the case L $= 12$, S $= 1$, K $= 0$ for which N* $= 3$, n $= 1$. The root equation in λ^2 can also be given as one in x $= 2\cos(k)$ using $\lambda^2 = (2 + x)/(2 - x)$; the equations are

$$55 - 505\lambda^2 + 582\lambda^4 + 78\lambda^6 - 45\lambda^8 - 5\lambda^{10} = 0\,, \quad 5 + 9x - 15x^2 - 2x^3 + 5x^4 - x^5 = 0 \tag{61}$$

and illustrate those in x typically have smaller coefficients. The roots of (61) give $\lambda = \pm 0.35796, \pm 0.83363, \pm 1.83377, \pm 3.03103i, \pm 1.99966i$ which together with the N* $= 3$ special λ can be identified with the even partitions (strings) of the 5 overturned spins, namely $1^3 2^1$ (3 cases) and $1^1 4^1$, $2^1 3^1$ (one case each) in agreement with the individual counts (49). Hao *et al* [3] report only 4 roots but the 'missing' $\lambda (= \pm 0.3579\ldots)$ is plausibly element 235 in their supplementary information Table 69, misidentified due to numerical inaccuracies.

For n $= 2$ the reduced BAE (59) can be simplified to the pair

$$\lambda_1^2 = Q^{N^*}_{L/2}(\lambda_2^2)/P^{N^*}_{L/2-1}(\lambda_2^2), \ \lambda_2^2 = Q^{N^*}_{L/2}(\lambda_1^2)/P^{N^*}_{L/2-1}(\lambda_1^2) \tag{62}$$

where the $P^{N^*}_{L/2-1}$ are the same polynomials that arose for n $= 1$; the $Q^{N^*}_{L/2}$ polynomials are new. Substituting either equation of the pair (62) into the other demands the vanishing of a degree $(L/2)^2$ polynomial. The numerical evidence is that this polynomial always factorizes giving

$$(\lambda^2 + 1)^{L-2}(\lambda^2 P^{N^*}_{L/2-1}(\lambda^2) - Q^{N^*}_{L/2}(\lambda^2)) R^{N^*}_{(L/2-1)(L/2-2)}(\lambda^2) = 0 \tag{63}$$

in which the L/2 roots of the middle factor are the $\lambda_1 = \lambda_2$ solutions of (62) and are to be discarded. Also to be discarded are the roots of the first factor in (63) which are the singular solutions already accounted for in the N* wave-vector list. The $(L/2 - 1)(L/2 - 2)$ roots of the R polynomial in (63) are to be paired using (62) and so exhaust the state counts (58) for n $= 2$. For L $= 10$, S $= 0$, K $= 5$ one has N* $= 1$, n $= 2$ and the R polynomial root equation, expressed in x, is

$$\begin{aligned} &1637 - 6346x + 2103x^2 + 11585x^3 - 10898x^4 - 1000x^5 + 6066x^6 \\ &- 3079x^7 - 55x^8 + 627x^9 - 258x^{10} + 45x^{11} - 3x^{12}. \end{aligned} \tag{64}$$

If the roots of (64) are ordered from 1 to 12 by non-decreasing real part, the Bethe solutions are the pairs [1, 9], [3, 10], [5, 11], [2, 4], [6, 7], [8, 12] obtained using (62). In explicit terms and including the N* $= 1$ root k $= \pi$ ($\lambda = 0$), the solutions in this sequence are, respectively

$$\begin{aligned} \lambda = &[\pm 0.23834, \pm 2.08921i, 0], \ [\pm 0.65226, \pm 2.00829i, 0], \ [\pm 1.50543, \pm 2.00166i, 0], \\ &[0, \pm 0.43240, \pm 1.19617], \ [0, \pm 1.02826 \pm 1.00383i], \ [\pm 4.32753i, \pm 2.00003i, 0] \end{aligned} \tag{65}$$

corresponding to the odd partitions of 5 overturned spins, namely $1^2 3^1$ (3 cases) and 1^5, $1^1 2^2$, 5^1 (one case each) again in agreement with (49).

I am unaware of any simple algebraic process that will find the analogs of polynomials (61) or (64) for n > 2. On the other hand, the existence of these polynomials has been confirmed in a number of cases either by direct construction from solutions of the BAE or more simply by use of the integer relation algorithm PSLQ [4]. For any given L, N* and n one need only find one BAE solution from which to pick a wave-vector k_1 and determine $x_1 = 2\cos(k_1)$ with a certain minimum accuracy. This x_1 is used to construct the list $[1, x_1, x_1^2, \ldots, x_1^{nD}]$ where D is the state counts from (58). This list serves as input to the PSLQ algorithm and provided the accuracy is adequate, the output will be the integer coefficient list $[a_0, a_1, a_2, \ldots, a_{nD}]$ in the polynomial $\sum a_i x^i$. Software packages such as Maple can efficiently find polynomial roots and what remains is then just a finite search process for D groups of n roots that satisfy the BAE.

The needed accuracy in x_1 for a successful PSLQ return is roughly nD times the number of digits in the coefficient a_i of largest magnitude. This can be a severe limitation but one can always reduce the PSLQ complexity by increasing the number of BAE solutions used for input. Instead of the single root power list one constructs the array, and by linear algebra, its triangular reduction

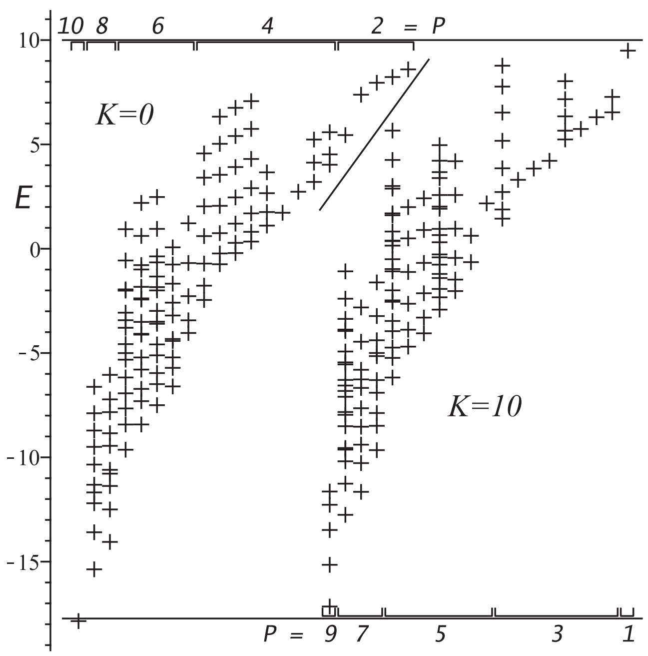

Figure 1. Non-degenerate L = 20 state energies at K = 0 and10, separated into partitions of 10 and grouped by particle number $P = \sum p_n$. The left-most column in each P group is the partition $1^{P-1}(11\text{-}P)^1$; partitions for the remaining columns are in the dictionary order given in Table 24.2 of AS [18]. The horizontal lines are the ferromagnetic (L/2) and limiting anti-ferromagnetic (L/2 − 2Lln(2)) energies.

$$\begin{bmatrix} 1\ x_1\ x_1^2\ \dots\ x_1^{nD} \\ 1\ x_2\ x_2^2 \dots x_2^{nD} \\ \dots \\ 1\ x_m\ x_m^2 \dots\ x_m^{nD} \end{bmatrix} \rightarrow \begin{bmatrix} 1 * * * \dots * \\ 0\ 1 * * \ \dots * \\ \dots \\ 0\ 0 \dots 0\ 1 \dots * \end{bmatrix} \tag{66}$$

which leaves, in the final row, nD − m + 2 non-zero elements that become the new input list into PSLQ. Back substitution of a successful PSLQ coefficient list return into the triangular reduction array yields successive polynomial coefficients. To within the floating-point accuracy used these are either integer or rational and in the latter case the entire (tentative) list can be converted to integer by an appropriate multiplication. It is advantageous to supply the PSLQ algorithm with real coefficients; complex x_i need not be discarded and instead the complex power list $[1, x_i, x_i^2, \dots, x_i^{nD}]$ should be input as the two lists which are its real and imaginary parts.

The largest L treated by this method has been L = 20 (D = 126) with PSLQ input reduced to less than 50 elements. The final 631(505) polynomial coefficients for K = 0(10) appear in the supplementary data file L20_nondegen.txt as lists Ih0S0L20 ($\hat{I}_0^0$) and Ih10S0L20 ($\hat{I}_{10}^0$). Also given are the corresponding energy ordered BAE solution lists $\hat{k}_0^0$ and $\hat{k}_{10}^0$ written as kh0S0L20 := [[70, 105, 146, 185, 238], …] and kh10S0L20 := [[56, 91, 127, 166], …] where the integers specify the location in the polynomial root lists x_i when ordered by non-decreasing real part as in the example leading to (65) (note for K = 10 each BAE solution consists of $\pm\lambda_i$ from the four listed x_i plus the $N^* = 2$ special $\pm$i). The D energies E_i for each K define a polynomial $\prod_i (E_i - E)$ that has been confirmed to have integer coefficients. These are the lists Ihe0S0L20 and Ihe10S0L20 and serve as useful checks. Every solution has been plausibly identified with a Bethe string solution and hence a partition of 10. To emphasize this and the agreement with the counts (49) all states have been separated by partition label with energies as shown in figure 1. Some of the state identifications might not be obvious at first sight. A K = 0 example is [1, 2, 564, 629, 630] which is

$$\lambda = [\pm 0.00188i,\ \pm 0.76047i,\ \pm 1.23953i,\ \pm 1.99994i,\ \pm 2.81271i] \tag{67}$$

and is identified as the P = 4 partition $1^1 2^1 3^1 4^1$. Here it is important to recognize that symmetry dictates that the nominal Bethe strings have the same (vanishing) real part which implies 2-fold λ root degeneracy at both $\pm$i and 0. This degeneracy must be lifted and (67) shows it is lifted by a spitting of the roots in the imaginary direction[5]. The splitting in (67) can be emphasized by writing the λ roots as

[5] There are examples where the splitting is in the real direction. For the K = 10 state [119, 380, 476, 477] which is identified as the P = 3 partition $2^1 3^1 5^1$, $\lambda \approx [\pm 0.550075, \pm i, \pm 0.550074 \pm 2.000001i, \pm 4.816316i]$.

