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LETTER TO THE EDITOR

Bethe-ansatz solutions of a non-string type: numerical results

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Abstract. For the integrable XXX antiferromagnetic ring of N spins s = 1 or $s = \frac{1}{2}$ the numerical solutions to the Bethe-ansatz equations are found, which involve non-string configurations, namely multiplets. The results up to sN = 150 are compared with higher-level Bethe-ansatz predictions. The absolute difference between the predicted and finite-N energies of the spin-zero states with a multiplet and four holes is of O(1/N). The coefficient is not the same as for the vacuum and depends on the positions of the holes. As has been expected, the multiplets are of an exponential accuracy in N, while sea strings are much more strongly deformed.

The problem of diagonalising the Hamiltonian for quantum integrable models in the context of the coordinate [1] or algebraic [2] Bethe ansatz is reduced to solving the system of the Bethe ansatz equations. For the simplest case of the XXX Heisenberg antiferromagnet and its integrable generalisation [3] to arbitrary spin s, the equations have the form

$$\frac{\lambda_j + is}{\lambda_j - is} = \prod_{k=1}^M \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i} \qquad j = 1, \dots, M.$$
(1)

Here, N is the number of sites of the spin ring; the number M of complex parameters λ_i may be $0, \ldots, sN$. The energies E are eigenvalues of the Hamiltonian

$$H = \sum_{n=1}^{N} h(\mathbf{S}_n \cdot \mathbf{S}_{n+1}) \qquad h(x) = -\sum_{j=0}^{2s-1} \left(\sum_{k=j+1}^{2s} \frac{1}{k} \right) \prod_{\substack{m=0 \ m\neq j}}^{2s} \frac{x - x_m}{x_j - x_m}$$
$$x_m = m(m+1)/2 - s(s+1) \qquad \mathbf{S}_n^2 = s(s+1) \qquad \mathbf{S}_{N+1} \equiv \mathbf{S}_1.$$

Momenta P, and spins S of the states are expressed through the solutions $\{\lambda_j\}_M$ of system (1):

$$E = -\sum_{j=1}^{M} \frac{s}{\lambda_j^2 + s^2} \qquad P \stackrel{2=\pi}{=} \frac{1}{i} \sum_{j=1}^{M} \ln\left(\frac{\lambda_j + is}{\lambda_j - is}\right) \qquad S = sN - M.$$
(2)

According to the 'string' hypothesis [1, 4, 5], every parameter λ should be a member of an *n*-string with an exponential accuracy as $N \rightarrow \infty$:

$$\lambda = x + i[\frac{1}{2}(n+1) - m] + O[\exp(-\alpha N)] \qquad m = 1, ..., n \quad \alpha > 0 \quad (3)$$

where an integer $n \ge 1$ specifies the length of the string, and a real x its centre position. The antiferromagnetic vacuum comprises a sea of M = sN 2s-strings [5].

The string hypothesis gives a rather good general qualitative classification of states, their total number being in agreement [6] with the assumption of completeness. However, the assertion about the exponential accuracy of strings proves to be wrong

in a number of cases. Even for $s = \frac{1}{2}$, on the background of the sea of real roots (1-strings), non-string configurations—quartets and wide pairs—have been predicted [7]. For $s > \frac{1}{2}$, quartets are changed to multiplets and narrow pairs may appear [8]. Deformations of the sea strings also become possible. Numerical computations [9] have shown that the minimal deviations from equation (3) for the vacuum and two-hole states behave as O(1/N) while the maximum is O(1). However, these considerable string deformations affect the energy rather weakly: the shift of the absolute energy both for the vacuum and excitations does not exceed O(1/N). The object of the present letter is to find out multiplet-type solutions explicitly and to study finite-size corrections for them.

