Записки научных
семинаров ПОМИ
Том 251, 1998 г.

H-P. Eckle

SPECTRAL GAPS IN THE XXZ QUANTUM SPIN CHAIN

Abstract. We report on the behavior of the finite-size energy spectrum of the Heisenberg–Ising (XXZ) quantum spin chain in the momentum π sector. Our numerical and perturbative results for the behavior of energy gaps are explained by considering the motion of string solutions of the Bethe-Ansatz equations.

1. Introduction

The analytical finite-size energy spectra of one-dimensional quantum many-body Hamiltonians have been of much interest in recent years. These calculations have been to a large extent motivated by the recent ideas of conformal invariance, which allow a computation of scaling indices and classification of universality classes, i.e. determination of the conformal anomaly number c, directly from the $1/L$ (L being the length of the one-dimensional system) behavior of a given critical model [1].

For example, the one-dimensional Hubbard model has been, a model of great interest in condensed matter physics, gas been studied from this point of view [2].

For one-dimensional systems, solvable by the Bethe-Ansatz method, the finite size spectra are accessible analytically by various methods and these models have thus been used as testing grounds for the general ideas of conformal invariance. In particular, the Heisenberg–Ising model of an anisotropic spin-1/2 chain has been studied in great detail [yy66]. It has been shown that its low energy spectrum in the large N limit can be classified as that of a $c = 1$ conformal field theory with marginally irrelevant operators giving rise to logarithmic corrections [4].

However, most studies of the Heisenberg–Ising model have been restricted to the antiferromagnetic critical region of the model [4, 5]. In the ferromagnetic interaction range, solutions of the Bethe-Ansatz equations for the low lying states correspond to complex roots arranged in strings and their behavior becomes increasingly complicated as the anisotropy approaches the ferromagnetic isotropic point [6].

In the present work, we shall reexamine the behavior of the spectrum and the corresponding states of the Heisenberg–Ising chain threaded by a magnetic flux Φ, which corresponds to twisted boundary conditions. As shown in [6], the adiabatic ground state for half-filling is periodic in Φ with a period equal to $2 \cdot 2\pi$ (2π is the flux quantum in appropriate units) for values of the interaction strength $\Delta = \cos(\pi/Q)$ with Q not an integer. This is due to the presence of a finite gap at $\Phi = 2\pi$. We show that this gap scales as a power of the system size, with variable exponent depending on Δ. For $\Delta \sim 0$, the exponent can be explicitly calculated by perturbation theory. For Q equal to an integer, however, the gap closes exactly and the periodicity of the ground state becomes macroscopic at half-filling, i. e. proportional to the system size. We show how this behavior can be understood in terms of the Bethe-Ansatz solution as a successive crossing of string solutions.

2. Closing of energy gaps at half-filling

As is well known, the Heisenberg–Ising model has an interpretation as a lattice gas of either fermions or bosons, where spin-down represents a particle and spin-up represents an empty site. The magnetic flux Φ modifies only the hopping term, such that the Hamiltonian is

$$H = -\frac{1}{2}\sum_{j=1}^{N}\{e^{i\Phi/N}c_j^{\dagger}c_{j+1} + \text{h.c.}\} + \cos\mu\sum_{j=1}^{N} n_j n_{j+1} + e_0, \qquad (2.1)$$

where $e_0 = \Delta(2M - N/2)$, N is the number of sites, M the number of particles and we reparametrized the anisotropy as $\Delta = -\cos(\mu)$. We note that the total momentum induced into the system by the flux is given as $P = M\Phi/N$. We further remark, that the repulsive region $0 \leq \mu < \pi/2$ and the attractive region $\pi/2 < \mu \leq \pi$ of the Heisenberg–Ising chain are related by an inversion of the spectrum: The behavior of the low-lying energy states in the attractive region will be mirrored to the behavior of the high energy states in the repulsive region and vice versa.

Let $E_0(\Phi)$ denote the ground state energy of the system with flux Φ. As is easy to see, $E_0(\Phi)$ has a periodicity of 2π in Φ, i.e.

$$E_0(\Phi + 2\pi) = E_0(-\Phi) = E_0(\Phi). \qquad (2.2)$$

However, the periodicity of a given state can be an integer multiple of the period of the energy. Following [5], we define a topological winding number n to be the number of times the flux Φ increases by 2π before the state returns to its initial value.