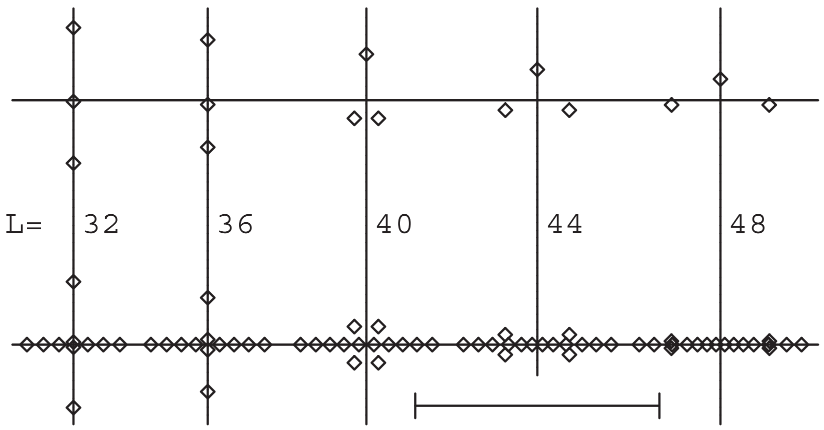

Figure 2. A sequence of complex λ-plane sections showing Bethe roots for partitions $1^{L/2-9}2^1 3^1 4^1$ at lengths L shown. The lower half planes, being the reflection of the upper half, have been truncated. The major horizontal and vertical lines intersect at the points $\lambda = 0$ and $\lambda = 2i$. The horizontal scale is indicated by a scale bar of length 2.

$$\lambda = [\pm e_0 i,\ \pm(1 - e_1 - e_Q)i,\ \pm(1 + e_1 - e_Q)i,\ \pm(2 - e_2)i, \pm(3 - e_3)i]$$
$$e_0 = 1.8798 \times 10^{-3},\ e_1 = 0.23953\ldots, e_Q = 1.4197 \times 10^{-17},\ e_2 = 5.9980 \times 10^{-5},\ e_3 = 0.18729 \quad (68)$$

and the very small e_Q shows how little the centroid of the nominally degenerate $\pm$i pair has shifted. The small e_Q also labels the state as a 'quartet' – a state in which two different λ_i have imaginary parts differing by $\approx$2. Since there has been some question in the literature [17] about the role that quartet states play in the BAE solutions it is instructive to see what happens to (68) with changes in L. For large L one can derive the asymptotic results

$$e_0 = 3^{-L/2}20\sqrt{21}\{1 + 2^{-L}128(150L - 1321) + O(L^{\omega}3^{-L})\},$$
$$e_1 = 2^{-L/2}60\sqrt{14}\{1 + 2^{-L}(3150L^2 - 95145L + 675329) + O(L^{\omega}3^{-L})\},$$
$$e_Q = (e_1/2)^L 45\{1 - 2^{-L}14(450L^2 - 11610L + 65189) + O(L^{\omega}3^{-L})\},$$
$$e_2 = 3^{-L}140\{60\mathrm{L} - 187 + 2^{-L}512(4500L^2 - 50820L + 79417) + O(L^{\omega}3^{-L})\},$$
$$e_3 = 2^{-L}840\{30\mathrm{L} - 337 + 2^{-L}6(10500L^3 - 597600L^2 + 9552665L - 47241816) + O(L^{\omega}3^{-L})\} \quad (69)$$

that even for $L = 20$ are in qualitative agreement with (68). One notes that e_Q becomes doubly exponentially small but does not in any way prevent the $\pm$i and 0 root splittings from becoming exponentially small.

A more interesting situation arises at $L > 20$ when the $(2^1 3^1 4^1)$-string combination with $L/2 - 9$ remaining 1-strings is kept as an $S = 0$ excitation. The number of such excitations based on (49) is $\binom{m+6}{m}$ for $L = 20 + 4$ m but I consider for each L only the one state in which the 1-string λ_i are in magnitude as small as possible and sandwiched between a symmetric set of 1-string large $|\lambda|$ holes[6]. The 1-strings interfere significantly with the $(2^1 3^1 4^1)$-string combination and lead to an increase in both e_0 and e_1 in (68) until a complex λ_i collision occurs and changes the qualitative character of the solution. This is illustrated in figure 2. That the states for $L \geqslant 40$ are indeed the continuation of those for $L < 40$ is confirmed by noting that the squares of the splitting between the colliding roots form a smooth sequence with a sign change at $L \approx 39$. The configuration at $L = 48$ when viewed in isolation would almost certainly be identified as an 'apparent' $1^{15}3^3$ partition rather than the Bethe $1^{15}2^1 3^1 4^1$. While this is just a more elaborate example of a complex root collision discussed following (19) and already observed by Bethe and others, it does illustrate that quartet configurations are typically unstable intermediate forms that facilitate transitions between states of different character.

BAE solutions for $L > 20$ such as those shown in figure 2 have been found by Newton-Raphson (NR) iteration. The $L = 20$ results are invaluable as a template for NR initialization for $L = 24$. For larger L, polynomial extrapolation in L (with allowance for root collision) is usually adequate for the complex root initialization. For real root initialization it is preferable to start with numerical approximations to the density $\rho = dn/d\lambda$ and extrapolate these in L. One then obtains λ_n by the integration $n = \int_0^{\lambda_n} \rho d\lambda$ with n either integer or half-integer. An adequate approximation to ρ in most cases is the Hulthén [19] ground state $\rho_0 = L/(4\cosh(\pi\lambda/2))$ plus polynomial and/or resonance (Lorentzian) functions. Many such calculations have been carried to $L \approx 1000$ with the goal of establishing the correspondence between Bethe string solutions and WZW model states. A graphical solution is facilitated if we rewrite (7) as

[6] This state is a local energy minimum and is appropriately called a cusp state. Quite generally, asymptotic $L \to \infty$ energies $\varepsilon = \varepsilon(K)$ in (7) for different 1-string arrangements but fixed (n>1)-strings fill a V-shaped 'cusp' region $\varepsilon(K) \geqslant \varepsilon(K_\varepsilon) + 2|K - K_\varepsilon|$ in energy versus momentum in the neighbourhood of a local minimum $\varepsilon(K_\varepsilon)$, K_ε.

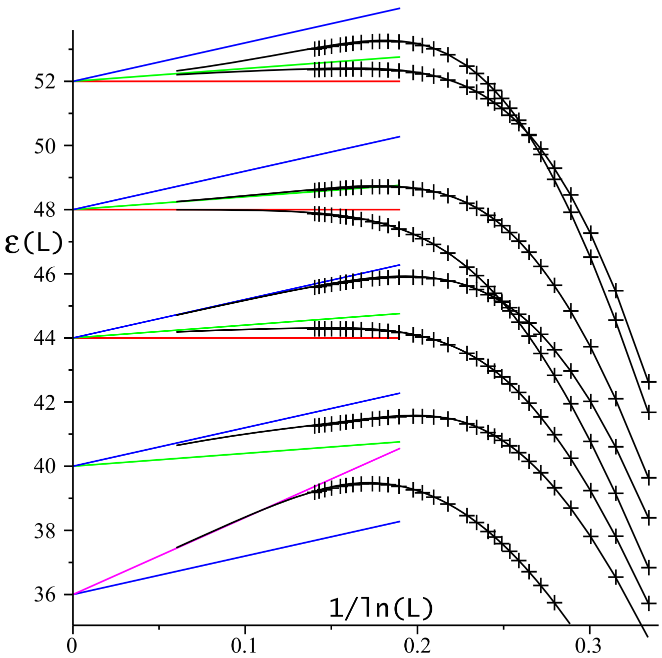

Figure 3. Crosses mark numerical ε(L) from (70) versus 1/ln(L), 20 ⩽ L ⩽ 1280, for configurations (reading upward at large L) 7^1, $2^1 6^1, 3^1 5^1, 2^2 5^1, 4^2, 2^1 3^1 4^1, 2^3 4^1, 3^3$ in the simplified notation that excludes the L- dependent 1-strings. Solid curves are interpolations plus extrapolations based on fits while the straight line segments are WZW asymptotes $\varepsilon + 2\, s(s+1)/\ln(L)$ for s = 0(red), 1(green), 2(blue) and 3(magenta).

$$\varepsilon(L) = \frac{L}{\pi^2}\left(E + L\left(2\ln(2) - \frac{1}{2}\right)\right) + \frac{1}{6} = \varepsilon + \frac{2s(s+1)}{\ln(L/L_0)} + o\left(\frac{1}{\ln(L)}\right). \tag{70}$$

Let the left hand side be numerical BAE solutions and the explicit terms with integer ε and 2 s on the right hand side be possible asymptotic WZW solutions. A sample of such paired graphs, including the $(2^1 3^1 4^1)$-string combination featured in figure 2, is shown in figure 3. It is apparent that in most cases a length L = 1280 is more than adequate to unambiguously establish the Bethe-WZW correspondence.

The results of the correspondence from figure 3 and many similar calculations are given in table 1. Empirical relations describing the Bethe-WZW correspondence for the states F_{nm} in table 1 are

$$\begin{aligned} &F_{n,m} = 1^{L/2-2-n}(m+1)^1(n-m+1)^1, \quad h_1 = 2n \quad (\textit{Bethe string}) \\ &\varepsilon = n^2 + 4m\,, \quad s\ (=s_L = s_R) = (n-2m)/2 \quad (\textit{WZW model}) \end{aligned} \tag{71}$$

for $m = 0, 1, \ldots \lfloor n/2 \rfloor$, $n = 0, 1, \ldots$ and can be understood to be the rules for all states with at most two (n>1)-strings. A more comprehensive set of rules and combinatorial relations will be given in section 7 after Bethe string configurations at general K have been discussed in sections 5 and 6.

I close this section with a discussion of a very different but intriguing state. It is the single particle P = 1, L/2-string state which appears in figure 1 as the lowest lying S = 0 excitation on the ground state of a *ferromagnetic* chain. This is the state [323, 341, 379, 468] which in λ representation is

$$\lambda = [\pm i,\ \pm(3 + 4.59 \times 10^{-9})i,\ \pm 5.001053i,\ \pm 7.23669i,\ \pm 13.08157i]. \tag{72}$$

The L = 22 state,

$$\lambda = [0,\ \pm(2 + 3.54 \times 10^{-17})i,\ \pm(4 + 4.60 \times 10^{-7})i,\ \pm 6.005167i,\ \pm 8.43462i,\ \pm 15.42998i]\,, \tag{73}$$

is the analogous single particle L/2-string for L/2 odd. The explicit (72) and (73) serve as useful templates for initial guesses for larger L and can be easily improved by NR iteration. Oscillations due to odd/even L/2 rapidly decay with increasing L and I find from an analysis of states to L = 60 that the energy is

$$E_L \approx \frac{L}{2} - \frac{\pi^2}{L}\left(1 - \frac{1.34630515852995}{L} + \frac{3.35506593315}{L^2} - \frac{6.18534702}{L^3} + \frac{12.96091}{L^4} - \frac{25.54}{L^5}\right) \tag{74}$$

where the π^2 has been inferred from numerical values but is not in doubt. Corresponding inference for the other numerical values in the series (74) has not been successful. The excitation energy $\propto 1/L$ implies this state is not two ferromagnetic domains separated by finite width domain walls. Another guess for a classical analog of this state is one in which the chain is cut and the ferromagnetic ground state twisted by 2π before reconnection. This state is not topologically distinct from the ground state but it is a highly degenerate stationary energy state since the vector defining the 2π rotation can have any orientation. In all such states neighbouring spins deviate by

Table 1. WZW asymptotic parameters ε and s together with Bethe 1-string hole count h_1 for the lowest energy cusp state picked from every column in figure 1. Each main configuration entry is the L = 20 Bethe (n>1)-string list; this is followed by a label in parentheses that is the 'apparent' large L string content if there are changes as a result of root interactions. For states labelled by F_{nm} see text; for a state designated with +n there are additional cusp states with energies ε greater by 4 m, m = 1 … n.