At large N, one can describe the sea of 2s-strings with a density function. The Bethe-ansatz equations for the sea are rewritten as an integral equation for the density, which may be solved by the Fourier transformation. The study of the equations for complex-root configurations on the sea background shows that there are only three possibilities [8]: free narrow pairs $|\text{Im } \lambda| < s - \frac{1}{2}$; wide pairs $|\text{Im } \lambda| > s + \frac{1}{2}$; and multiplets

$$\lambda \simeq x \pm i(y+s-m) \qquad m=0,\ldots,2s \quad 0 < y < \frac{1}{2}.$$
(4)

Real parameters x and y determine the positions of all the pairs of the multiplet, 2s-1 narrow pairs and two intermediate pairs with $||\text{Im }\lambda| - s| < \frac{1}{2}$. As well as in strings, for each complex root of a multiplet λ (except lower members of its intermediate pairs) there is a successor λ' lying an imaginary unit below it. The deviations $\Delta x + i\Delta y = \lambda - \lambda' - i$ should be exponentially small [8]

$$\Delta x^2 + \Delta y^2 = \exp(-KN) \qquad \qquad K = \ln \frac{\cosh(\pi x) + \cos(\pi y)}{\cosh(\pi x) - \cos(\pi y)}. \tag{5}$$

The sea contributions to the equations for the allowed configurations can be evaluated. Thereafter, the equations are reduced to the higher-level Bethe-ansatz form, where the N factors of equations (1) are cancelled. Contributions of the complex roots to the energy and momentum are exactly compensated for by the backflow reaction of the sea. Thus, the energy and momentum are completely determined by physical excitations, i.e. holes in the sea. In the limit of an infinite size of the ring, their positions may be arbitrary. However, at finite N they are discrete and correspond to half-integer values of the integral of the density for 2s-strings together with holes. This can also be written [9] as higher-level Bethe-ansatz equations.

In the present letter the simplest multiplet-type solutions are considered, with one quartet $(s = \frac{1}{2})$ or sextet (s = 1) at even N and the minimal number of holes (i.e. four holes) with total spin S = 0. For this case the higher-level Bethe-ansatz equations [8] are reduced to the form

$$\prod_{j=1}^{4} \frac{x - x_j + i(y + \frac{1}{2})}{x - x_j + i(y - \frac{1}{2})} = \frac{2y + 1}{2y - 1}$$
(6)

$$\pi Q_j = N[\pi/4 - \tan^{-1} \exp(-\pi x_j)] + \tan^{-1} \left(\frac{x - x_j}{y + \frac{1}{2}}\right) + \tan^{-1} \left(\frac{x - x_j}{\frac{1}{2} - y}\right) + \int_0^\infty \frac{dp}{p} \sum_{k=1}^4 \sin[(x_j - x_k)p] \\
+ \int_0^\infty \frac{dp}{p} \sum_{k=1}^4 \sin[(x_j - x_k)p] \\
\times \frac{2 \exp[(s - \frac{1}{2})p] - \exp[-(s - \frac{1}{2})p] - \exp[-(s + \frac{1}{2})p]}{2 \cosh(p/2)2 \sinh(sp)} \qquad j = 1, \dots, 4 \quad (7)$$

where Q_j are (half-) integer numbers—according to $Q_{\max} = \frac{1}{4}N + \frac{1}{2} - (2s)^{-1}$ —which specify the hole positions; $|Q_j| \le Q_{\max}$.

Equation (6) for the parameters of the multiplet can be solved exactly. After eliminating the denominator and taking the imaginary part, one gets $y(4y^2-1) \times (x_1+x_2+x_3+x_4-4x) = 0$. It follows then that, for the multiplet solution (4),

$$x = \frac{1}{4}(x_1 + x_2 + x_3 + x_4). \tag{8}$$

The real part, after formula (8) is substituted, gives a biquadratic equation for y. Its solution can be represented as

$$y = \left\{\frac{1}{6}\left[\frac{1}{2} - 2A_2 \pm (1 + 4A_2 + 28A_2^2 - 12A_4)^{1/2}\right]\right\}^{1/2} \qquad A_n = \frac{1}{4}\sum_{j=1}^4 (x_j - x)^n.$$
(9)

Equations (7) have to be solved numerically. One iterates the hole coordinates, using formulae (8) and (9) at every step. The result allows one to compute the leading approximation in $N \rightarrow \infty$ for the energy and momentum of the state

$$E_{\infty} = \sum_{j=1}^{4} \frac{1}{2}\pi / \cosh(\pi x_j) - N \times \begin{cases} \sum_{n=1}^{s} (2n-1)^{-1} & \text{integer } S \\ \ln 2 + \sum_{n=1}^{s-1/2} (2n)^{-1} & \text{half-integer } S \end{cases}$$
(10)

$$P \stackrel{2\pi}{=} \pi s N - 2 \sum_{j=1}^{4} \tan^{-1} \exp(-\pi x_j).$$
(11)

