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LETTER TO THE EDITOR

The lowest excitations in the spin-s XXX magnet and conformal invariance

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Abstract. The Bethe-ansatz equations for the integrable spin-s isotropic Heisenberg antiferromagnet are solved numerically at a finite number of sites N. The vacuum and the lowest singlet and triplet solutions are presented for $s=\frac{1}{2},\ldots,2$ up to $sN=240$. Through extrapolation of the finite-size data, the central charge and anomalous dimensions of the scaling operators for the underlying conformal field theory are calculated and found to agree with the expected theoretical values. The status of the Bethe string hypothesis about the structure of the solutions is discussed based on the obtained computer data up to $s=\frac{9}{2}$.

The study of low-lying excitations in finite-size one-dimensional quantum systems without a mass gap is of interest because of their relation to conformal invariance. The behaviour of finite-size energy corrections in the scaling region allows one to determine the parameters of the underlying conformal field theory relevant to critical phenomena [1]. The Bethe ansatz [2, 3] reduces the solution of an integrable model to a system of coupled equations. This permits reaching a larger size and performing a more definite check of conformal-invariance predictions.

The integrable spin-s generalisation [4-6] of the Heisenberg ring of N spins leads to the following Bethe-ansatz equations

$$\left(\frac{\lambda_j+\mathrm{i}s}{\lambda_j-\mathrm{i}s}\right)^N=-\prod_{k=1}^{M}\frac{\lambda_j-\lambda_k+\mathrm{i}}{\lambda_j-\lambda_k-\mathrm{i}}\qquad j=1,\ldots,M \tag{1}$$

where $0\leqslant M\leqslant sN$. A solution set of complex numbers $\{\lambda_j\}^M$ determines the energy E, momentum P, and spin S of a state

$$E=-\sum_{j=1}^{M}\frac{s}{\lambda_j^2+s^2}\qquad P\overset{2\pi}{=}\mathrm{i}^{-1}\sum_{j=1}^{M}\ln\frac{\lambda_j+\mathrm{i}s}{\lambda_j-\mathrm{i}s}\qquad S=sN-M. \tag{2}$$

Conformal invariance predicts [1] that with periodic boundary conditions as $N\to\infty$ the ground-state and excitation energies should behave like

$$E_v=e_\infty N-\tfrac{1}{6}\pi vN^{-1}[c+\mathrm{O}(\ln^{-3}N)] \tag{3}$$

$$E_\alpha-E_v=2\pi vN^{-1}[x_\alpha+d_\alpha/\ln N+\mathrm{o}(\ln^{-1}N)] \tag{4}$$

where a central charge c, scaling dimensions x_α, and slopes d_α are parameters of a universality class, while e_∞ and v are specific of a particular model. Equation (4) refers to the lowest state of a 'tower' of states with

$$E_\alpha^{(m,n)}\simeq E_\alpha+2\pi vN^{-1}(m+n)\qquad P_\alpha^{(m,n)}=P_\alpha+2\pi N^{-1}(m-n) \tag{5}$$

where m, $n\geqslant 0$ are integers.

For the present model, $e_\infty = \Sigma_{n=1}^{s}(2n-1)^{-1}$ if s is an integer, and $e_\infty = \ln 2 + \Sigma_{n=1}^{s-1/2}(2n)^{-1}$ for a half-odd-integer s [5, 6]. The effective velocity of sound $v = \pi/2$ is extracted from the dispersion relation for elementary excitations (holes) [5-8], which should reproduce formula (5) as $N \to \infty$. The conjectured value of the central charge is [8]

$$c = 3s/(s+1). \tag{6}$$

It agrees with the specific heat capacity at low temperatures [6] which should be $C_N/N \simeq \frac{1}{3}\pi c v^{-1} T$. The conjecture for the underlying conformal field theory is the SU(2) $k = 2s$ Wess-Zumino-Novikov-Witten σ model [9]. In that case, primary field operators should have the following scaling dimensions [10]

$$x_j = j(j+1)/(s+1) \qquad j = 0, \tfrac{1}{2}, \ldots, s. \tag{7}$$

For the simplest case of $s = \frac{1}{2}$, when the bulk of the configuration comprises a sea of real roots, powerful analytic methods have been developed to evaluate finite-size corrections [11-13]. The results agree with the numerical computations [14, 15], although the logarithmic corrections in formulae (3) and (4) make the extrapolation, even for $N \leqslant 1024$ [15], rather hard [13].

