

XXX Spin Chain: from Bethe Solution to Open Problems

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Our understanding of Bethe Ansatz has improved a lot over the last 75 years. This was clear from the many excellent lectures on the conference. But there are still unanswered questions and actually this lecture will concentrate on three open problems. Two of the problems are related to the correlations functions of the XXX spin chain and the XXZ spin chain and one to the entropy of subsystems.

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1. Introduction

Originally introduced in 1931 by Hans Bethe in order to solve the isotropic Heisenberg spin chain, the Bethe Ansatz, with its numerous generalizations and refinements has been proven an invaluable tool in the field of exactly solved models. The versatility of this method is exemplified by the multitude of physical models and problems in which it proved useful. Some of these are: δ -function Bose gas, massive Thirring model, Hubbard model, XXX, XXZ and the XYZ spin chains, six-vertex and eight-vertex models and the list could go on.

Even though our understanding of exactly solved models has improved a lot there is still a large number of unsolved problems. The purpose of this lecture is to present some of them.

2. The Heisenberg Spin Chain and Number Theory

Our first open problem is related to the model that was the starting point for the Bethe Ansatz. Consider the antiferromagnetic spin 1/2 Heisenberg XXX spin chain with the hamiltonian

$$\mathcal{H}_{XXX} = \sum_{j=-\infty}^{\infty} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z \right) \quad (2.1)$$

where $\sigma_i^x, \sigma_i^y, \sigma_i^z$ are the Pauli matrices and we will denote σ^0 the 2×2 unit matrix

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

As we have said this hamiltonian was diagonalized in 1931 by means of what today we call coordinate Bethe Ansatz [1]. The unique antiferromagnetic ground state in the thermodynamic limit was investigated by Hulthen in 1938 [2] and the spectrum of excitations which consists of magnons of spin 1/2 was correctly described for the first time by Faddeev and Takhtajan [3].

2.1 Correlation Functions

The correlation functions of the XXX spin chain are defined as follows: consider n sequential lattice sites and in each site pick up $\sigma_k^{a_k} \in \{\sigma_k^0, \sigma_k^x, \sigma_k^y, \sigma_k^z\}$. The average of this operator with respect to the ground state $|GS\rangle$

$$\left\langle \prod_{k=1}^n \sigma_k^{a_k} \right\rangle = \langle GS | \prod_{k=1}^n \sigma_k^{a_k} | GS \rangle \quad (2.2)$$

is called a correlation function. An example is *emptiness formation probability* which is defined as

$$P(n) = \langle GS | \prod_{j=1}^n P_j | GS \rangle \quad (2.3)$$

where $P_j = (\sigma_j^z + 1)/2$ is the projector on the state with the spin up in the j -th lattice site. $P(n)$ is the probability of formation of a ferromagnetic string of length n in the antiferromagnetic ground state.

We will show that there is a strong connection between the correlation functions of the XXX spin chain and Riemann zeta function at odd arguments, but first we need to introduce some preliminary notions.

2.2 Number Theory and Riemann Zeta Function with Odd Arguments

The roots of all the polynomials with rational coefficients

$$r_n x^n + r_{n-1} x^{n-1} + \dots + r_1 x + r_0 = 0, \quad r_i \in \mathbb{Q}$$

(where we denote by \mathbb{Q} the field of rational numbers) are called algebraic numbers. The transcendental numbers are not roots of any polynomials with rational coefficients (i.e. $\ln 2, \pi, e$). We say that x, y are algebraically dependent if

$$r_{nm} x^n y^m + \sum_{a=0}^{n-1} \sum_{b=0}^{m-1} r_{ab} x^a y^b = 0, \quad r_{ij} \in \mathbb{Q}$$

and algebraically independent if

$$r_{nm} x^n y^m + \sum_{a=0}^{n-1} \sum_{b=0}^{m-1} r_{ab} x^a y^b \neq 0, \quad r_{ij} \in \mathbb{Q}$$

Also we say that t_1, \dots, t_k are algebraically independent transcendental numbers

$$\sum_{\{a_j\}} r_{a_1 \dots a_k} t_1^{a_1} t_2^{a_2} \dots t_k^{a_k} \neq 0, \quad a_j = \text{integers}, \quad r_{a_1 \dots a_k} \in \mathbb{Q}$$

