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THE LOWEST EXCITATIONS IN THE SPIN-S XXX MAGNET AND CONFORMAL INVARIANCE

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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

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

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

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

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

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

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

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

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

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

For the present model, $e_\infty=\sum_{n=1}^{s}(2n-1)^{-1}$ if s is an integer, and $e_\infty=\ln 2+\sum_{n=1}^{s-1/2}(2n)^{-1}$ 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]

$$c=3s/(s+1). \qquad (6)$$

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]

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

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 $N\le 1024$ [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

$$\lambda_m \simeq x+i\left[(n+1)/2-m\right] \qquad m=1,\ldots,n \qquad (8)$$

with deviations of $O\left[\exp(-aN)\right]$. 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 nonanalytic 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, $\Delta x+i\Delta y=\lambda_m-\lambda_{m+1}-i$, are shown. The minimum Δy is multiplied by N and then extrapolated to $N\to\infty$ from the computer results for $sN\le 128$ [20]. This $N\Delta y^{ex}_{min}$ is presented in conjunction with the theoretical predictions [23] $N\Delta y^{th}_{min}$ for $1\le s\le\frac{9}{2}$. A perfect agreement is observed within extrapolation errors, presumably of $O(1/N)$.

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

$2s$	$N\Delta y^{ex}_{min}$	$N\Delta y^{th}_{min}$	$2s$	$N\Delta y^{ex}_{min}$	$N\Delta y^{th}_{min}$
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

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

Re λ	Im λ	Im λ^{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

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 $O(1/N)$.

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 an 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

$$f = (E-e_\infty N)\, N/(2\pi v). \tag{9}$$

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 $-1/12$, $-1/8$, $-3/20$, $-1/6$, and $-9/44$. 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 $5/12$, $1/4$, $3/20$, $1/12$, and $-3/44$ 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.