We write the shift of the ground state energy as a function of flux as

$$\Delta E_0(\Phi) \equiv E_0(\Phi) - E_0(0) \equiv D\Phi^2/2N + O(\Phi^4), \tag{2.3}$$

where D has been called the stiffness constant [5]. For $0 \leq \mu \leq \pi/2$ and a half-filled band ($M = N/2$), the stiffness has been calculated exactly as $D = v_s/2(\pi - \mu)$ for flux values $|\Phi| \leq 2(\pi - \mu)$; the spin-wave velocity is given by $v_s = \pi \sin\mu/\mu$ [3].

At half-filling, we now adiabatically boost the zero momentum ground state until we have $\Phi = 2\pi$ and $P = \pi$. For $0 \leq \mu < \pi/2$, we then observe a finite gap ΔE between the boosted ground state and the first excited state in this momentum π sector and so the winding number of the zero momentum ground state is $n = 2$. For the non-interacting case of $\mu = \pi/2$, the gap closes and $n = N$ which correctly implies free acceleration in the thermodynamic limit.

For $\mu > \pi/2$, the situation is more complicated: As has already been noted in [6], there are special values of the interaction strength $\mu_Q = (Q-1)\pi/Q$ at which the winding number becomes again macroscopic.

Note that not only the ground state gap closes at $\Phi = 2\pi$, but also various higher lying states become degenerate. Moreover, the closing of the gap at the special values μ_Q for $Q = 2, 3, \ldots, N$ occurs for *all* lattices sizes N.

In order to further understand this interesting behavior of the energy spectrum, we studied the Bethe Ansatz equations of the Heisenberg–Ising chain with flux. The equations are given as [5]

$$N\theta(\alpha, \mu) = 2\pi I + \Phi + \sum_{\alpha'}^{M} \theta(\alpha - \alpha', \mu), \tag{2.4}$$

where we have used Yang's [3] change of variables for the pseudomomenta such that

$$p = \theta(\alpha, \mu) \equiv 2\arctan[\cot(\mu/2)\tanh(\alpha/2)]. \tag{2.5}$$

The quantum numbers $\{I\}$ are integers or half-odd integers and specify the states. The ground state is given by $\{I\} = \{-(M-1)/2, \ldots, (M-1)/2\}$.

Let us briefly recall the behavior of the roots $\{\alpha\}$ for the ground state as we adiabatically turn on the flux: The largest root α_M goes to ∞ exactly at $\Phi = 2(\pi - \mu)$ and the remaining $M - 1$ roots are distributed symmetrically around 0. The energy of the system is now equal to $M-1$ particles on a chain of length N with $\Phi = 0$ – the ground state in the $S^z = 1$ sector. For $0 \leq \mu \leq \pi/2$, further increase of Φ renders α_M complex and it moves backwards along the line $i\pi$ with decreasing real part until at $\Phi = 2\pi$ it has the value $\alpha_M = i\pi \equiv \lambda_1$. Again, the remaining $M-1$ real roots have been distributed symmetrically around 0. However, the energy now is not related to the $S^z = 1$ ground state in a simple way.

For $\pi/2 \leq \mu \leq 2\pi/3$ and at $\Phi = 2\pi$, we have two complex roots with zero real part, i.e. $\lambda_{1,2} = i(\pi \pm (\pi - \mu))$, i.e. a two-string. And in general we find that at $\Phi = 2\pi$ in the interaction interval $(Q-1)\pi/Q \leq \mu \leq (Q)\pi/(Q+1)$, we have a Q-string sitting on the imaginary axis symmetrically around $i\pi$ with individual roots given by

$$\lambda_a = i\pi + i\beta_a \equiv i\pi + i(\pi - \mu)(Q + 1 - 2a) + i\delta_L. \tag{2.6}$$

δ_L represents an exponentially small finite-size correction, which is exactly zero for a 1-string, a 2-string and the two complex roots closest to $i\pi$ in a Q-string with Q even. The remaining $M-Q$ real roots are distributed symmetrically around 0.