F_{nm}, +n	Configuration (at K = 0)	ε	2 × s	$h_1 \div 2$	line #	F_{nm}, +n	Configuration (at K = L/2)	ε	2 × s	$h_1 \div 2$
F_{00}	Ground state	0	0	0	1					
F_{20}	3^1	4	2	2	2	F_{10}	2^1	1	1	1
F_{21}	2^2	8	0	2	3	F_{30}	4^1	9	3	3
F_{40}	5^1	16	4	4	4	F_{31}	$2^1 3^1$ (2^3)	13	1	3
F_{41}	$2^1 4^1$ ($2^2 3^1$)	20	2	4	5		2^3	17	1	3
F_{42}	3^2	24	0	4	6	F_{50}	6^1	25	5	5
+1	$2^2 3^1$	24	2	4	7	F_{51}	$2^1 5^1$ ($2^2 4^1$)	29	3	5
	2^4	32	0	4	8	F_{52}	$3^1 4^1$ ($2^1 3^2$)	33	1	5
F_{60}	7^1	36	6	6	9	+2	$2^2 4^1$	33	3	5
F_{61}	$2^1 6^1$ ($2^2 5^1$)	40	4	6	10		$2^1 3^2$	37	1	5
F_{62}	$3^1 5^1$ (3^3)	44	2	6	11	+1	$2^3 3^1$ (2^5)	41	1	5
F_{63}	4^2	48	0	6	12		2^5	49	1	5
+3	$2^2 5^1$	44	4	6	13	F_{70}	8^1	49	7	7
	$2^1 3^1 4^1$ (3^3)	48	2	6	14	F_{71}	$2^1 7^1$ ($2^2 6^1$)	53	5	7
	3^3	52	2	6	15	F_{72}	$3^1 6^1$ ($3^2 4^1$)	57	3	7
+2	$2^3 4^1$ ($2^4 3^1$)	52	2	6	16	F_{73}	$4^1 5^1$ ($2^1 4^2$)	61	1	7
+2	$2^2 3^2$	56	0	6	17	+4	$2^2 6^1$	57	5	7
F_{80}	9^1	64	8	8	18		$2^1 3^1 5^1$ ($3^2 4^1$)	61	3	7
F_{81}	$2^1 8^1$ ($2^2 7^1$)	68	6	8	19		$2^1 4^2$	65	1	7
F_{82}	$3^1 7^1$ ($3^2 5^1$)	72	4	8	20	+1	$3^2 4^1$	65	3	7
F_{83}	$4^1 6^1$ ($3^1 4^2$)	76	2	8	21	F_{90}	10^1	81	9	9
F_{84}	5^2	80	0	8	22					

angle $2\pi/L$ so that

$$E_L^{Classical} = \frac{L}{2}\cos\left(\frac{2\pi}{L}\right) = \frac{L}{2} - \frac{\pi^2}{L} + O(L^{-3}) \tag{75}$$

and the agreement of the leading terms in (74) and (75) suggests this is indeed the correct analog state. Confirmation comes from a comparison of spin-spin correlations which classically are simply

$$\langle \vec{s}_i \cdot \vec{s}_{i+j}\rangle / |\vec{s}\,|^2|^{Classical} = \cos\left(\frac{2\pi}{L}j\right) \tag{76}$$

and imply long range order with spins separated by L/2 strictly anti-parallel.

For the s = ½ quantum chain correlations I have solved the Hamiltonian (1) eigenvalue/eigenvector problem by generating a basis recursively starting with $|\psi_0\rangle = 0$ and

$$|\psi_1\rangle = \prod_{j=1}^{L/2} (\uparrow\downarrow - \uparrow\downarrow)_{j,j+L/2} \tag{77}$$

which is a product of singlet states of spin pairs separated by L/2. Besides the desired property that spins separated by L/2 are strictly anti-parallel, (77) is shown by translation $j \to j+1$ to be an eigenstate of total momentum K = L/2. Additional bases are defined by $|\psi_{n+1}\rangle = H|\psi_n\rangle - \varepsilon_n|\psi_n\rangle - a_n|\psi_{n-1}\rangle$ where ε_n and a_n are chosen to guarantee the orthogonality $\langle\psi_n|\ \psi_{n+1}\rangle = \langle\psi_{n-1}|\ \psi_{n+1}\rangle = 0$. Iteration stops when one observes $|\psi_{D+1}\rangle = 0$; this happens when $D = \begin{pmatrix} L/2 - 1 \\ \lfloor L/4 \rfloor \end{pmatrix}$, the dimension given in (57). If the states are left unnormalized as written above and we define the normalization constants $N_n = \langle\psi_n|\psi_n\rangle$, the tri-diagonal Hamiltonian matrix in a normalized basis has elements $H_{n,n} = \varepsilon_n$ and $H_{n,n+1} = H_{n+1,n} = \sqrt{N_{n+1}/N_n}$. The characteristic (eigenvalue) polynomial of this matrix agrees with that found by Bethe ansatz for all cases considered. The highest energy eigenvalue is that of the single particle L/2-string state and the spin-spin correlations found from the associated eigenvectors for even L from 4 to 20 are shown in figure 4. The j = 1 correlation C_1 is related to the energy (74) by $C_1 = 2E_L/(3L)$ while the factor 3 enhancement of the j = 0 correlation C_0 over that of the asymptotic C_1 in figure 4 is the s = ½ distinction between spin length squared s(s + 1) = 3/4 for a single quantum spin and the maximum $\langle \vec{s}_1 \cdot \vec{s}_2\rangle = s^2 = ¼$ for distinct (parallel) spins. This obvious quantum effect has no classical analog. The data in figure 4 for L = 20 has the Fourier decomposition

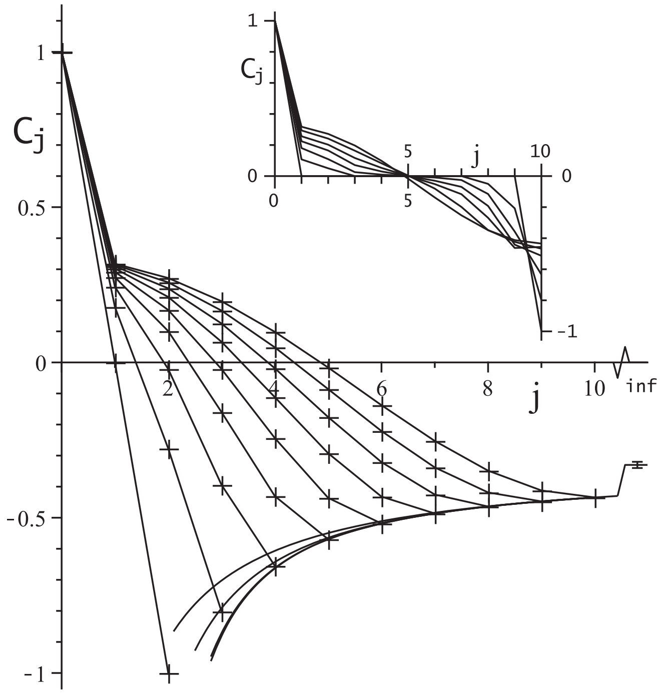

Figure 4. Spin-½ model spin-spin correlations $C_j = \langle \vec{s_i} \cdot \vec{s}_{i+j} \rangle / (s(s+1))$ versus site separation j in the single particle P = 1, L/2-string state for chains of length 4, 6, …, 20. Lines connecting C_j, $0 \leqslant j \leqslant L/2$ at the same L are a guide to the eye. The remaining lines are polynomial in 1/L fits to $C_{L/2}$ for the largest L and these extrapolate to $C_\infty = -0.33(1)$ as shown. The inset shows the convergence of C_j for L = 20 when only contributions from bases $|\psi_1\rangle$ through $|\psi_n\rangle$ are kept. The extremes are $C_j = \delta_{j,0} - \delta_{j,L/2}$ for n = 1 and the exact C_j for n = 126. Intermediate curves are n = 2, 3, 4, 5 and 7.

$$C_j = 0.6666625\delta_{j,0} - 0.033331 + 0.383518 \cos\left(\frac{2\pi}{L}j\right) - 0.017072 \cos\left(\frac{4\pi}{L}j\right) + 0.000538 \cos\left(\frac{6\pi}{L}j\right) - \ldots + 1.78 \times 10^{-7} \cos\left(\frac{18\pi}{L}j\right) \tag{78}$$

and from various fits, including the extrapolation $C_{L/2} = -0.33(1)$ for $L \to \infty$ from figure 4, I conclude

$$C_j = \frac{2}{3}\delta_{j,0} + \frac{1}{3}\cos\left(\frac{2\pi}{L}j\right) - \frac{1}{L}\left(\frac{2}{3} - 0.93(2)\cos\left(\frac{2\pi}{L}j\right) + 0.24(3)\cos\left(\frac{4\pi}{L}j\right) + 0.03(3)\cos\left(\frac{6\pi}{L}j\right) + \ldots\right) + O(L^{-2}) \tag{79}$$

in the $L \to \infty$ limit. The first correction $-2/(3L)$ in (79) is required by the sum rule $\sum_j C_j = 0$ while the sum $2/3 - 0.93(2) + 0.24(3) + \ldots$ must vanish because there are no $O(1/L)$ corrections to C_1. Finally, because $\cos(2\pi j/L)$ is the only surviving cosine mode in (79) for $L \to \infty$ in agreement with (76) we have confirmed the suggested identity of the analog classical state.

5. States of 3 overturned spins for general K

This section confirms the structures (5) and (6) for the case of 3 overturned spins and Bethe string configurations 1^3, $1^1 2^1$ and 3^1. The results are coefficient lists reported in 3_overturned_spins.txt based on the following notation and conventions. The data for given L starts with the state count list in the form (23), $NS\$:= [\hat{\nu}_0,\ \nu_0,\ \nu_K (0 < K < L/2),\ \nu_{L/2},\ \hat{\nu}_{L/2}]$, where \$ is the numerical value of the spin S and defines also L = 6 + 2 S. The number of states $\hat{\nu}_0 + 2\nu_0$, $\nu_K (0 < K < L/2)$ and $2\nu_{L/2} + \hat{\nu}_{L/2}$ at each K together with $\nu_{-K} = \nu_K$ are given by (41) followed by (42). There is only the $\hat{\nu}_0 = 1$ symmetric non-degenerate K = 0, E = L/2–6 state $[\pi/2 + i\infty, \pi/2 - i\infty, \pi]$ which is the $N^* = 3$, n = 0 case in (58). At K = L/2 there are $\hat{\nu}_{L/2} =$ L/2–1 symmetric non-degenerate states $[\pi, k, -k]$ based on $N^* = 1$, n=1. The non-trivial momenta are k = arccos(x/2) with x in turn each root of the polynomial $\hat{P}_{L/2} = \sum_{i=0}^{L/2-1} \hat{I}^S_{L/2,i} x^i$ derived as described for (59) and (60). The coefficient list defining this polynomial is denoted $Ih\$S\$:= [\hat{I}^S_{L/2,i},\ i = 0,\ 1,\ \ldots,\hat{\nu}_{L/2}]$ with \$ being placeholders for the numerical K = L/2 and S respectively. To completely describe the BAE solutions via (5) and (6) requires and additional L/2 + 1 analogous coefficient lists $IKS\$:= [I^S_{K,i},\ \ i = 0,\ 1,\ldots,3\nu_K]$, $0 \leqslant K \leqslant L/2$.

For K = 0, L/6, L/4, L/3 or L/2 the polynomial $P_K(x) = \sum_{i=0}^{3\nu_K} I_{K,i}^S x^i$ is defined by the single list '$IKS\exists$' but for K an element of block K_d with $M_d = \varphi(L/d)/2 \geqslant 2$ elements as described following (28), $P_K(x)$ depends on a superposition of M_d lists. Let the elements of K_d be labelled and ordered as $K_d^{[0]} < K_d^{[1]} < \ldots < K_d^{[M_d-1]}$ in which case the list sum

$$`IK_d^{[0]}S\$` + 2\sum_{m=1}^{M_d-1} \cos(2\pi mK/L)`IK_d^{[m]}S\$` \tag{80}$$

replaces the single list '$IKS\$$' used to define $P_K(x)$ as in the (29) example. The $3\nu_K$ roots of $P_K(x)$ define the 3 Bethe wave-vectors for all of the ν_K states. These states are represented as the list k\$S\$:= [[n_1, n_2, n_3], [n_4, n_5, n_6], …, […, $n_{3\nu_K}$]] where the \$ are numerical K and S as before while the $|n_i|$ are position pointers to the root list. It is to be understood that the roots x_i are arranged in non-decreasing $\Re(x_i)$ order with the Bethe momentum k_{n_i} associated with n_i then uniquely given by (26). The list '$k\$S\$$' is energy ordered with the energy of each state given by (4). A check is provided by energy polynomial coefficient lists '$IeKS\$$' that are the analog of '$IKS\$$' but define polynomials $P_K(E)$ whose ν_K roots are the energies of the states in the '$kKS\$$' lists. The analogy between '$IeKS\$$' and '$IKS\$$' extends to the combining rule (80) that is applicable to both lists. One final list '$Ihe\$S\$$' provides the energies for the states generated from '$Ih\$S\$$' at K = L/2.