The Riemann zeta function is defined as [4]

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \quad \Re(s) > 1 \quad (2.4)$$

and it can also be represented as a product with respect to all the prime numbers p (Euler's product)

$$\zeta(s) = \prod_p \frac{1}{1 - p^{-s}} \quad (2.5)$$

For the characterization of the correlation functions it will also be useful to use the alternating zeta series (the value of the polylogarithm at root of unity)

$$\zeta_a(s) = \sum_{n>0} \frac{(-1)^{n-1}}{n^s} = -\text{Li}_s(-1) \quad (2.6)$$

where $\text{Li}_s(x)$ is the polylogarithm. The connection between the Riemann zeta function and the alternating zeta series is

$$\zeta(s) = \frac{1}{1 - 2^{1-s}} \zeta_a(s) \quad (2.7)$$

where $s \neq 1$. Unlike the Riemann zeta function which has a pole at $s = 1$ the alternating zeta function has a limit when $s \rightarrow 1$.

$$\zeta_a(1) = \ln 2 \quad (2.8)$$

It is known that at even values of the argument the zeta function can be expressed in terms of powers of π but at odd arguments the situation is more complicated. R. Apéry proved first that $\zeta(3)$ is irrational [5] and T. Rivoal showed that the zeta function at odd arguments takes an infinite number of irrational values [6] (see also [7]). In fact it was conjectured that the values of the zeta function at odd arguments are all irrational even algebraically independent transcendental numbers (Don Zagier [8], P. Cartier [9]).

2.3 Quantum Correlations and Number Theory

In 2001 H.Boos and one of the authors were able to calculate exactly the emptiness formation probability $P(n)$ for small strings ($n = 1, \dots, 4$) obtaining the following results

$$\begin{aligned}
 P(1) &= \frac{1}{2} = 0.5, \\
 P(2) &= \frac{1}{3} - \frac{1}{3} \ln 2 \\
 P(3) &= \frac{1}{4} - \ln 2 + \frac{3}{8} \zeta(3) = 0.007624158, \\
 P(4) &= \frac{1}{5} - 2 \ln 2 + \frac{173}{60} \zeta(3) - \frac{11}{6} \ln 2 \cdot \zeta(3) - \frac{51}{80} \zeta^2(3) \\
 &\quad - \frac{55}{24} \zeta(5) + \frac{85}{24} \ln 2 \cdot \zeta(5) = 0.000206270.
 \end{aligned}$$

$P(1)$ is obvious from symmetry and $P(2)$ can be obtained from the result of Hulthen [2] for the ground state energy. $P(3)$ can be obtained from Takahashi's result [10] for the nearest neighbor correlation (see also [11]) and $P(4)$ was obtained from the integral representation derived in [12] based on the vertex operator approach [52]. Subsequent computations of $P(5)$ in [15] and $P(6)$ in [14] showed that the emptiness formation probability for small strings share the same structure. This led to the following conjecture

Conjecture. 1. (Boos, Korepin 2001) Any correlation function of the XXX spin chain can be represented as a polynomial in $\ln 2$ and values of Riemann zeta function at odd arguments with rational coefficients [13],[14].

The conjecture was sustained also by computations of different correlation functions such as two-point spin-spin correlators some examples being listed bellow

$$\begin{aligned}
 \langle S_j^z S_{j+1}^z \rangle &= \frac{1}{12} - \frac{1}{3} \zeta_a(1) = -0.147715726853315 \\
 \langle S_j^z S_{j+2}^z \rangle &= \frac{1}{12} - \frac{4}{3} \zeta_a(1) + \zeta_a(3) \\
 &= 0.060679769956435 \\
 \langle S_j^z S_{j+4}^z \rangle &= \frac{1}{12} - \frac{16}{3} \zeta_a(1) + \frac{290}{9} \zeta_a(3) - 72 \zeta_a(1) \zeta_a(3) \\
 &\quad - \frac{1172}{9} \zeta_a(3)^2 - \frac{700}{9} \zeta_a(5) \\
 &\quad + \frac{4640}{9} \zeta_a(1) \zeta_a(5) - \frac{220}{9} \zeta_a(3) \zeta_a(5) - \frac{400}{3} \zeta_a(5)^2 \\
 &\quad + \frac{455}{9} \zeta_a(7) - \frac{3920}{9} \zeta_a(1) \zeta_a(7) + 280 \zeta_a(3) \zeta_a(7) \\
 &= 0.034652776982728
 \end{aligned}$$