Note that at values of the interaction strength equal to μ_Q, both a $(Q-1)$-string and Q-string coexist in the degenerate ground state. The energies associated with these strings are $E_Q(\mu_Q) = 0$ and $E_{Q-1}(\mu_Q) = 2(\cos\mu_Q + 1)$ [s94]. This suggests, that for $(Q-1)\pi/Q \leq \mu \leq (Q)\pi/(Q+1)$, when the Q-string corresponds to the ground state, the first exited state corresponds to the $(Q+1)$-string.

We have therefore rewritten the Bethe-Ansatz equations (2.4) in order to incorporate the Q-strings sitting on the imaginary axis. The equations now are

$$N\theta_{00}(\alpha, \mu) = 2\pi I + \sum_{\alpha'}^{M-Q} \theta_{00}(\alpha - \alpha', 2\mu) + \sum_{\beta'}^{Q} \theta_{01}(\alpha, \beta', \mu), \tag{2.7}$$

$$N\theta_{11}(\beta, \pi - \mu) = 0 + \sum_{\alpha'}^{M-Q} \theta_{10}(\alpha', \beta, \mu) + \sum_{\beta'}^{Q} \theta_{11}(\beta - \beta', 2(\pi - \mu)), \tag{2.8}$$

with

$$\theta_{00}(\alpha, \mu) \equiv \theta(\alpha, \mu) \tag{2.9}$$

the phase shift of real roots α,

$$\theta_{11}(\beta, \mu) \equiv \mathrm{Re}\{2\mathrm{arctanh}[\tan(\beta/2)/\tan(\mu/2)]\} \tag{2.10}$$

the phase shift of complex roots and

$$\theta_{01}(\alpha,\beta,\mu) \equiv \mathrm{Re}\{2\arctan[\coth[(\alpha - i\beta)/2)/\tan(\mu)]\}, \tag{2.11}$$

$$\theta_{10}(\alpha,\beta,\mu) \equiv -\frac{1}{2}\log[(\cos(\beta+2\mu)+\cosh(\alpha))/(\cos(\beta-2\mu)+\cosh(\alpha))] \tag{2.12}$$

the mixed phase shifts of a real with a complex root. The quantum numbers for the $\{\beta\}$'s are zero and the flux $\Phi = 2\pi$ has been incorporated into the $\{I\}$ quantum numbers. We caution the reader that care has to be taken in regard to the branch cuts of these phase shifts. The existence of roots on different branches is equal to a net shift of the quantum numbers and thus a different state. A detailed account of the motion of string solutions of the Heisenberg–Ising ring has recently been given in [8]. Excited states in the twisted XXZ spin chain are, with a different objective, also considered by Nassar and Tirkkonen [9].

These considerations have been confirmed with high precision by a numerical iteration of the Bethe-Ansatz equations [10].

We have also determined numerically the energy difference $\Delta E \equiv E_1 - E_0$ at $\Phi = 2\pi$ as a function of μ. The closing of the gap at the special points μ_Q can be clearly observed.

As $N \to \infty$, the gaps for $\mu \neq \mu_Q$ should close as $\Delta E \sim N^{-\gamma}$. ¿From numerical calculations of up to $N = 14$ sites and various values of μ, it is apparent that γ varies continuously with μ for all $0 \leq \mu \leq \pi$ [10].

Alcaraz et al. [4] have argued that both 1-string and 2-string for $0 \leq \mu \leq \pi/2$ have the same scaling dimension. Therefore, the energy gap ΔE measures finite size behavior beyond simple conformal $1/N$ formulas and we interpret the continuous variation of γ as indicating the presence of higher order corrections which may be logarithmic depending on the value of μ.

A direct analytical calculation of these corrections in the Heisenberg–Ising chain has so far been done only at the isotropic point, $\mu = 0$, where they have been found to be indeed logarithmic [4].

However, at $\mu \sim \pi/2$ ($\Delta \sim 0$), i.e. in the vicinity of the non-interacting point, we can calculate γ directly by perturbation theory in Δ [11].