The results presented in 3_overturned_spins.txt include all even L, $8 \leqslant L \leqslant 26$. The L = 8 data, part of which is

$$\begin{aligned}
&I1S1: =[384, -896, -208, 1248, -436, -328, 292, -52, -8, 0, -2, 6, -1];\\
&I3S1: =[256, -512, -464, 1088, 92, -856, 262, 274, -152, -4, 21, -5, 1];\\
&k1S1: =[[-1, 3, 5], [2, -9, -10], [-4, 7, 8], [-6, 11, 12]];\\
&k3S1 : =[[-1, -3, 6], [2, 7, -8], [-4, -9, -10], [5, 11, 12]];\\
&Ie1S1: =[0, -16, -6, 4, 1]; \quad Ie3S1: =[-8, 0, 4, 1, 0]; ,
\end{aligned} \tag{81}$$

is here used to illustrate that the lists '$IK_dS\$$' for $M_d > 1$ are not unique. The coefficient lists

$$\begin{aligned}
&J1S1: =[896, -1920, -1136, 3424, -252, -2040, 816, 496, -312, -8, 40, -4, 1];\\
&J3S1: =[640, -1408, -672, 2336, -344, -1184, 554, 222, -160, -4, 19, 1, 0];
\end{aligned} \tag{82}$$

are alternatives to '$I1S1$' and '$I3S1$' respectively. They are related by

$$\begin{aligned}
\prod_{i=1}^{12} (x - x_i^{(K)}) &= `J1S1` + 2\cos\left(\frac{\pi}{4}K\right)`J3S1`\\
&= \left(1 + 2\cos\left(\frac{\pi}{4}K\right)\right)\left(`I1S1` + 2\cos\left(\frac{\pi}{4}K\right)`I3S1`\right), \quad K = 1,\ 3
\end{aligned} \tag{83}$$

where $x_i^{(K)}$ are the roots of the associated polynomials $P_K(x)$ of either coefficient list. Only the result following the first equality conforms to that in (6) but the second form with irrational multipliers is more typically found when obtaining the polynomials by PSLQ. Since such different forms give identical roots, supplementary data that is equivalent to (6), as in L = 8 above, has been left unchanged. The remaining data in (81) can be used to verify that the roots of $P_K(E)$ determined from the list sum '$Ie1S1$' + 2 cos (K/4)'$Ie3S1$' are the energies calculated from lists '$kKS1$' for K = 1 and 3 using (4).

The maximum L = 26 exceeds the L ≈ 21.86 critical value where (19) shows the first complex root collision for 2 overturned spins and this allows us to explore more fully string interactions. As a specific example, figure 5 shows how strings in $1^1 2^1$ interact and modify bare 2^1 behaviour. The main indicators of interaction are the approximately linear drifts from the marker values and a pronounced level repulsion around the line $2k_1 = k_2 \bmod 2\pi$. 2-string root collisions are first observed at L = 24, a marginal shift from L = 22 expected based on (19), for 22 distinct k_1 values. In contrast for the 23rd k_1, the collision seen in the L = 74 inset is suppressed until L = 56. For states with root collision expected at L ≈ 61.35 based on (19), the 2-string remains complex in two states with k_1 above the line $2k_1 = k_2 \bmod 2\pi$ at L = 74.

6. L = 16 singlet states for general K

This section provides further confirmation of (5) and (6) but more importantly provides the BAE solutions that serve as templates for the calculations of much longer chains. The notation and conventions follow those in section 5 and start with the S = 0, L = 16 state count

$$[\hat{\nu}_0,\ \nu_0,\ \nu_K(0 < K < 8),\ \nu_8,\ \hat{\nu}_8] = [35,\ 30,\ 85,\ 93,\ 85,\ 94,\ 85,\ 93,\ 85,\ 30,\ 35] \tag{84}$$

determined from (41), (42) and (58). A minor change is that labels for lists reported as supplementary data in L16_singlet.txt are truncated versions '$Ih\$$', '$I\$$', '$kh\$$', '$k\$$', '$Ihe\$$' and '$Ie\$$' with \$ the numerical momentum K. The symmetric non-degenerate states at K = 0 are $N^* = 0$, n = 4 versions of (58) and of the form [$k_i, -k_i$, i = 1..4]. They are listed as [n_i, i = 1..4] in '$kh0$' with $k_i = \arccos(x_{n_i}/2)$ and x_{n_i} the n_i^{th} root of P(x) of degree

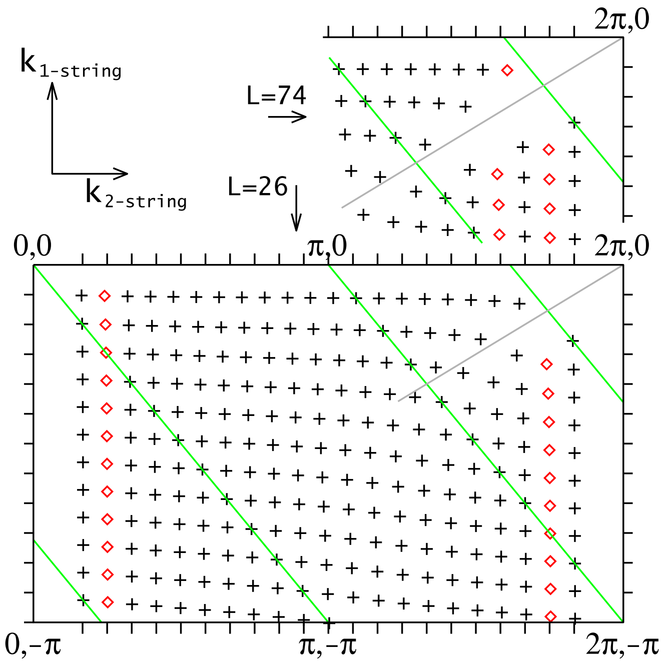

Figure 5. Momentum correlations for BAE $1^1 2^1$ configuration solutions in a (half) periodic cell. The 242 states shown for L = 26 plus 241 additional states obtained by inversion about $(\pi, -\pi)$ make up the total 23 × 21 from (43). The k_i markers are at $2\pi n/(L-2)$, n integer. Diagonals indicate constant $k_1 + k_2 = 2\pi K/L$ shown at K = −10, 0, 13 and 21 for L = 26 and matching L − 13 and L − 5 for L = 74. Crosses label complex 2-strings; diamonds are real 2-strings following root collision.

$4\hat{\nu}_0$ with coefficients listed in '*Ih0*'. The corresponding symmetric non-degenerate states at K = 8 are $N^* = 2$, n = 3 versions of (58) and of the form $[\pi/2 + i\infty, \pi/2 - i\infty, k_i, -k_i, i = 1..3]$. The non-trivial momenta are listed as $[n_i, i = 1..3]$ in '*kh8*' with $k_i = \arccos(x_{n_i}/2)$ and x_{n_i} the n_i^{th} root of P(x) of degree $3\hat{\nu}_0$ with coefficients listed in '*Ih8*'. All other states are of the form $[k_i, i=1..8]$ listed as $[n_i, i = 1..8]$ in '*kK*'. Now however signs are important and k_i is given by (26) with the $x_{|n_i|}$ the roots of a $P_K(x)$ of degree $8\nu_K$. For K = 0, 4 or 8 the coefficients of P_K are the lists '*IK*'; for K a member of the block $K_1 = 1, 3, 5, 7$ or $K_2 = 2, 6$ the superposition rules of (80) apply. Similarly for the energy polynomial lists '*IeK*'.

Solutions are plausibly identified with Bethe string configurations that are partitions of 8 and confirm the counts (45). Energy versus momentum of all states, separated by partition, is shown in figures 6–8. Of particular note are cusp states defined as those for which all 1-strings occupy adjacent positions with no intervening holes. In the limit of large L these are local energy minima with respect to 1-string excitation and a particularly important set of low energy states called current excitations by Bortz *et al* [20]. Many such large L (≈1000) solutions have been found by NR and analyzed similarly to that described in the text leading to (70). The results for all cusp states supplementing the odd ε cases from table 1 are shown in figure 9 for $\varepsilon \leqslant 41$. The state labelling conforms to that used in figures 6–8. Combinatorial rules that predict the location of states in the $L \to \infty$ limit shown in figure 9 are found to be a simple modification of the standard Bethe rules and are described in the next section. Here I only note that while the Bethe string labelling is an essential component of these rules, a different 'apparent' string labelling is often a much better indicator of the solution rapidities in the complex λ plane.

Very clear patterns are seen in figure 9 of which the most striking is that all state counts are consistent with products of the (left and right moving) $\pm\kappa$ excitation counts appearing in the single row diagonals $\varepsilon = (n-1)^2 + 2|\kappa|$ terminating at the single n-string values at $\kappa = 0$. This is as expected for the WZW model and is also explored in more detail in the next section which concludes with a conjecture for the string content of all left and right tower states in the total S = 0 sector. Another observation is that any cusp state associated with WZW spin s contains at least one n-string with n > 2 s; this is shown to follow from the string content conjecture.

7. Low energy S = 0 state counting for $L \to \infty$

The cusp state examples described in sections 4 and 6 lead naturally to conjectures for the multiplicity of all low lying singlet states as $L \to \infty$. An important parameter in the cusp state classification is the number of 1-string holes $h_1 = 2\sum(n\text{-}1)p_n$ (cf (43) and subsequent discussion) which is necessarily even and fixed by the n-string

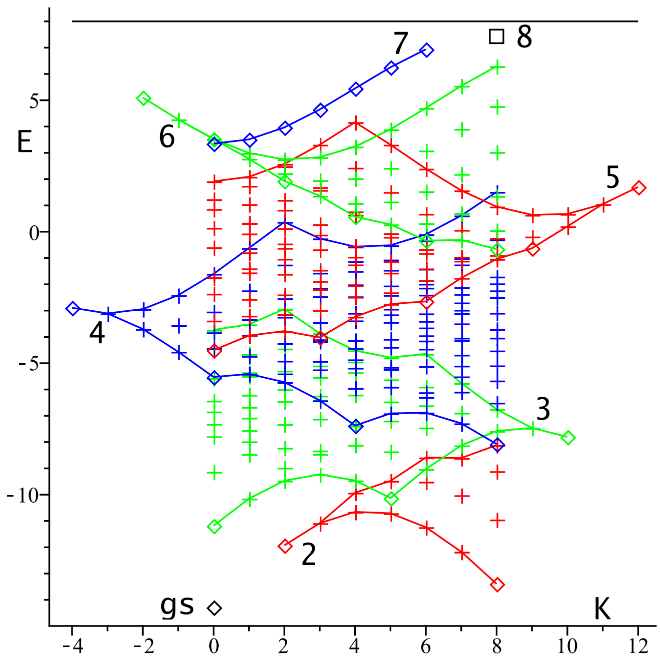

Figure 6. Energy E versus (quasi) momentum K for Bethe $1^{8-n}n^1$ (P = 9-n) configurations. Only the (n>1)-string component is used as plot label. Lines connect upper and lower boundary states for each n as a guide to the eye. For clarity the K (mod L) for each state has been chosen such that only after including reflection about K = 0(L/2) for states of even(odd) particle number P will the display be in explicit agreement with the counts (45). Diamonds replace crosses for the ground state (gs) and cusp states described in the text. Configurations with no 1-strings are also potential cusp states and are marked as squares. The horizontal line of length L (one periodic cell) marks the ferromagnetic energy L/2.