For $s > \frac{1}{2}$, another difficulty arises, concerning the accuracy of the Bethe string hypothesis [2, 16] used in references [5, 6]. The hypothesis claims that, as $N \to \infty$, any solution of equations (1) should consist of some n-strings

$$\lambda_m \simeq x + \mathrm{i}[(n+1)/2 - m] \qquad m = 1, \ldots, n \tag{8}$$

with deviations of $O[\exp(-aN)]$. Already at $s = \frac{1}{2}$, some non-string configurations appear [17, 18]. A relaxed version [19] of the string hypothesis involves these configurations on the background of the sea of perfect $2s$-strings. However, the numerical computations [20-22] show that at least $O(1/N)$ deformations of the sea strings occur. As a result, the analytic estimate that does not take these deformations into account leads to $c = 1$ irrespective of s [22], which contradicts the numerical data [18, 20-22] supporting formula (6).

An important step to the analytic description of the string deformations has recently been made by de Vega and Woynarovich [23]. They succeeded in analytically estimating the leading correction to the imaginary parts of the roots (8) for the vacuum solution through a generalisation of the Euler-Maclaurin integration formula to include non-analytic contributions in N^{-1}. It is worth comparing their estimate, which describes the asymptotics in $N \to \infty$ for the bulk of the deformations (except the ends of the string distribution), with the computer data. In table 1, data for deviations of the distance between successive members of a string (8) from the imaginary unit, $\Delta x + \mathrm{i}\Delta y = \lambda_m - \lambda_{m+1} - \mathrm{i}$, are shown. The minimum Δy is multiplied by N and then extrapolated

Table 1. The extrapolated minimum string deformation $N\Delta y_{\min}^{\mathrm{ex}}$ and its theoretical prediction $N\Delta y_{\min}^{\mathrm{th}}$ for different s.

$2s$	$N\Delta y_{\min}^{\mathrm{ex}}$	$N\Delta y_{\min}^{\mathrm{th}}$	$2s$	$N\Delta y_{\min}^{\mathrm{ex}}$	$N\Delta y_{\min}^{\mathrm{th}}$
2	0.220	0.220 635 600	6	0.053	0.050 403 474
3	0.153	0.153 174 481	7	0.043	0.040 913 071
4	0.093	0.091 572 048	8	0.034	0.031 946 720
5	0.072	0.070 258 730	9	0.030	0.026 892 235

to $N \to \infty$ from the computer results for $sN \leqslant 128$ [20]. This $N\Delta y^{\rm ex}_{\rm min}$ is presented in conjunction with the theoretical predictions [23] $N\Delta y^{\rm th}_{\rm min}$ for $1 \leqslant s \leqslant \frac{9}{2}$. A perfect agreement is observed within extrapolation errors, presumably of $O(1/N)$.

A comparison of internal deformations of a sea string near the origin for the $s = \frac{9}{2}$, $N = 52$ vacuum with the asymptotics [23] is presented in table 2. The roots of equations (1), computed numerically, and their imaginary parts in the asymptotic approximation [23], taking into account the real-root position, are presented. One can see that the theoretical predictions underestimate by 7–20% the actual string deformations. The error seems to be of $O(1/N)$.

Table 2. Numerical solutions λ and theoretical predictions $\lambda^{\rm th}$ for the roots of a 9-string at $s = 9/2$, $N = 52$.

Re λ	Im λ	Im $\lambda^{\rm th}$
0.019 295 132 866	0	0
0.019 294 724 871	±1.000 617 287 46	±1.000 518 108 80
0.019 293 355 234	±2.001 329 577 57	±2.001 136 553 89
0.019 290 441 652	±3.002 323 601 98	±3.002 054 142 55
0.019 284 156 898	±4.004 290 492 52	±4.003 997 205 57

Nonetheless, for excited states there are still no analytic results taking into account string deformations which are not smaller than $O(1/N)$, as we have seen. Thus, numerical computations may provide important information. The results of the present letter (tables 2–5) have been obtained by a Newton-type method for the logarithms of equations (1) [20], regrouped [18] according to the chain configuration of strings [16] and multiplets [19], to localise singularities in internal deformations of the chains.