The difference between the primary values (2) derived from the solutions to equations (1), on the one hand, and the higher-level approximation (5)-(11), on the other hand, is due to finite-size corrections. As a consequence of equations (6) and (7), formula (11) for the momentum proves to be exact because its values are multiples of $2\pi/N$. Numerical data presented below demonstrate that the absolute energy correction $E - E_{\infty}$ behaves like O(1/N), i.e. in the same way as for the vacuum and simplest excitations [9-11].

The numerical computations are performed by the Newton method for the logarithms of equations (1) [9]. Since multiplets should have exponentially small deviations from formula (4), quantities of essentially different scales may be present in the problem. Thus, because the computer precision is limited, one has to store for each complex root, besides its absolute position, the value of $\Delta x + i\Delta y$. Furthermore, to improve the linear system solved at every step of the iterations, the equations are modified as follows. To each equation for a member of a string-like chain, the equations for all its successors are added. This eliminates singularities in internal deformations of the chains from the equations for their higher members.

The results of computing multiplet-type states with different N but about the same hole positions are presented in tables 1 and 2. The index ∞ relates to the higher-level Bethe-ansatz approximation (5)-(10). On the other hand, the real and imaginary parts of the highest multiplet member $\lambda_{\max}(\text{Im} \simeq y_{\infty} + s)$, the coefficient K = $-\ln(\Delta x^2 + \Delta y^2)_{\max}/N$ characterising its deviation from the successor, the momentum and energy of the state (2) are computed through the solutions to equations (1). The quantity $\delta = (E - E_{\infty})N$ controls the accuracy of the approximation (10); the δ_v values correspond to the vacuum solutions.

For s = 1 we also present information about the sea-string deformations, namely Δ_{\max} and Δ_{\max} , the maximum and average values of Δy over all the string-like chains. It should be noted that at the points x_j the sign of the deformations alters, as in two-hole states [9]. This is reflected in the average and maximum values.

N	Q_j	$x_{j\infty}$	$x_{\infty}, y_{\infty}; \lambda_{\max}$	K_{∞}, K	$P\frac{N}{2\pi}$, E, δ , δ_v
50	-12	-1.252 832 0	0.406 961 9	0.223	-3
	10	0.653 101 12	0.431 076 6	0.305	-33.965 296 076 7
	11	0.862 333 72	0.415 359 545		-0.890 181
	12	1.365 244 8	0.929 075 272		-0.824 79 465 969
80	-19.5	-1.403 916 72	0.482 866 2	0.305	37
	17.5	0.803 357 612	0.382 315 4	0.342	-55.017 755 873 5
	18.5	1.012 484 691	0.491 795 306		-0.895 606
	19.5	1.519 539 278	0.878 948 890		-0.824 136 394 052
128	-31.5	-1.555 931 0	0.466 372 6	0.364	59
	28.5	0.826 307 48	0.365 157 5	0.388	-88.298 064 364 7
	29.5	0.952 866 74	0.473 087 495		-0.893 067
	31.5	1.642 247 31	0.861 554 593		-0.823 697 869 135
200	-48.5	-1.235 321 67	0.450 874 7	0.300	92
	44.5	0.805 860 239	0.394 788 6	0.313	-138.110 673 055
	46.5	0.963 748 648	0.456 742 522		-0.865 510
	48.5	1.269 211 69	0.894 007 428		-0.823 428 050 508
300	-72.5	-1.184 032 24	0.463 133 7	0.289	139
	67.5	0.828 597 34	0.394 891 8	0.296	-207.433 923 708
	70.5	1.002 305 24	0.468 814 566		-0.859 953 1
	72.5	1.205 664 62	0.894 719 545		-0.828 254 238 795

Table 1. Quartet-type solutions $(s = \frac{1}{2}, S = 0)$: N dependence. (Note that $-\pi^2/12 = -0.822467033424$.)