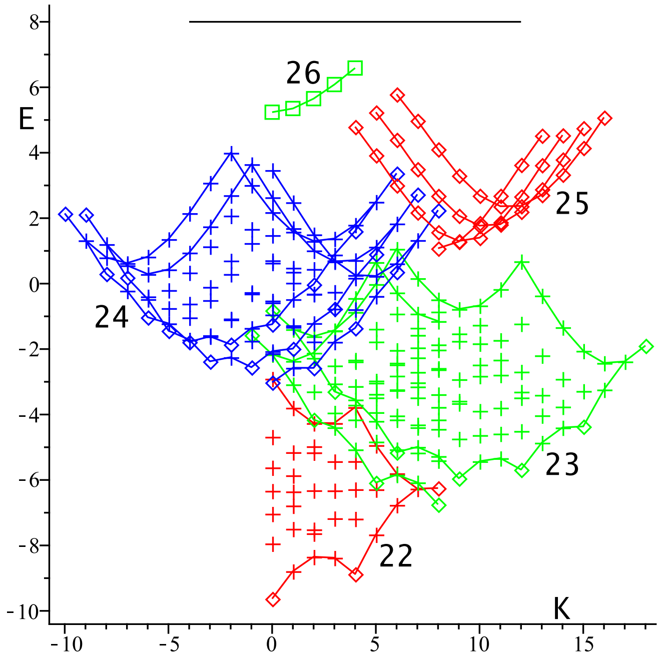

Figure 7. E versus K for Bethe $1^{6-n}2^1n^1$ (P = 8-n) configurations. Only the (n>1)-string components are used as plot labels (with $22 \rightarrow 2^2, 23 \rightarrow 2^13^1$, etc). Conventions as in figure 6.

content for $n > 1$. Thus h_1 is decoupled from L and our analysis does not require any specific value for L beyond L even and $L \gg h_1$. The complete list of possible $\{p_{n>1}\}_{h_1} = (p_2, p_3, \dots)$ for any h_1 is the list of the partitions of $h_1/2$ with every integer in a partition incremented by one. For example, for $h_1 = 10$, the partitions of 5 ($1^5, 1^32^1, 1^23^1, 1^12^2, 1^14^1, 2^13^1, 5^1$) after incrementing are the cusp state configurations $\{p_{n>1}\}_{10}$ ($2^5, 2^33^1, 2^24^1, 2^13^2, 2^15^1, 3^14^1, 6^1$). Define $\tilde{P} = \sum_{n>1} p_n$ and $\tilde{N} = \sum_{n>1} np_n$, the total number of 'particles' and overturned spins

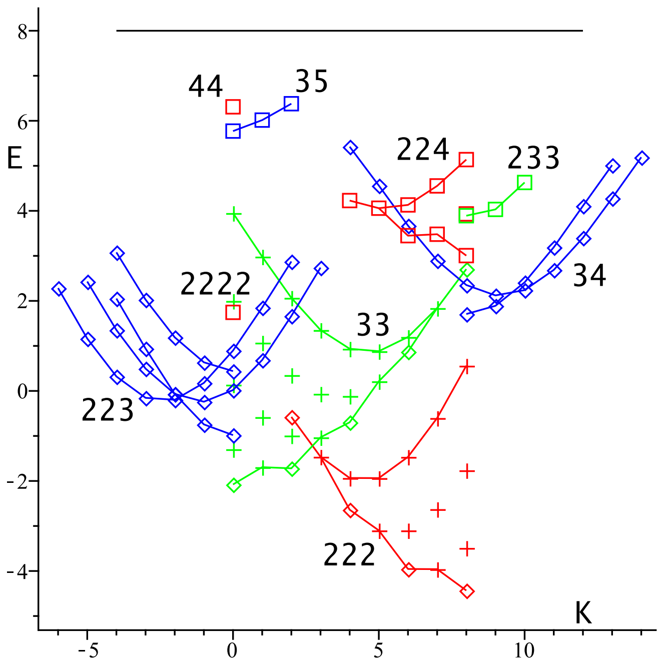

Figure 8. E versus K for Bethe configurations not shown in figures 6 and 7. Conventions as in figures 6, 7.

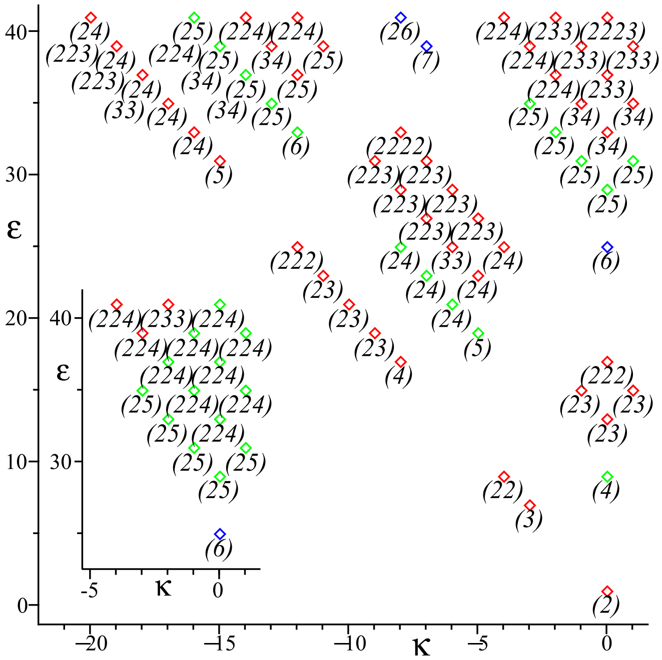

Figure 9. Bethe configuration labelled cusp state asymptotic energy ε from (7) versus momentum $\kappa = K - K_c, K_c = 0(L/2)$ for L/2 odd(even). States are distinguished by WZW model $s = s_L = s_R = 1/2$(red), 3/2(green) and 5/2(blue). States at $\kappa > 0$ are obtained by reflection about $\kappa = 0$. There are hidden $s = 3/2$ states near $\kappa = 0, \varepsilon = 37$; for these see the lower left corner insert which hides the $s = 1/2$ states instead. The data for the lowest excited state shown has been carried to $L = 16384$ in [21].

respectively in the (n>1)-strings. For the example list, $\tilde{P} = 5, 4, 3, 3, 2, 2, 1$ and in general $\tilde{N} = \tilde{P} + h_1/2$ with $1 \leqslant \tilde{P} \leqslant h_1/2$.

Any particular $\{p_{n>1}\}$ appears as a distinct cusp state for each division of h_1 into exclusively left h_L and right h_R holes. In the symmetric case, $h_L = h_R = h_1/2$, there is a trivial generalization of the generator (45) to the cusp state generator[7].

[7] $\begin{bmatrix} p_n + h_n \\ h_n \end{bmatrix}_q = \begin{bmatrix} p_n + h_n \\ p_n \end{bmatrix}_q$ and the lower element in the Gaussian binomial in a Bethe product is always to be understood to be p_n in this section.

$$\tilde{Z}(\{p_{n>1}\})_q^{Sym} = q^{((L+h_1)/2 \bmod 2)L/2} \prod_{n>1} \begin{bmatrix} p_n + h_n \\ p_n \end{bmatrix}_q, \quad h_n = 2\sum\nolimits_{m>n}(m-n)p_m, \tag{85}$$

where use has been made of the relation $h_1 = L - 2P$ derived in the discussion following (43). To get from the symmetric case to $h_L = h_1/2 + m$, $h_R = h_1/2 - m$ requires moving each of $p_1 = L/2 - \tilde{N}$ 1-strings by m steps. Each step shifts momentum K by one so the effect is to multiply (85) by $q^{m(L/2-\tilde{N})}$. The $q^{mL/2}$ factor can be accommodated by replacing $h_1/2$ in the first factor in (85) by h_L to give the general result

$$\tilde{Z}_{h_L,h_R}(\{p_{n>1}\})_q = q^{(L/2+h_L \bmod 2)L/2} q^{(h_R-h_L)\tilde{N}/2} \prod_{n>1} \begin{bmatrix} p_n + h_n \\ p_n \end{bmatrix}_q, \quad \tilde{N} = \sum\nolimits_{n>1} np_n. \tag{86}$$

To efficiently evaluate configuration sums of expressions such as (86) it is useful to first determine amplitudes $A_{i,j}$, $i = 1, 2, \ldots, 1 \leqslant j \leqslant i$, which are sums of the products $\Pi[\ldots]_q$ appearing in (85) and (86) subject to the constraints $h_1 = 2i$, $\tilde{P} = j$ (or $\tilde{N} = i + j$). Endpoint values are $A_{i,1} = A_{i,i} = 1$ arising from configurations $(i+1)^1$ and 2^i respectively. Intermediate cases for the partition of 5 list above are

$$\begin{aligned} A_{5,2} &= \underbrace{\begin{bmatrix} 7 \\ 1 \end{bmatrix}_q}_{2^1 5^1} + \underbrace{\begin{bmatrix} 3 \\ 1 \end{bmatrix}_q}_{3^1 4^1} = q^{-3} + q^{-2} + 2q^{-1} + 2 + 2q + q^2 + q^3, \\ A_{5,3} &= \underbrace{\begin{bmatrix} 5 \\ 1 \end{bmatrix}_q}_{2^1 3^2} + \underbrace{\begin{bmatrix} 6 \\ 2 \end{bmatrix}_q}_{2^2 4^1} = q^{-4} + q^{-3} + 3q^{-2} + 3q^{-1} + 4 + 3q + 3q^2 + q^3 + q^4, \\ A_{5,4} &= \underbrace{\begin{bmatrix} 5 \\ 3 \end{bmatrix}_q}_{2^3 3^1} = q^{-3} + q^{-2} + 2q^{-1} + 2 + 2q + q^2 + q^3 = A_{5,2}. \end{aligned} \tag{87}$$

Based on many more examples I conjecture but have not proved $A_{i,j} = A_{i,i-j+1}$ for all i, j. On the other hand, the sum rule $A_{i,j}|_{q=1} = \frac{1}{j}\binom{i}{j-1}\binom{i-1}{j-1}$ is easily verified by noting the Gaussian binomials at $q = 1$ are ordinary binomials after which follows a one to one correspondence between the sums here and Bethe's constrained sums $D(L, S, P)$ in (52). What are L and P with $S = 0$ in (52) are here h_1 and $\tilde{P}$ respectively as a consequence of our transcription of partitions into the cusp state configurations $\{p_{n>1}\}$. The symmetry $A_{i,j+1} = A_{i,i-j}$ allows us to restrict our explicit amplitude calculation to $A_{i,i-j}$ with $1 \leqslant j \leqslant (i-1)/2$ in which case every Gaussian binomial product contains some $f_2 = \begin{bmatrix} p_2 + h_2 \\ p_2 \end{bmatrix}_q$ together with other factors that are incremented partition analogs of the $\{p_{n>1}\}$. These remaining factors in all terms with a common f_2 combine into an amplitude of the same structure as $A_{i,j}$ but of lower order. The result, together with $A_{i,1} = A_{i,i} = 1$, is the recursion formula

$$A_{i,j+1} = A_{i,i-j} = \sum_{k=1}^{j} \begin{bmatrix} i+j-k \\ 2j \end{bmatrix}_q A_{j,k}, \quad 1 \leqslant j \leqslant (i-1)/2. \tag{88}$$

The generator for all cusp states obtained by summing (86) over configurations are usefully separated as

$$\tilde{Z}(q) = q^{(L/2 \bmod 2)L/2} \tilde{Z}^{(even)} + q^{(L/2+1 \bmod 2)L/2} \tilde{Z}^{(odd)}, \quad \tilde{Z}(q)^{(e/o)} = \sum_{h_L,h_R}^{(e/o)} B_{h_L,h_R}(q) \tag{89}$$

where

$$\begin{aligned} B_{h_L,h_R}(q) &= \sum_{\{p_{n>1}\}} q^{(h_R-h_L)\tilde{N}/2} \prod_{n>1} \begin{bmatrix} p_n + h_n \\ p_n \end{bmatrix}_q \\ &= \sum_{\tilde{N}=h_1/2+1}^{h_1} q^{(h_R-h_L)\tilde{N}/2} A_{h_1/2,\tilde{N}-h_1/2}, \quad h_1 = h_L + h_R. \end{aligned} \tag{90}$$