To extract the critical parameters, it is convenient to consider the following finite-size energy correction:

$$f = (E - e_\infty N)N/(2\pi v). \qquad (9)$$

According to formulae (3) and (6), we expect that for the vacuum solutions, as $N \to \infty$, f_v should approach the limit of $-\frac{1}{4}s/(s+1)$, proportional to the central charge. Thus, for $2s = 1$, 2, 3, 4, and 9, we get $-\frac{1}{12}$, $-\frac{1}{8}$, $-\frac{3}{20}$, $-\frac{1}{6}$ and $-\frac{9}{44}$. Besides the vacuum, for each s and N, two lowest excitations are computed, the singlet (with the total spin $S = 0$) and the triplet ($S = 1$). Solutions of the latter type have already been studied [21, 22] (sector $r = 1$); in the domain of overlap, the results are in agreement with ours which extend to larger N. A conjecture to be verified in tables 3 and 4 is that the conformal dimensions both for the singlet and triplet are given by formula (7) with $j = \frac{1}{2}$, $x_s = x_t = \frac{3}{4}/(s+1)$. Hence, the finite-size energy corrections should approach f_s, $f_t \to \frac{1}{4}(3-s)/(s+1)$, which equals $\frac{5}{12}$, $\frac{1}{4}$, $\frac{3}{20}$, $\frac{1}{12}$, and $-\frac{3}{44}$ for $2s = 1$, 2, 3, 4, and 9. The normalisation factors in tables 3 and 4 involve the denominators of the expected limit values, to make the comparison easier.

The data are extrapolated to zero in $1/(\ln N)$ linearly (using two last rows) and quadratically (three last rows). The extrapolation of the vacuum correction f_v includes the terms $\ln^{-3} N$ (3) and $\ln^{-4} N$. For estimating extrapolation errors and getting improved values, the results of the higher-level Bethe-ansatz approximation [17–20] are included in table 3. The corresponding values of F_s and F_t for the singlet and

Table 3. Finite-size energy corrections for the vacuum and the lowest singlet and triplet excitations $f_{v,s,t}$ in conjunction with the higher-level Bethe-ansatz approximation $F_{s,t}$ and their extrapolations to $N \to \infty$.

$2s$	N	$12 f_v$	$12 f_s$	$12 f_t$	$2F_s$	$2F_t$	$6 f_s/F_s$	$6 f_t/F_t$
1	8	−1.030 226 965	8.224 517 330	4.053 739 432	1.570 173	0.785 3180	5.237 968	5.161 908
1	16	−1.010 452 107	7.660 999 337	4.245 728 069	1.476 720	0.834 0110	5.187 850	5.090 734
1	32	−1.004 496 374	7.215 404 226	4.372 415 266	1.398 626	0.865 2650	5.158 924	5.053 267
1	64	−1.002 395 300	6.884 567 681	4.460 947 747	1.339 303	0.886 6113	5.140 409	5.031 458
1	128	−1.001 496 517	6.636 183 286	4.526 381 344	1.294 293	0.902 0666	5.127 267	5.017 791
1	256	−1.001 032 325	6.444 842 550	4.576 935 359	1.259 447	0.913 7852	5.117 198	5.008 765
1	480	−1.000 776 452	6.306 267 178	4.613 901 699	1.234 159	0.922 2146	5.109 770	5.003 068
Linear slope		−1.000 103	5.0838	4.9400	1.0111	0.996 57	5.0442	4.9528
		−0.158	7.55	−2.01	1.38	−0.459	0.405	0.310
Quadratic slope		−1.000 124	5.0045	4.9737	0.9947	0.999 36	5.0351	4.9793
		−0.141	8.48	−2.41	1.57	−0.492	0.511	−0.0003
$2s$	N	$8 f_v$	$4 f_s$	$4 f_t$	$4F_s$	$4F_t$	f_s/F_s	f_t/F_t
2	4	−1.137 330	2.431 708	0.810 5695	2.756 87	0.743 625	0.882 055	1.090 024
2	6	−1.066 802	2.234 402	0.819 6859	2.483 54	0.757 523	0.899 685	1.082 061
2	8	−1.041 970	2.099 851	0.826 1490	2.302 65	0.765 811	0.911 929	1.078 789
2	10	−1.030 016	2.007 762	0.831 0068	2.180 85	0.771 894	0.920 631	1.076 582
2	26	−1.009 235	1.728 184	0.850 3551	1.824 06	0.797 284	0.947 440	1.066 565
2	64	−1.004 321	1.575 870	0.866 6106	1.640 28	0.820 388	0.960 731	1.056 343
2	126	−1.002 850	1.499 143	0.877 4451	1.550 94	0.836 315	0.966 604	1.049 181
2	240	−1.002 065	1.444 068	0.886 6011	1.488 05	0.849 924	0.970 447	1.043 153
Linear slope		−1.000 34	1.030 7	0.955 3	1.016 0	0.952 1	0.999 3	0.997 9
		−0.284	2.27	−0.377	2.59	−0.560	−0.158	0.248
Quadratic slope		−1.000 42	1.0389	0.991	1.0588	1.0086	0.9886	0.9750
		−0.240	2.18	−0.745	2.15	−1.14	−0.048	0.485