Table 2. Sextet-type solutions (s = 1, S = 0): N dependence. (Note that $-\pi^2/8 = -1.23370055014$.)

N	Q_j	$x_{j\infty}$	$x_{\infty}, y_{\infty}; \lambda_{\max}$	K_{∞}, K	$P\frac{N}{2\pi}, E, \delta, \delta_{v}$	$\Delta_{\max}, \Delta_{mean}$
30	-7.5	-1.266 2	0.442 8	0.120	13	-0.052 827 9
	5.5	0.587 47	0.459 35	0.296	-29.242 077 802 2	-0.012 479 9
	6.5	0.872 13	0.461 383 788		-0.273	
	7.5	1.577 61	1.463 892 21		-1.243 593 960 24	
50	-12.5	-1.427 391 6	0.527 411	0.189	23	-0.055 786 7
	10.5	0.750 800 6	0.447 459	0.236	-49.540 440 441 1	-0.012 966 2
	11.5	1.035 817 1	0.548 039 600		-0.212 63	
	12.5	1.750 416 8	1.423 892 89		-1.240 083 196 75	
80	-20	-1.581 445	0.555 043	0.183	37	-0.057 110 0
	17	0.740 698	0.413 279	0.198	79.590 490 309 4	-0.009 917 90
	19	1.176 765	0.578 650 910		-0.187 48	
	20	1.884 152	1.423 775 51		-1.238 295 840 77	
128	-31	-1.125 783 9	0.468 014	0.234	59	0.076 985 0
	28	0.773 952 8	0.414 146	0.253	-127.435 220 911	-0.001 247 05
	30	1.006 604 1	0.478 827 931		-0.249 32	
	31	1.217 283 7	1.415 264 22		-1.237 186 501 32	
150	-36.5	-1.176 467 48	0.472 369	0.233	69	0.077 194 9
	32.5	0.747 517 12	0.413 384	0.246	-149.452 818 318	-0.001 269 93
	35.5	1.054 620 39	0.483 363 361		-0.237 879	
	36.5	1.263 806 19	1.415 000 05		-1.236 904 878 80	

Another projection, different multiplet-type states at the same N, is presented in tables 3 and 4. One can observe how the parameters of the multiplets vary with a shifting of the holes.

The following general conclusion can be made from the computations. As well as strings, multiplets are perfectly reliable configurations for sufficiently large N. They may degenerate into strings only when y approaches $\frac{1}{2}$ or 0. Moreover, the deviations from the multiplet structure (4) are in fact exponentially small: K behaves like O(1) and agrees reasonably with the predicted values (5). At the same time, deformations of the sea strings (at s = 1) are more considerable, between O(1/N) and O(1). The average deformation may probably be diminished in the 'thermodynamic' limit of a very large number of excitations, only owing to deformation-sign changes at the hole positions.

The higher-level Bethe ansatz (6)-(11) provides a rather good approximation. One sees from tables 1 and 2 that the quantity δ at large N approaches a constant (fluctuations are due to some drift of the holes). Hence, the finite-size absolute correction to both the ground-state and excitation energy is O(1/N). The leading asymptotics coefficient for the vacuum (for previous numerical results see [10] ($s = \frac{1}{2}$), [11] (s = 1) and [9] (s up to $\frac{9}{2}$)) agrees well with the value of the central charge in the conformal field theory [12]

$$\delta_{v} = (E - E_{\infty})_{v} N \xrightarrow[N \to \infty]{} -\frac{1}{12} \pi^{2} c \qquad c = 3s/(s+1).$$
(12)

For the excited states, δ differs from formula (12) and depends on the hole positions (tables 3 4). The comparison with the anomalous dimensions of the scaling operators [13] is, however, difficult because the states considered are too highly excited. The low-lying two-hole excitations [9] would be more appropriate, but there are also