The sum in the first equality in (90) is over configurations $\{p_{n>1}\}$ understood to be $\{p_{n>1}\}_{h_1}$ as described in the first paragraph of this section and $\tilde{N} = \sum_{n>1} np_n$ as in (86). In the second equality $\tilde{N}$ has become a dummy summation variable indexing the very restricted configuration information available in the $A_{i,j}$. By excluding the power of q factors in (89) from the definition of $\tilde{Z}^{(e/o)}$ the latter become generators in which κ in q^{κ} is the momentum K relative to a central K_c that is either 0 or L/2. To make contact with WZW model results I expand $B_{h_L,h_R}(q)$ from (90) as a sum of products[8] of independent left and right cusp generators $B_h^{(2s)}(x)$ carrying a

[8] To avoid exceptions in product formulas it is convenient to define the ground state as a cusp state also. Then (89) and (90) are understood to be supplemented with the definition $B_{0,0} = 1$.

common $2s = 2s_L = 2s_R$ WZW spin label and differing only in argument in the left and right cases. For $h < 2s$, $B_h^{(2s)}(x) = 0$, while $B_{2s}^{(2s)}(x) = 1$. The defining equations (notationally collapsed into one with (e/o) indicating h_L, h_R and 2 s are all either even or odd integers),

$$B_{h_L,h_R}(q) = \sum_{2s=0/1}^{(e/o)} B_{h_L}^{(2s)}(1/q)B_{h_R}^{(2s)}(q), \tag{91}$$

considered as identities in h_L and h_R have a structure that allows all remaining $B_h^{(2s)}$ to be determined recursively from B_{h_L,h_R} starting from the smallest $2s = 0$ or 1. To illustrate, consider the odd case in (91) and set $h_L = 1$ to get $B_{1,h_R}(q) = B_{h_R}^{(1)}(q)$. For $h_R = 1$, $B_1^{(1)} = B_{1,1} = A_{1,1}$, the last equality coming from (90) and confirming $B_1^{(1)} = 1$. As a few additional cases, again using (90) and $A_{i,j}$ from (88),

$$\begin{aligned} B_3^{(1)}(q) &= B_{1,3} = q^3A_{2,1} + q^4A_{2,2} = q^3 + q^4,\\ B_5^{(1)}(q) &= B_{1,5} = \sum_{n=1}^{3} q^{6+2n}A_{3,n} = q^8 + q^9 + q^{10} + q^{11} + q^{12},\\ B_7^{(1)}(q) &= B_{1,7} = \sum_{n=1}^{4} q^{12+3n}A_{4,n}\\ &= q^{15} + q^{16} + q^{17} + 2q^{18} + 2q^{19} + 2q^{20} + 2q^{21} + q^{22} + q^{23} + q^{24}. \end{aligned} \tag{92}$$

Had we kept configuration information by utilizing the first equality in (90) rather than the $A_{i,j}$ form we could have sourced $B_1^{(1)}$ and each term in (92) by its $\{p_{n>1}\}$ configuration. The result is

$$\begin{aligned} &B_1^{(1)} = \underbrace{1}_{2^1}, \quad B_3^{(1)}(q) = \underbrace{q^3}_{3^1} + \underbrace{q^4}_{2^2}, \quad B_5^{(1)}(q) = \underbrace{q^8}_{4^1} + \underbrace{q^{10}\begin{bmatrix}3\\1\end{bmatrix}_q}_{2^13^1} + \underbrace{q^{12}}_{2^3},\\ &B_7^{(1)}(q) = \underbrace{q^{15}}_{5^1} + \underbrace{q^{18}\begin{bmatrix}5\\1\end{bmatrix}_q}_{2^14^1} + \underbrace{q^{18}}_{3^2} + \underbrace{q^{21}\begin{bmatrix}4\\2\end{bmatrix}_q}_{2^23^1} + \underbrace{q^{24}}_{2^4} \end{aligned} \tag{93}$$

and with the replacement $q \to 1/q$ we see all the terms in (93) can be identified with the terms on a single (lowest) diagonal of energy versus momentum in figure 9.

For the determination of $B_h^{(3)}$ set $h_L = 3$ in (91) to get $B_{3,h_R}(q) = B_3^{(1)}(1/q)B_{h_R}^{(1)}(q) + B_{h_R}^{(3)}(q)$. For confirmation, using $B_{3,3} = \sum_{n=1}^{3} A_{3,n}$, we get $B_3^{(3)} = q^{-1} + 3 + q - (q^{-3} + q^{-4})(q^3 + q^4) = 1$. A few higher order terms are

$$\begin{aligned} B_5^{(3)}(q) &= \sum_{n=1}^{4} q^{4+n}A_{4,n} - B_3^{(1)}(1/q)B_5^{(1)}(q) = q^5 + q^6 + q^7 + q^8,\\ B_7^{(3)}(q) &= \sum_{n=1}^{5} q^{10+2n}A_{5,n} - B_3^{(1)}(1/q)B_7^{(1)}(q)\\ &= q^{12} + q^{13} + 2q^{14} + 2q^{15} + 2q^{16} + 2q^{17} + 2q^{18} + q^{19} + q^{20}. \end{aligned} \tag{94}$$

To get the analog of (93) we must supplement the product count rules with configuration product rules. For the simpler case of the subtraction $B_{2+2\nu}^{(2)}(q) = B_{2,2+2\nu}(q) - B_2^{(0)}(1/q)B_{2+2\nu}^{(0)}(q)$, $\nu = 0, 1, 2, \ldots$, we meet only the products 2^1 from $B_2^{(0)}$ times $(p_2, p_3, \ldots)$ from $B_{2+2\nu}^{(0)}$. The result $2^1 \times (p_2, p_3, \ldots) = (p_2 + 1, p_3, \ldots)$ is just a special case of ordinary multiplication $(p'_2, p'_3, \ldots)(p_2, p_3, \ldots) = (p_2 + p'_2, p_3 + p'_3, \ldots)$. Clearly no subtraction occurs if $p_2 = 0$ in the configuration $\{p_{n>1}\}$ that contributes to $B_{2,2+2\nu}(q)$. If $p_2 > 0$ in $\{p_{n>1}\}$ I find the effect of the subtraction is to make the contribution to $B_{2+2\nu}^{(2)}(q)$ to be that for $B_{2,2+2\nu}(q)$ modified by the Gaussian binomial replacement

$$\begin{bmatrix} p_2 + h_2\\ p_2 \end{bmatrix}_q \to q^{p_2/2}\begin{bmatrix} p_2 + h_2 - 1\\ p_2 \end{bmatrix}_q. \tag{95}$$

Note that the replacement (95) implies the $h_2 = 0$ configuration $2^{2+\nu}$ does not contribute to $B_{2+2\nu}^{(2)}$. This is a special case of an observed general rule that only configurations $\{p_{n>1}\}$ with at least one m-string, $m > 2s$, contribute to $B_{2s+2\nu}^{(2s)}$. It is also the case that in general every contribution to $B_{2s+2\nu}^{(2s)}$ is found to be of the form of the contribution to $B_{2s,2s+2\nu}$ but with modified Gaussian binomials. Returning now to the terms in (94), the configuration version of $B_3^{(1)}(1/q)B_{h_R}^{(1)}(q)$ involves new considerations. First, it is necessary to follow every product $\{p_{n>1}\}_{4s+2\mu} \times \{p_{n>1}\}_{4s+2\nu}$ in $B_{2s+2\mu}^{(2s)}(1/q)B_{2s+2\nu}^{(2s)}(q)$ by division by some $\{p_{n>1}\}_{4s}$. Second, it may also be necessary to replace $\{p_{n>1}\}_{4s+2\mu}$ by some other configuration with the same h_1. This introduces ambiguities which for low order terms can be resolved on a case by case basis without having to resort to long chain calculations. From examples for the $B_3^{(1)}(1/q)B_{3+2\nu}^{(1)}(q)$ product like those given in appendix A, I infer as a general result that the contribution to $B_{3+2\nu}^{(3)}(q)$ is the $B_{3,3+2\nu}(q)$ contribution modified by the two Gaussian binomial replacements

$$\begin{bmatrix} p_2 + h_2 \\ p_2 \end{bmatrix}_q \to q^{p_2}\begin{bmatrix} p_2 + h_2 - 2 \\ p_2 \end{bmatrix}_q, \quad \begin{bmatrix} p_3 + h_3 \\ p_3 \end{bmatrix}_q \to q^{p_3/2}\begin{bmatrix} p_3 + h_3 - 1 \\ p_3 \end{bmatrix}_q \tag{96}$$

similar in form to (95). The results for the configuration sources for the terms in (94),

$$B_3^{(3)} = \underbrace{1}_{4^1}, \quad B_5^{(3)}(q) = \underbrace{q^5}_{5^1} + \underbrace{q^7\begin{bmatrix} 3 \\ 1 \end{bmatrix}_q}_{2^1 4^1}, \quad B_7^{(3)}(q) = \underbrace{q^{12}}_{6^1} + \underbrace{q^{15}\begin{bmatrix} 5 \\ 1 \end{bmatrix}_q}_{2^1 5^1} + \underbrace{q^{\frac{29}{2}}\begin{bmatrix} 2 \\ 1 \end{bmatrix}_q}_{3^1 4^1} + \underbrace{q^{18}\begin{bmatrix} 4 \\ 2 \end{bmatrix}_q}_{2^2 4^1}, \tag{97}$$

identify with the terms on the second diagonal in figure 9.

The process for getting the independent left and right cusp count generators illustrated by the examples above extends to the general case. Equations (90) and (91) rewritten as

$$\begin{aligned} B_{2s,2s+2\nu}(q) &= \sum_{\mu=1}^{2s+\nu} q^{(2s+\nu+\mu)\nu} A_{2s+\nu,\mu}, \\ B_{2s+2\nu}^{(2s)}(q) &= B_{2s,2s+2\nu}(q) - \sum_{\mu=1}^{\lfloor s \rfloor} B_{2s}^{(2s-2\mu)}(1/q) B_{2s+2\nu}^{(2s-2\mu)}(q), \quad \nu = 0, 1, 2, \ldots \end{aligned} \tag{98}$$

are applicable to both even and odd 2s and as recursions together with (88) for $A_{i,j}$ provide everything needed for the cusp count generator $\tilde{Z}(q)$ in (89) or its WZW product form

$$\tilde{Z}(q)^{(e/o)} = \sum_{2s=0/1}^{(e/o)} \left(\sum_{\nu_L=0} B_{2s+2\nu_L}^{(2s)}(1/q) \right) \left(\sum_{\nu_R=0} B_{2s+2\nu_R}^{(2s)}(q) \right). \tag{99}$$

From (95) and (96) and a few higher order analogs I conjecture the configuration sourced version of (98) is

$$B_{2s+2\nu}^{(2s)}(q) = \sum_{\{p_{n>1}\}_{4s+2\nu}} \prod_{n, p_n > 0} q^{\nu n p_n} \times \begin{cases} q^{(2s-n+1)p_n/2} \begin{bmatrix} p_n + h_n - 2s + n - 1 \\ p_n \end{bmatrix}_q, & n \leqslant 2s \\ \begin{bmatrix} p_n + h_n \\ p_n \end{bmatrix}_q, & n > 2s. \end{cases} \tag{100}$$

The configurations $\{p_{n>1}\}_{h_1}$, $h_1 = 4s + 2\nu$, contributing to the sum (100) are as described in the first paragraph of this section while the product is over those n for which p_n is non-vanishing. The Gaussian binomial $\begin{bmatrix} a \\ b \end{bmatrix}_q$ is to be understood to vanish when $a < b$ which happens when n is its maximum n_{max} (making $h_n = 0$, cf (85)) and $n_{max} \leqslant 2s$; this is the basis for the rule that there is no contribution to $B_{2s+2\nu}^{(2s)}(q)$ from a configuration that does not contain at least one string with length greater than 2 s. Conversely, every configuration with $n_{max} > 2s$ contributes; for a proof it suffices to show $h_n - 2s + n - 1 \geqslant 0$ for every $n \leqslant 2s$ in (100). Now $h_n = 2\sum_{m>n}(m - n)p_m \geqslant 2(n_{max} - n) \geqslant n_{max} - n + 1 > 2s - n + 1$ which is the required result. Agreement between (98) and (100) has been confirmed numerically to high order.