Again the nearest neighbor correlator was obtained from Hulthen result [2] and the second-neighbor correlator was obtained by Takahashi in 1977 [10] using the strong coupling expansion

of the ground state energy of the half-filled Hubbard chain. The next nearest correlators were calculated in [16],[17].

The conjecture was finally proved in 2006 by H. Boos, M. Jimbo, T. Miwa, F. Smirnov and Y. Takeyama [18]. However we still not have explicit expressions for the rational coefficients that enter in the expression for the correlation functions as polynomials in $\ln 2$ and Riemann zeta function at odd arguments. Such a description will provide a tractable formula for the correlations of the XXX spin chain.

Open problem: Efficient description of the rational coefficients which appear in the expression for the correlation functions of the XXX spin chain as a polynomial in alternating zeta series at odd arguments.

3. Entropy of Subsystems

We are interested in the following physical situation. Consider a one-dimensional system of interacting spins (we can also consider particles interacting) in the ground-state denoted by $|GS\rangle$. We will treat the whole ground state as a binary system A and B where A is a block of neighboring spins and B is the rest of the spins in the ground state. The density matrix of the entire system is

$$\rho_{A\&B} = |GS\rangle\langle GS| \quad (3.1)$$

and the density matrix of the subsystem A obtained by tracing away the B degrees of freedom is

$$\rho_A = Tr_B(\rho_{A\&B}) \quad (3.2)$$

In a seminal paper [19] Bennet, Bernstein, Popescu and Schumacher discovered that the von Neumann entropy of a subsystem A

$$S(\rho_A) = -Tr(\rho_A \ln \rho_A) \quad (3.3)$$

is a measure of entanglement. Entanglement is the fundamental resource used in quantum computation and quantum information. A better understanding of entanglement will provide further insight in the theory of quantum phase transitions but also in the physics of strongly correlated quantum systems where deeply entangled ground-states play a major role in the understanding of these quantum collective phenomena. Consequently a large amount of effort was invested in studying the entropy of subsystems in a large class of quantum systems.

3.1 General results

If we consider the doubling scaling limit in which the size of the block of spins is much larger than one but much smaller than the length of the entire chain we can present some general results about the behavior of the entropy of subsystems.

In the case of 1D critical models (gap-less) the entropy of the subsystems scales logarithmically with the size of the block. More precisely for a block of n spins we have

$$S(n) = \frac{c}{3} \ln n \quad n \rightarrow \infty \quad (3.4)$$

where c is the central charge of the associated conformal field theory that describes the critical model. This formula was first derived for the geometrical entropy (the analogous of (3.3) for

conformal field theory) by Holzhey, Larsen and Wilczek in [20] (see also [21],[22],[28]). Some examples are: Hubbard model, XX0 (or isotropic XY) spin chain, higher spin generalization of the isotropic XXX antiferromagnetic spin chain, Bose gas with δ interaction etc.

In the case of non-critical models (gap-full) it was conjectured in [21] (based on numerical evidence for some spin chains) that the entropy of subsystems will increase with the size of the subsystem until it will reach a limiting value $S(\infty)$. This was proved for the XY spin chain in [30],[31] where the limiting value was analytical computed and also checked for the spin chain introduced by Affleck, Kennedy, Lieb, Tasaki ([23] AKLT model) in [24] where it was showed that $S(\infty) = 2$. This explains why the Density Matrix Renormalization Group [25](DMRG) technique works so well for the AKLT model and fails to reproduce quantum critical behavior. It was noted in [21] that in order for the DMRG technique to work we need to have for the $S(\rho_A)$ a limiting value as the size of the subsystem increases (this is equivalent with a bounded rank for ρ_A) and as we have shown this is not the case in critical models.