Q_j	$x_{j\infty}$	$x_{\infty}, y_{\infty}; \lambda_{\max}$	K_{∞}, K	$P\frac{N}{2\pi}$, E, δ
-73.5	-1.364 821 57	0.587 937 6	0.380 8	145
71.5	1.094 332 26	0.290 619 1	0.379 9	-207.696 353 473
72.5	1.216 142 73	0.595 746 011		-0.868 34
73.5	1.406 097 20	0.789 259 871		
-73.5	-1.363 640 14	0.72 300 6	0.544 6	118
62.5	0.655 947 17	0.401 130 3	0.586 2	-206.817 631 923
63.5	0.683 452 20	0.168 892 334		-0.852 31
64.5	0.713 442 96	0.896 267 176		
-73.5	-1.363 810 05	-0.064 776 9	0.351 9	64
44.5	0.356 686 17	0.443 105 6	0.390 5	-205.206 089 162
45.5	0.368 119 28	-0.071 645 209		-0.832 73
46.5	0.379 897 02	0.938 997 428		
-73.5	-1.364 804 79	-0.244 137 4	0.167 3	-17
17.5	0.122 220 59	0.465 1560 0	0.197 3	-203.556 189 286
18.5	0.129 397 48	-0.252 869 538		-0.807 541
19.5	0.136 636 94	0.961 900 751		
-73.5	-1.369 625 06	-0.536 278 4	0.028 6	121
-36.5	-0.267 482 56	0.487 321 8	0.055 8	-204.409 235 838
-35.5	-0.258 439 97	-0.547 265 385		-0.787 864
-34.5	-0.249 566 19	0.985 490 076		

Table 3. Quartet-type solutions $(s = \frac{1}{2}, N = 300, S = 0)$: Q dependence.

Q_j	$x_{j\infty}$	$x_{\infty}, y_{\infty}; \lambda_{\max}$	K_{∞}, K	$P\frac{N}{2\pi}$, E, δ	$\Delta_{\max}, \Delta_{\max}$
-37.5	-1.784 453	0.705 753	0.325	73	-0.058 475 0
35.5	1.100 561	0.231 061	0.295	-149.846 266 281	-0.008 951 29
36.5	1.387 729	0,729 061 176		-0.132 87	
37.5	2.119 174	1.248 480 914			
-37.5	-1.770 189 3	0.372 806 1	1.006	70	0.70 843 0
34.5	0.924 332 2	0.193 250 1	1.117	-149.648 265 432	-0.005 959 21
35.5	1.061 094 3	0.368 102 324		-0.143 13	
36.5	1.275 987 1	1.154 708 082			
-37.5	-1.765 015 46	0.172 158 3	1.247	64	0.084 035 2
32.5	0.738 942 90	0.280 394 2	1.474	-149.256 159 171	-0.004 126 34
33.5	0.811 524 92	0.160 400 989		-0.166 79	
34.5	0.903 180 69	1.250 735 093			
-37.5	-1.762 330 77	-0.006 741 4	1.020	52	0.090 990 2
28.5	0.538 436 98	0.344 188 1	1.205	-148.490 623 758	-0.002 579 04
29.5	0.576 872 37	-0.023 845 271		-0.207 09	
30.5	0.620 055 85	1.320 130 172			
-37.5	-1.761 956 49	-0.149 269 4	0.669	34	0.094 104 0
22.5	0.364 446 98	0.383 285 4	0.784	-147.427 735 359	-0.001 457 36
23.5	0.387 795 68	-0.170 197 903		0.274 93	
24.5	0.412 636 09	1.362 607 767			
-37.5	-1.764 783 69	-0.318 320 0	0.330	-2	0.095 862 8
10.5	0.148 924 74	0.418 808 6	0.399	-145.842 065 398	-0.000 275 055
11.5	0.163 725 58	-0.343 302 354		-0.457 89	
12.5	0.178 853 36	1.401 552 230			
37.5	-1.770 475 69	-0.444 898 2	0.177	-38	0.096 323 5
-1.5	-0.016 236 79	0.439 181 6	0.231	-145.283 023 731	0.000 500 191
-0.5	-0.003 036 83	-0.472 627 654		-0.684 93	
0.5	0.010 156 57	1.424 216 927			

Table 4. Sextet-type solutions (s = 1, N = 150, S = 0): Q dependence.

problems with them, due to the presence of $O[1/(N \ln N)]$ corrections [8, 9, 14] in addition to O(1/N) corrections. Although the shift of the sea strings can be estimated [14], there are still no efficient exact methods for describing their deformation, essential for computing the central charge and anomalous dimensions analytically.

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