Many regularities are observed in the solutions (98) and (100). Of particular note, the terms $c_\kappa q^\kappa$ in $B_{2s+2\nu}^{(2s)}(q)$ are constrained by $\nu(2s + \nu + 1) \leqslant \kappa \leqslant 2\nu(2s + \nu)$ with the coefficient $c_{\nu(2s+\nu+1)}$ in the leading term always unity and sourced by the single $(2s + \nu + 1)$-string configuration. The coefficients c_κ are symmetric under reflection of κ about the midpoint of its allowed range and a similar reflection symmetry applies to any subset of coefficients sourced by a particular $\{p_{n>1}\}$ configuration. The number of configurations contributing to $B_{2s+2\nu}^{(2s)}(q)$, $C_\nu^{(2s)} = \sum c_\kappa = B_{2s+2\nu}^{(2s)}(q = 1)$, is the coefficient of x^ν in the generator

$$C^{(2s)} = \sum_{\nu=0} B_{2s+2\nu}^{(2s)}(q = 1)x^\nu = (2/(1 - 2x + \sqrt{1 - 4x}))^{(2s+1)/2}. \tag{101}$$

The formulas for $C^{(1)}$ and $C^{(0)} = 1 + xC^{(1)}$ can be derived using the $A_{i,j}$ sum rule in the discussion following (87) and supplemented with $\sum_{j=1}^{i} A_{i,j}|_{q=1} = (2i)!/(i!(i + 1)!)$; formulas for $C^{(2s)}$ for some $2s > 1$ have been confirmed analytically based on the recursions (98) while others have been checked numerically. An explicit independent formula is

$$C^{(2s)} = \sum_{\mu=0}^{\nu} \frac{1}{\mu + 1}\binom{\nu}{\mu}\left\{\binom{2s + \nu - 1}{\mu} + 2s\binom{2s + \nu - 1}{\mu - 1}\right\} \tag{102}$$

in which the μ^{th} term in the sum is the number of contributions from configurations of fixed $\tilde{N} = 2s + \nu + \mu + 1$ in (100).

Because of the observation made in connection with (93) and (97) and illustrated in figure 9 that the contributions to $B_{2s+2\nu}^{(2s)}$ lie on single row diagonals, the $\tilde{Z}(q)$ from (99) is easily modified to the generator $\tilde{Z}(e, q)$

of cusp state counts in both energy and momentum. With the normalization of ε as chosen in the energy formula (7),

$$\tilde{Z}(e,\, q)^{(e/o)} = \sum_{2s=0/1}^{(e/o)} e^{(2s)^2}\left(\sum_{h_L=2s}^{(e/o)} B_{h_L}^{(2s)}(e^2/q)\right)\left(\sum_{h_R=2s}^{(e/o)} B_{h_R}^{(2s)}(e^2 q)\right) \tag{103}$$

where the coefficient of $e^{\varepsilon}q^{k}$ is the number of cusp states at ε and κ. The factor $e^{(2s)^2}$ incorporated into (103) accounts for the observation that $B_{2s}^{(2s)}$, which identifies with the single (2s + 1)-string configuration at $\kappa = 0$, has $\varepsilon = (2s)^2$ as seen in the many examples in table 1. The arguments e^2/q and e^2q replacing those in (91) account for the observed increase in ε of two units for every unit shift of κ away from $\kappa = 0$.

No counter examples to (103) have been found in the many computations of cusp energies in long chains. On the other hand, a general rule for handling configuration products, as distinct from configuration *count* products, has not been found. In the search for possible systematics I have included cases where $B_{h_L}^{(2s)}$ contains a term $n(e^2/q)^{\omega}$ with n > 1. Multiplication with the corresponding $B_{h_R}^{(2s)}$ term $n(e^2q)^{\omega}$ and factor $e^{(2s)^2}$ implies a multiplicity of n^2 at $\kappa = 0$ and $\varepsilon = (2s)^2 + 4\omega$ of which n should be non-degenerate and $(n^2\text{-}n)/2$ doubly degenerate. The lowest energy example of this is the configuration combination 2^15^1 and 3^14^1 in $B_7^{(3)}$ at $\kappa = 14$ (cf (94) and (97) or figure 9) which implies multiplicity 4 at 2s = 3, $\kappa = 0$, $\varepsilon = 65$. The observed Bethe and 'apparent' (in parentheses) configurations followed by the complex Bethe roots λ at length L = 640 are

$$\begin{aligned}
&3^24^1(3^1|4^1|\,3^1)\!:\ \pm 3.17920 \pm (2 - 7.627 \times 10^{-6})i,\ \pm i,\ \pm 3.97827i\\
&2^35^1(2^2|4^1|\,2^2)\!:\ \pm 2.51180 \pm (1 - 4.926 \times 10^{-13})i,\ \pm 0.93741 \pm (1 - 1.024 \times 10^{-130})i,\ \pm i,\ \pm 6.77476i\\
&2^13^15^1(3^1|4^1|\,2^2)\!:\ -3.35607 \pm 1.9997104i,\ 0.85154 \pm 5.50177i,\ 1.38330304024 \pm 0.06388218267i,\\
&\quad 1.38330300552 \pm 1.93611787368i,\ 2.46892 \pm (1 - 8.379 \times 10^{-14})i
\end{aligned} \tag{104}$$

with a 4th one obtained from the 3rd by reversal of all signs. The strings in the apparent configurations are separated into left, central and right; that for the 3rd root assumes the quartet with real parts near 1.3833 will at some longer length split into two 2-strings, one central and the other right. The apparent configurations suggest a product form $(3^1 + 2^2|4^1|3^1 + 2^2)$ and a special role for the 4(=2s + 1)-string, expected because we are dealing with a $B^{(2s)}B^{(2s)}$ configuration product. Allowance for string replacement $5^1 \to 2^14^1$ analogous to that in (A.2) is required to get the resultant strings, namely $3^14^1 \times 3^14^1 = (3^14^1)(3^14^1)/4^1 = 3^24^1$, $2^15^1 \times 2^15^1 \to (2^15^1)(2^24^1)/4^1 = 2^35^1$ and $3^14^1 \times 2^15^1 = (3^14^1)(2^15^1)/4^1 = 2^13^15^1$. Another example is the configuration combination 2^14^1 and 3^2 in $B_7^{(1)}$ at $\kappa = 18$ (cf (92) and (93) or figure 9) which implies multiplicity 4 at 2 s = 1, $\kappa = 0$, $\varepsilon = 73$. The analog of (104) is

$$\begin{aligned}
&2^23^14^1(2^13^1|2^1|\,2^13^1)\!:\ \pm 2.84490 \pm (1 + 1.136 \times 10^{-8})i,\ \pm 1.67148 \pm 2.05580i,\ \pm i\\
&2^13^3(2^13^1|2^1|\,2^13^1)\!:\ \pm 4.08785 \pm 1.98750i,\ \pm 0.89428 \pm (1 - 2.938 \times 10^{-140})i,\ \pm i\\
&2^23^14^1(3^1|2^1|\,4^12^1)\!:\ -4.17364 \pm 1.98721i,\ -1.40196 \pm (1 - 1.988 \times 10^{-63})i,\ 2.39321 \pm 3.24675i,\\
&2.40291 \pm (1 + 1.937 \times 10^{-15})i,\ 2.90420 \pm (1 + 3.126 \times 10^{-8})i
\end{aligned} \tag{105}$$

Here the apparent configurations are not of product form but do single out the 2(=2s + 1)-string as special. After allowance for string replacements $4^1 \to 2^13^1$ and $3^1 \to 2^2$ we get $2^14^1 \times 2^14^1 \to (2^14^1)(2^23^1)/2^1 = 2^23^14^1$, $3^2 \times 3^2 \to (3^2)(2^23^1)/2^1 = 2^13^3$ and $2^14^1 \times 3^2 \to (2^14^1)(2^23^1)/2^1 = 2^23^14^1$. A final, different example is the product 4^1 ($B_4^{(2)}$ at $\kappa = -4$) $\times$ 2^14^1 ($B_6^{(2)}$ at $\kappa = 11$) that results in 3^14^1 at 2 s = 2, $\kappa = 7$, $\varepsilon = 34$. This requires the string replacement $4^1 \to 2^13^1$ and the divisor choice 2^2 rather than 3^1 (a 2s + 1-string was the divisor for a $B^{(2s)}B^{(2s)}$ product in all the other examples above). The absence of any obvious pattern in these configuration products is in stark contrast to the simple explicit formula (100) for the WZW tower excitations $B_{2s+2\nu}^{(2s)}$.

Equation (103) can be modified to become the generator $Z(e,\, q)$ for all states by incorporating the generators for 1-string excitations into the available left h_L and right h_R holes. These $G_h(x)$ are most easily found as the $p \to \infty$ limit of $\begin{bmatrix} p + h \\ h \end{bmatrix}_x$ giving

$$G_h(x) = 1/(x)_h, \quad (x)_h = \prod_{n=1}^{h} (1 - x^n), \tag{106}$$

where $x = e^2/q$ for $h = h_L$ and e^2q for $h = h_R$. The result, reproduced in (8), for the all state generator is

$$Z(e,\, q)^{(e/o)} = \sum_{2s=0/1}^{(e/o)} e^{(2s)^2}\left(\sum_{h_L=2s}^{(e/o)} B_{h_L}^{(2s)}(e^2/q)G_{h_L}(e^2/q)\right)\left(\sum_{h_R=2s}^{(e/o)} B_{h_R}^{(2s)}(e^2q)G_{h_R}(e^2q)\right) \tag{107}$$

considered as a series expansion in e. Evidence that (107) is correct comes from the separate left/right excitation count sum rules

$$\sum_{h=2s}^{(e/o)} B_h^{(2s)}(x)G_h(x) = (1 - x^{2s+1})G_\infty(x) \tag{108}$$

determined by explicit calculation, in many cases to an excess of a hundred terms. The right hand side of (108) involves $G_\infty(x) = \lim_{h\to\infty} G_h(x) = 1 + \sum_{n=1}^{\infty} p(n)x^n$ which is Euler's generating function for p(n), the number of partitions of n. This is known to be the multiplicity of states $m(s_z)$ at fixed s_z in the WZW model with $n = 0$ always understood to be a point on the parabola s_z^2. The multiplicity at fixed s given by the generator (108) is the difference $m(s_z = s) - m(s_z = s + 1)$ and the factor x^{2s+1} accounts for the shift $\Delta n = (s + 1)^2 - s^2$ between the two $m(s_z)$ multiplicity expressions. This can be seen more directly by writing the factor $e^{(2s)^2}$ in (107) as the product $(e^2/q)^{s^2}(e^2q)^{s^2}$ and incorporating these terms separately into the left and right factors. The sum rules involving the new left/right factors take the form (9) and are explicit realizations of the characters noted in equation (159) of [22], chapter 9.