We find that $\gamma = 3$ at $\Delta = 0$ and $\Phi = 2\pi$. This agrees quite well with the numerical results, which were obtained for small systems of up to $N = 14$ sites and $M = 7$ particles [10].

3. Conclusions

We have presented numerical and perturbative evidence for degeneracies in the momentum π sector of the half-filled critical Heisenberg–Ising model on a finite ring.

Furthermore, we have shown by exact diagonalization and numerical iteration of the Bethe-Ansatz equations that the gap at $\Phi = 2\pi$ ($P = \pi$) and half-filling scales as power of the system size with variable exponent γ depending on the interaction strength. An analytical calculation of γ would be very desirable, albeit encumbered with a large technical expense as the earlier $\mu = 0$ calculation already suggests [4].

In [10], it is also shown that for $1/r$ filling with r an integer, the periodicity is again not the expected r flux quanta and we observe exact degeneracies between ground state and first excited state at various values of Φ. This is true for *all* values of the interaction strength and not only at isolated points. The numerical results are confirmed by second order perturbation theory, due to a remarkable cancellation of various diagrams.

Furthermore, adding a non-integrable, say, next-nearest neighbor interaction $W = \omega \sum_{j=1}^{N} n_j n_{j+2}$ to the Hamiltonian (2.1), *all* the degeneracies discussed above for $\mu \neq \pi/2$ are lifted and therefore all gap-closings disappear [10].

It is an interesting question, if our results can be found also in other one-dimnesional quantum systems such as the long-ranged Haldane–Shastry chains.

We close this paper by noting that as shown in [12], the here considered structure of low-lying states in the Heisenberg–Ising chain is qualitatively the same in the SC model [13]. Therefore the results presented here will also hold in the SC model, up to the renormalization of quantities such as the spin wave velocity v_s.

Acknowledgments

The author is a Alexander-von-Humboldt Award Fellow of the Finnish Academy. He is grateful to Rudolf Römer and Bill Sutherland for collaboration on the research summarized in this report. He also thanks Olav Tirkkonen for discussions of his results prior to publication.

References

1. J. L. Cardy, in "Phase Transitions and Critical Phenomena," edited by C. Domb and J. L. Lebowitz (Academic, London, 1987) and references cited therein.
2. F. Woynarovich and H.-P. Eckle, J. Phys. A **20** (1987), L443.

3. C. N. Yang and C. P. Yang, Phys. Rev. **147** (1966), 303; Phys. Rev. **150** (1966), 321; Phys. Rev. **150** (1966), 327; Phys. Rev. **151** (1966), 258.
4. F. Woynarovich and H.-P. Eckle, J. Phys. A **20** (1987), L97; F. Woynarovich, Phys. Rev. Lett. **59** (1987), 259; (unpublished); F. C. Alcaraz, M. N. Barber and M. T. Batchelor, Phys. Rev. Lett. **58** (1987), 771; Ann. Phys. **182** (1988), 283.
5. B. Sutherland and B. S. Shastry, Phys. Rev. Lett. **65** (1990), 1833; H.-P. Eckle and C. J. Hamer, J. Phys. A **24** (1991), 191.
6. B. Sutherland, (unpublished) N. Yu and M. Fowler, Phys. Rev. B **46** (1993), 14583.
7. B. Sutherland, in *Festschrift Volume for C. N. Yang's 70th Birthday*, S. T. Yau, editor, (International, Hong Kong, to be published 1994).
8. N. Fumita, H. Itoyama and T. Oota, Int. J. Mod. Phys. A **12** (1997), 801.
9. T. Nassar and O. Tirkkonen, NORDITA preprint 97/33 P, hep-th/9707098.
10. R. A. Römer, H.-P. Eckle and B. Sutherland, Phys. Rev. B **52** (1995), 1656.
11. B. S. Shastry, (private communication).
12. B. Sutherland and R. A. Römer, Phys. Rev. B **50** (1994), 15389.
13. B. Sutherland and R. A. Römer, Phys. Rev. Lett. **71** (1993), 2789.

Department of Physics
University of Jyväskylä
PO Box 35
FIN–40351 Jyväskylä
Finland

Поступило 26 января 1998 г.