$2s$	N	$20f_v$	$20f_s$	$20f_t$	$6F_s$	$6F_t$	$\frac{20}{6}f_s/F_s$	$\frac{20}{6}f_t/F_t$
3	4	−3.490 868 892	10.709 417 289	2.643 473 002	3.606 8028	0.596 2761	2.969 2273	4.433 304
3	6	−3.244 435 482	9.343 252 931	2.575 037 327	3.052 5433	0.619 1811	3.060 8093	4.158 779
3	10	−3.114 022 321	8.001 326 652	2.524 656 864	2.578 3797	0.648 6945	3.103 2383	3.891 904
3	16	−3.062 823 024	7.134 320 243	2.501 313 682	2.304 2864	0.674 9355	3.096 1083	3.706 004
3	26	−3.037 601 313	6.494 951 720	2.492 871 472	2.113 8863	0.700 1552	3.072 5170	3.560 456
3	50	−3.025 799 850	6.074 165 793	2.494 478 363	1.991 3278	0.720 5798	3.050 3093	3.461 766
3	62	−3.018 728 833	5.742 731 519	2.501 946 584	1.894 6959	0.739 4034	3.030 9515	3.383 737
3	100	−3.013 963 517	5.459 236 739	2.514 362 496	1.810 8580	0.757 7759	3.014 7240	3.318 082
3	160	−3.010 906 701	5.237 036 288	2.529 100 458	1.743 7189	0.773 8251	3.003 3718	3.268 310
Linear slope		−3.0019	3.060	2.674	1.086	0.9311	2.892	2.781
		−1.18	11.05	−0.73	3.34	−0.80	0.56	2.48
Quadratic slope		−3.0022	3.270	2.900	1.081	0.9950	2.968	2.909
		−1.04	9.02	−2.92	3.39	1.42	−0.17	1.24

$2s$	n	$6f_v$	$12f_s$	$12f_t$	$8F_s$	$8F_t$	$\frac{3}{2}f_s/F_s$	$\frac{3}{2}f_t/F_t$
4	4	−1.186 270 420	5.795 418 190	0.987 925 3647	2.832 9156	0.402 5179	2.0457 433	2.454 364
4	8	−1.061 444 973	4.305 101 542	0.880 465 5114	2.645 9815	0.491 9038	1.6270 339	1.789 914
4	10	−1.045 259 988	3.968 295 267	0.857 609 5788	2.579 6557	0.517 1779	1.5383 042	1.658 249
4	16	−1.025 588 378	3.427 593 389	0.822 136 1611	2.442 8800	0.564 5979	1.4030 953	1.456 145
4	26	−1.015 661 836	3.036 512 152	0.799 017 2040	2.312 8686	0.605 8917	1.3128 771	1.318 746
4	32	−1.013 050 093	2.905 099 355	0.792 264 9391	2.261 7229	0.621 4359	1.2844 630	1.274 894
4	50	−1.009 249 467	2.674 360 758	0.782 531 7684	2.161 1126	0.651 1501	1.2374 925	1.201 769
4	80	−1.006 822 136	2.487 515 932	0.777 604 5460	2.068 2094	0.677 8084	1.2027 389	1.147 233
4	120	−1.005 442 677	2.359 142 928	0.776 458 8581	1.997 7301	0.697 6837	1.1809 117	1.112 910
Linear slope		−1.000 91	0.972	0.764	1.236	0.912	0.945	0.742
		−0.498	6.64	0.06	3.65	−1.03	1.13	1.78
Quadratic slope		−1.001 05	1.148	0.887	0.973	0.970	1.086	0.959
		−0.443	5.03	−1.07	6.06	−1.55	−0.16	−0.22

Table 4. The finite-size energy corrections for the vacuum and the lowest singlet and triplet excitations at $s=\frac{9}{2}$.