8. Conclusions

Examples have been provided in support of the conjecture that all BAE solutions for spin-½ isotropic Heisenberg chains in fixed total spin and momentum sectors can be obtained as roots of single variable polynomials with integer (5) or integer based (6) coefficients. The most important examples are those such as the $L = 16$ states in figures 6–8 which were used to obtain BAE solutions by NR for longer chains extending to $L \approx 1000$. These long chain solutions have provided the basis for a conjecture on the relation between Bethe's string configuration labelling and the asymptotic $L \to \infty$, $k = 1$, SU(2) WZW model states in the $S = 0$ sector. The WZW states are characterized by left and right moving excitations labelled by a WZW spin $s = s_L = s_R$ and an example of the Bethe-WZW relation is shown in figure 9 for odd 2 s. The general conjecture is (8) which expresses the state multiplicity generating function in energy and momentum in the expected WZW left times right tower excitation product form. The tower generator $B_h^{(2s)}(x)/(x)_h$ in (8), equivalently $B_h^{(2s)}G_h$ in (107), contains the generator $G_h(x) = 1/(x)_h$ of 1-string excitations and a polynomial $B_h^{(2s)}(x)$ as generator for the (n>1)-string parts of Bethe's string labelled configurations. The $B_h^{(2s)}$ explicit formula (100) provides every tower state in the $L \to \infty$ limit with a Bethe string configuration label; the alternative (98) together with the recurrences (88) can be used if only multiplicities without string labelling are desired. The additional (numerical) reduction via the sum rule (9), equivalently (108), confirms the multiplicities are those expected from the WZW model. The methods described in this paper are expected to apply also to the extension of the Bethe-WZW correspondence to $S > 0$ states.

The successful assignment of Bethe string configuration labels to every state in the WZW left/right towers in the critical region at large L could be viewed as nothing more than some (yet to be proved) combinatorial identities. However, results such as (100) are more than a tautology as they rely on the observation that the tower states in an energy versus momentum plane lie on single row diagonals as illustrated in figure 9 and thus involve more than just Bethe combinatorics. I have found no counter examples in the calculation of the energy of any particular state based on the assignment of Bethe string labels by the observed complex rapidities λ at small L and the use of continuity in L to track λ to large L. It is unclear whether this always is, or can be turned into, a rigorous procedure since Bethe string identification at small L might ultimately fail to be unambiguous and, because L is discrete, continuity in L is not a well defined concept.

Because so many of the large L solutions that have been observed have complex λ that are qualitatively different from those at small L, the paper explores the possibility that there exists an 'apparent' string labelling appropriate for $L \to \infty$. While many plausible examples are found there are also counter examples such as (105) which do not fit into a consistent classification scheme. It appears that Bethe's string labelling remains as the only viable alternative even though its implementation at large L is computationally involved.

Finally, there remains the challenge of actually proving the combinatorial identities require to go from the Bethe string representation (100) to the final sum rule (108) that expresses multiplicities in terms of Euler's generating function for p(n), the number of partitions of n.

Appendix

Configuration product examples

The ambiguities and their resolution in the subtraction process

$$B_{3+2\nu}^{(3)}(q) = B_{3,3+2\nu}(q) - B_3^{(1)}(1/q)B_{3+2\nu}^{(1)}(q), \quad B_3^{(1)}(1/q) = \underbrace{q^{-3}}_{3^1} + \underbrace{q^{-4}}_{2^2} \tag{A.1}$$

are illustrated for $\nu = 1, 2$ and 3. If we write a configuration in the $B_{3+2\nu}^{(1)}(q)$ factor as $(p_2, p_3, \ldots)$ we find all observations are consistent with the products

$$2^2 \times (p_2, p_3, \ldots) = (p_2 + 1, p_3, \ldots), \quad 3^1 \times (p_2, p_3, \ldots) = \begin{cases} (p_2 + 1, p_3, \ldots), & case\ c1\ or \\ (p_2 - 1, p_3 + 1, \ldots), & case\ c2 \end{cases} \tag{A.2}$$

which corresponds to ordinary multiplication and division $(p'_2, p'_3, \ldots)(p_2, p_3, \ldots)/2^1 = (p_2 + p'_2 - 1, p_3 + p'_3, \ldots)$. Two possibilities for the 3^1 product are required to correctly generate all terms in (A.1) with case c1 arising from the replacement $3^1 \to 2^2$ that maintains $h_1 = 4$ as noted in the remarks following (95).

Consider first the generation of $B_5^{(3)}(q)$. From (106) we have

$$B_{3,5}(q) = \underbrace{q^5}_{5^1} + \underbrace{q^6 \begin{bmatrix} 5 \\ 1 \end{bmatrix}_q}_{2^1 4^1} + \underbrace{q^6}_{3^2} + \underbrace{q^7 \begin{bmatrix} 4 \\ 2 \end{bmatrix}_q}_{2^2 3^1} + \underbrace{q^8}_{2^4} \tag{A.3}$$

which together with $B_5^{(1)}(q)$ from (93) and the product rule (A.2) gives

$$\begin{aligned} U_5 &= B_{3,5}(q) - \underbrace{q^{-4}}_{2^2} \times (\underbrace{q^8}_{4^1} + \underbrace{q^9 + q^{10} + q^{11}}_{2^1 3^1} + \underbrace{q^{12}}_{2^3}) \\ &= \underbrace{q^5}_{5^1} + \underbrace{q^5 + q^6 + q^7 + q^8}_{2^1 4^1} + \underbrace{q^6}_{3^2} + \underbrace{q^7 + q^8 + q^9}_{2^2 3^1} \end{aligned} \tag{A.4}$$

as the unambiguous part of the subtraction in (A.1). For the final result

$$B_5^{(3)}(q) = U_5 - \underbrace{q^{-3}}_{3^1} \times (\overbrace{\underbrace{q^8}_{4^1}}^{c1} + \underbrace{\overbrace{q^9}^{c2} + \overbrace{q^{10} + q^{11}}^{c1}}_{2^1 3^1} + \overbrace{\underbrace{q^{12}}_{2^3}}^{c2}) \tag{A.5}$$

we need to compare terms to see, for example, that $3^1 \times 4^1 = (3^1)(4^1)/2^1$ can only be $2^1 4^1$(c1) while $3^1 \times 2^1 3^1 = (3^1)(2^1 3^1)/2^1$ is either $2^2 3^1$(c1) or 3^2(c2) and a unique choice is dictated by the terms in U_5 available for cancellation. All uniquely fixed products are indicated by the (A.2) case markers above the $B_5^{(1)}(q)$ terms in (A.5) and yield, after subtraction,

$$B_5^{(3)}(q) = \underbrace{q^5}_{5^1} + \underbrace{q^6 + q^7 + q^8}_{2^1 4^1} = \underbrace{q^5}_{5^1} + \underbrace{q^7 \begin{bmatrix} 3 \\ 1 \end{bmatrix}_q}_{2^1 4^1} \tag{A.6}$$

which is that reported in (97). Comparison with (A.3) confirms both the cancellation of all terms not containing strings longer than 2 s = 3 and the form invariance with modified Gaussian binomials in the remaining terms.

A similar calculation starting from

$$B_{3,7}(q) = \underbrace{q^{12}}_{6^1} + \underbrace{q^{14} \begin{bmatrix} 7 \\ 1 \end{bmatrix}_q}_{2^1 5^1} + \underbrace{q^{14} \begin{bmatrix} 3 \\ 1 \end{bmatrix}_q}_{3^1 4^1} + \underbrace{q^{16} \begin{bmatrix} 5 \\ 1 \end{bmatrix}_q}_{2^1 3^2} + \underbrace{q^{16} \begin{bmatrix} 6 \\ 2 \end{bmatrix}_q}_{2^2 4^1} + \underbrace{q^{18} \begin{bmatrix} 5 \\ 3 \end{bmatrix}_q}_{2^3 3^1} + \underbrace{q^{20}}_{2^5} \tag{A.7}$$

yields a U_7 analog of (A.4) given by

$$\begin{aligned} U_7 = {} & \underbrace{q^{12}}_{6^1} + \underbrace{q^{12} + q^{13} + q^{14} + q^{15} + q^{16} + q^{17}}_{2^1 5^1} + \underbrace{q^{13} + q^{14} + q^{15}}_{3^1 4^1} + \underbrace{q^{15} + q^{16} + q^{17} + q^{18}}_{2^1 3^2} \\ & + \underbrace{q^{14} + q^{15} + 2q^{16} + 2q^{17} + 2q^{18} + q^{19} + q^{20}}_{2^2 4^1} + \underbrace{q^{18} + q^{19} + q^{20} + q^{21}}_{2^3 3^1} \end{aligned} \tag{A.8}$$

and, accepting the need to cancel all terms with no string longer than 2 s = 3, a final

$$\begin{aligned} B_7^{(3)}(q) = U_7 - \underbrace{q^{-3}}_{3^1} \times (& \overbrace{\underbrace{q^{15}}_{5^1}}^{c1} + \underbrace{\overbrace{q^{16}}^{c2} + \overbrace{q^{17} + q^{18}}^{??} + \overbrace{q^{19} + q^{20}}^{c1}}_{2^1 4^1} \\ & + \overbrace{\underbrace{q^{18}}_{3^2}}^{c1} + \underbrace{\overbrace{q^{19} + q^{20} + q^{21}}^{c2} + \overbrace{q^{21} + q^{22} + q^{23}}^{c1}}_{2^2 3^1} + \overbrace{\underbrace{q^{24}}_{2^4}}^{c2}). \end{aligned} \tag{A.9}$$

The uncertain terms in (A.9) indicated by question marks could default to either $3^1 4^1$ or $2^2 4^1$ and are resolved as type c1 if we demand form invariance which only allows for a changed Gaussian binomial in the term sourced by $2^2 4^1$. Explicit long chain calculation confirms this is the correct choice and on collecting terms, (A.9) reduces to

$$B_7^{(3)}(q) = \underbrace{q^{12}}_{6^1} + \underbrace{q^{15} \begin{bmatrix} 5 \\ 1 \end{bmatrix}_q}_{2^1 5^1} + \underbrace{q^{29/2} \begin{bmatrix} 2 \\ 1 \end{bmatrix}_q}_{3^1 4^1} + \underbrace{q^{18} \begin{bmatrix} 4 \\ 2 \end{bmatrix}_q}_{2^2 4^1}, \tag{A.10}$$

again recorded in (97).

Form invariance has been checked to be sufficient for a unique $B_9^{(3)}(q)$ and $B_{11}^{(3)}(q)$. The result for $B_9^{(3)}(q)$ is the first to show what happens in the case of a Gaussian binomial product. We have

$$B_{3,9}(q) = \underbrace{q^{21}}_{7^1} + \underbrace{q^{24}\begin{bmatrix}9\\1\end{bmatrix}_q}_{2^16^1} + \underbrace{q^{24}\begin{bmatrix}5\\1\end{bmatrix}_q}_{3^15^1} + \underbrace{q^{24}}_{4^2} + \underbrace{q^{27}\begin{bmatrix}8\\2\end{bmatrix}_q}_{2^25^1} + \underbrace{q^{27}\begin{bmatrix}7\\1\end{bmatrix}_q\begin{bmatrix}3\\1\end{bmatrix}_q}_{2^13^14^1} + \underbrace{q^{30}\begin{bmatrix}7\\3\end{bmatrix}_q}_{2^34^1} + \dots \qquad (A.11)$$

where the ellipsis indicates terms without any strings longer than $2\,s = 3$ and

$$B_9^{(3)}(q) = \underbrace{q^{21}}_{7^1} + \underbrace{q^{25}\begin{bmatrix}7\\1\end{bmatrix}_q}_{2^16^1} + \underbrace{q^{49/2}\begin{bmatrix}4\\1\end{bmatrix}_q}_{3^15^1} + \underbrace{q^{24}}_{4^2} + \underbrace{q^{29}\begin{bmatrix}6\\2\end{bmatrix}_q}_{2^25^1} + \underbrace{q^{57/2}\begin{bmatrix}5\\1\end{bmatrix}_q\begin{bmatrix}2\\1\end{bmatrix}_q}_{2^13^14^1} + \underbrace{q^{33}\begin{bmatrix}5\\3\end{bmatrix}_q}_{2^34^1}. \qquad (A.12)$$

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