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	$12\,f_v$	$12\,f_s$	$12\,f_t$	$2\,F_s$	$2\,F_t$	$6\,f_s/F_s$	$6\,f_t/F_t$
1	8	-1.030226965	8.224517330	4.053739432	1.570173	0.7853180	5.237968	5.161908
1	16	-1.010452107	7.660999337	4.245728069	1.476720	0.8340110	5.187850	5.090734
1	32	-1.004496374	7.215404226	4.372415266	1.398626	0.8652650	5.158924	5.053267
1	64	-1.002395300	6.884567681	4.460947747	1.339303	0.8866113	5.140409	5.031458
1	128	-1.001496517	6.636183286	4.526381344	1.294293	0.9020666	5.127267	5.017791
1	256	-1.001032325	6.444842550	4.576935359	1.259447	0.9137852	5.117198	5.008765
1	480	-1.000776452	6.306267178	4.613901699	1.234159	0.9222146	5.109770	5.003068
Linear		-1.000103	5.0838	4.9400	1.0111	0.99657	5.0442	4.9528
slope		-0.158	7.55	-2.01	1.38	-0.459	0.405	0.310
Quadr.		-1.000124	5.0045	4.9737	0.9947	0.99936	5.0351	4.9793
slope		-0.141	8.48	-2.41	1.57	-0.492	0.511	-0.0003
$2s$	N	$8\,f_v$	$4\,f_s$	$4\,f_t$	$4\,F_s$	$4\,F_t$	f_s/F_s	f_t/F_t
2	4	-1.137330	2.431708	0.8105695	2.75687	0.743625	0.882055	1.090024
2	6	-1.066802	2.234402	0.8196859	2.48354	0.757523	0.899685	1.082061
2	8	-1.041970	2.099851	0.8261490	2.30265	0.765811	0.911929	1.078789
2	10	-1.030016	2.007762	0.8310068	2.18085	0.771894	0.920631	1.076582
2	26	-1.009235	1.728184	0.8503551	1.82406	0.797284	0.947440	1.066565
2	64	-1.004321	1.575870	0.8666106	1.64028	0.820388	0.960731	1.056343
2	126	-1.002850	1.499143	0.8774451	1.55094	0.836315	0.966604	1.049181
2	240	-1.002065	1.444068	0.8866011	1.48805	0.849924	0.970447	1.043153
Linear		-1.00034	1.0307	0.9553	1.0160	0.9521	0.9993	0.9979
slope		-0.284	2.27	-0.377	2.59	-0.560	-0.158	0.248
Quadr.		-1.00042	1.0389	0.9911	1.0588	1.0086	0.9886	0.9750
slope		-0.240	2.18	-0.745	2.15	-1.14	-0.048	0.485
$2s$	N	$20\,f_v$	$20\,f_s$	$20\,f_t$	$6\,F_s$	$6\,F_t$	$\frac{20}{6}\,f_s/F_s$	$\frac{20}{6}\,f_t/F_t$
3	4	-3.490868892	10.709417289	2.643473002	3.6068028	0.5962761	2.9692273	4.433304
3	6	-3.244435482	9.343252931	2.575037327	3.0525433	0.6191811	3.0608093	4.158779
3	10	-3.114022321	8.001326652	2.524656864	2.5783797	0.6486945	3.1032383	3.891904
3	16	-3.062823024	7.134320243	2.501313682	2.3042864	0.6749355	3.0961083	3.706004
3	26	-3.037601313	6.494951720	2.492871472	2.1138863	0.7001552	3.0725170	3.560456
3	40	-3.025799850	6.074165793	2.494478363	1.9913278	0.7205798	3.0503093	3.461766
3	62	-3.018728833	5.742731519	2.501946584	1.8946959	0.7394034	3.0309515	3.383737
3	100	-3.013963517	5.459236739	2.514362496	1.8108580	0.7577759	3.0147240	3.318082
3	160	-3.010906701	5.237036288	2.529100458	1.7437189	0.7738251	3.0033718	3.268310
Linear		-3.0019	3.060	2.674	1.086	0.9311	2.892	2.781
slope		-1.18	11.05	-0.73	3.34	-0.80	0.56	2.48
Quadr.		-3.0022	3.270	2.900	1.081	0.9950	2.968	2.909
slope		-1.04	9.02	-2.92	3.39	-1.42	-0.17	1.24
$2s$	N	$6\,f_v$	$12\,f_s$	$12\,f_t$	$8\,F_s$	$8\,F_t$	$\frac{3}{2}\,f_s/F_s$	$\frac{3}{2}\,f_t/F_t$
4	4	-1.186270420	5.795418190	0.9879253647	2.8329156	0.4025179	2.0457433	2.454364
4	8	-1.061444973	4.305101542	0.8804655114	2.6459815	0.4919038	1.6270339	1.789914
4	10	-1.045259988	3.968295267	0.8576095788	2.5796557	0.5171779	1.5383042	1.658249
4	16	-1.025588378	3.427593389	0.8221361611	2.4428800	0.5645979	1.4030953	1.456145
4	26	-1.015661836	3.036512152	0.7990172040	2.3128686	0.6058917	1.3128771	1.318746
4	32	-1.013050093	2.905099355	0.7922649391	2.2617229	0.6214359	1.2844630	1.274894
4	50	-1.009249467	2.674360758	0.7825317684	2.1611126	0.6511501	1.2374925	1.201769
4	80	-1.006822136	2.487515932	0.7776045460	2.0682094	0.6778084	1.2027389	1.147233
4	120	-1.005442677	2.359142928	0.7764588581	1.9977301	0.6976837	1.1809117	1.112910
Linear		-1.00091	0.972	0.764	1.236	0.912	0.945	0.742
slope		-0.498	6.64	0.06	3.65	-1.03	1.13	1.78
Quadr.		-1.00105	1.148	0.887	0.973	0.970	1.086	0.959
slope		-0.443	5.03	-1.07	6.06	-1.55	-0.16	-0.22

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 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]

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

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

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.

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

$2s$	N	$44\,f_v$		$44\,f_s$		$44\,f_t$	
9	4	-11.403 963 293 5		14.947 317 867		-2.072 071 145 09	
9	8	-9.869 320 377 8		8.396 161 215		-2.446 699 736 15	
9	16	-9.404 174 577 7		5.150 993 725			
9	32	-9.225 067 528 1		3.321 264 333			
9	52	-9.161 563 651 6					
Linear		-9.030		-3.998		-3.196	
slope			-8.13		25.4		1.56
Quadr.		-9.022		-3.117			
slope			-9.63		19.9		

In the considered excitations, 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 $\frac{1}{2}+O(1/N)$, 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.

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

Re λ	|Im λ|	|Re λ|	|Im λ|
		0.033 407 335 76	0
0	0.672 911 205 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

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 nonmonotonous 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

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

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

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

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]. 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 nonanalytic contributions [23] may be essential.

Finally, it is worth mentioning that, according to all the available data, the *XXZ* model (with the anisotropy that does not lead to a mass gap) belongs to the same universality class as the *XXX* model. Thus, the results obtained here may apply to the integrable *XXZ* gapless magnet of spin *s* as well.

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