$2s$	N	$44f_v$	$44f_s$	$44f_t$
9	4	−11.403 963 2935	14.947 317 867	−2.072 071 145 09
9	8	−9.869 320 3778	8.396 161 215	−2.446 699 736 15
9	16	−9.404 174 5777	5.150 993 725	
9	32	−9.225 067 5281	3.321 264 333	
9	52	−9.161 563 6516		
Linear slope		−9.030	−3.998	−3.196
		−8.13	25.4	1.56
Quadratic slope		−9.022	−3.117	
		−9.63	19.9	

triplet take into account non-string narrow pairs [19] on the background of the sea of perfect $2s$-strings. The asymptotic behaviour of these values is known [20, 22]

$$F_s=\tfrac{1}{4}[s^{-1}+3\ln^{-1}N-3\ln(8s/\pi)\ln^{-2}N+\mathrm{O}(\ln^{-3}N)] \tag{10}$$

$$F_t=\tfrac{1}{4}[s^{-1}-\ln^{-1}N+\ln(8s/\pi)\ln^{-2}N+\mathrm{O}(\ln^{-3}N)] \tag{11}$$

therefore they can be used to improve the extrapolation, since logarithmic corrections may be noticeably diminished in the ratios f_s/F_s and f_t/F_t.

In the excitations considered, one of the sea $2s$-strings should be replaced by a $(2s-1)$-string; in the singlet, another $2s$-string is replaced by a perfect $(2s+1)$-string at zero, without any deviations [24] from formula (8). However, for the $(2s-1)$-string, a strong violation of the string hypothesis occurs: the imaginary parts of all its complex pairs get incremented by $\frac{1}{2}+\mathrm{O}(1/N)$, and thus, the pairs are 'dissolved' in the sea of the deformed $2s$-strings. This is the limit picture. For high s at a finite N, an intermediate structure may be observed, when the higher members of the $(2s-1)$-string have already 'stretched' to the size of $2s$-strings while the lower members are still near their prescribed positions (8). An example—the $s=\frac{9}{2}$, $N=32$ singlet—is shown in table 5. Also, large Δx-type deformations may be present. These facts entail numerical instabilities due to difficulties in finding a good initial guess to start iterations.

As concerns the logarithmic slopes d_α in formula (4), their numerical estimates are very rough. For high s, when large values of n can hardly be achieved, even the signs for d_α may be wrong. This is seen from a non-monotonous behaviour of f_t at $2s=3$ in table 3. Also, a difference is observed between the values extracted from the direct extrapolation of $f_{s,t}$ and from $f_{s,t}/F_{s,t}$. A fit of the data, which is consistent with the analytic result for the triplet at $s=\frac{1}{2}$ [12], looks like

$$d_s=\tfrac{3}{8}[1+(2s)^{-1}] \qquad d_t=-\tfrac{1}{8}[1+(2s)^{-1}]. \tag{12}$$

Table 5. The deformed $(2s-1)$-string and the nearest roots of the $2s$-string sea for the lowest singlet excitation at $s=\frac{9}{2}$, $N=32$.

Re λ	$\lvert\mathrm{Im}\,\lambda\rvert$	$\lvert\mathrm{Re}\,\lambda\rvert$	$\lvert\mathrm{Im}\,\lambda\rvert$
		0.033 407 335 76	0
0	0.672 011 205 07	0.033 780 700 97	0.988 594 504 52
0	1.975 275 811 40	0.060 405 731 44	1.975 929 581 81
0	2.992 299 887 69	0.064 637 337 32	2.992 150 519 94
0	4.001 160 600 99	0.065 131 269 86	4.001 176 260 26

For the vacuum, however, the values of the leading logarithmic-correction coefficient are more reliable. The vacuum finite-size energy corrections in table 3 are well described by the formula

$$f_v \simeq -(c/12)[1+r_v \ln^{-3} N + \mathrm{O}(\ln^{-4} N)] \qquad r_v = s/(s+3). \tag{13}$$

Our fit $r_v = \frac{1}{7}$ at $s = \frac{1}{2}$ agrees neither with the earlier renormalisation-group prediction $r_v = \frac{3}{4}$ [1], nor with the analytic estimate $r_v = 0.3433$ [12, 13]. Strangely enough, the inadequacy of the latter value has not been noticed in the more advanced data [15]. Although the behaviour of further terms is unknown and something like $\mathrm{O}[\ln(\ln N)/\ln^4 N]$ may appear, the leading correction $\ln^{-3} N$ is small enough for plausibility of our result. Besides, when including $\ln^{-4} N$ ('quadratic' extrapolation in table 3), we obtain even a steeper slope which is farther from the analytic estimate and closer to the fit (13). An explanation of the contradiction may be the dropping of higher-order terms at the very beginning of the analytic calculation when a sum is replaced by an integral. In fact, the next term diverges, and non-analytic contributions [23] may be essential.

Finally, it is worth mentioning that the *XXZ* model (with the anisotropy that does not lead to a mass gap) appears to belong to the same universality class as the *XXX* model, at least as concerns the central charge and the lowest excitations considered in the present letter. Thus, the results obtained here may apply to the integrable *XXZ* gapless magnet of spin s as well.

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