3.2 An example: the XY spin chain

We can make all these general considerations more exact by presenting the results for the XY spin chain in magnetic field with the hamiltonian

$$\mathcal{H}_{XY} = - \sum_{j=-\infty}^{\infty} \left((1 + \gamma) \sigma_j^x \sigma_{j+1}^x + (1 - \gamma) \sigma_j^y \sigma_{j+1}^y + h \sigma_j^z \right)$$

where $0 < \gamma < 1$ is the anisotropy parameter and h is the magnetic field. The model was solved by E.H. Lieb, T. Schulz and D. Mattis in zero magnetic field case [32] and by E. Barouch and B.M. McCoy in the presence of a constant magnetic field [26]. The ground state is unique and in general there is a gap in the spectrum.

The density matrix of a block of n neighboring spins in the ground state can be expressed as

$$\rho(n) = \frac{1}{2^n} \sum_{\substack{\{a_j\} \\ j=1..n}} \left(\prod_{j=1}^n \sigma_j^{a_j} \right) \langle GS | \prod_{k=1}^n \sigma_k^{a_k} | GS \rangle$$

and the limiting value of the entropy in the double scaling limit depends on the isotropy and magnetic field. We can distinguish three cases:

- Case Ia: moderate magnetic field $2\sqrt{1-\gamma^2} < h < 2$
- Case Ib: weak magnetic field including zero magnetic field $0 \leq h < 2\sqrt{1-\gamma^2}$
- Case II: strong magnetic field $h > 2$

The result for these regions obtained in [30] (we denote by $S(\infty)$ the limiting value of $S(\rho(n))$ when $n \rightarrow \infty$) is

$$S(\infty) = \frac{\pi}{2} \int_0^\infty \ln \left(\frac{\theta_3(ix + \frac{\sigma\tau}{2}) \theta_3(ix - \frac{\sigma\tau}{2})}{\theta_3^2(\frac{\sigma\tau}{2})} \right) \frac{dx}{\sinh^2(\pi x)}$$

where the modulus k of the theta function is different in the three regions; $\tau = I(k')/I(k)$ where $I(k)$ is the complete elliptic integral of modulus k , $k' = \sqrt{1-k^2}$ is the complementary modulus

and $\sigma = 1$ in Case I and $\sigma = 0$ in Case II. Using the approach of [28] I. Peschel independently calculated and simplified the results in region (Ia) and (II) obtaining

$$S(\infty) = \frac{1}{6} \left[\ln \left(\frac{k^2}{16k'} \right) + \left(1 - \frac{k^2}{2} \right) \frac{4I(k)I(k')}{\pi} \right] + \ln 2 \quad \text{with} \quad k = \frac{\sqrt{(h/2)^2 + \gamma^2 - 1}}{\gamma} \quad (\text{Ia})$$

$$S(\infty) = \frac{1}{12} \left[\ln \frac{16}{k^2 k'^2} + (k^2 - k'^2) \frac{4I(k)I(k')}{\pi} \right] \quad \text{with} \quad k = \frac{\gamma}{\sqrt{(h/2)^2 + \gamma^2 - 1}} \quad (\text{II})$$

and the simplified result for the region (Ib) was finally obtained in [30]

$$S(\infty) = \frac{1}{6} \left[\ln \left(\frac{k^2}{16k'} \right) + \left(1 - \frac{k^2}{2} \right) \frac{4I(k)I(k')}{\pi} \right] + \ln 2 \quad \text{with} \quad k = \frac{\sqrt{1 - \gamma^2 - (h/2)^2}}{\sqrt{1 - (h/2)^2}} \quad (\text{Ib})$$

In the isotropic case $\gamma = 0$ the ground-state is again unique but now the model is critical for $h < 2$. We expect that the entropy will scale logarithmically and indeed it was showed in [27] that

$$S(\rho(n)) = \frac{1}{3} \ln(n\sqrt{4-h^2}) - \int_0^\infty dt \left\{ \frac{e^{-3t}}{3t} + \frac{1}{t \sinh^2(t/2)} - \frac{\cosh t/2}{2 \sinh^3(t/2)} \right\}$$

We see that the result of applying the magnetic field is very simple effectively reducing the size of the subsystem. If the magnetic field is larger than the critical value 2 then the ground-state is ferromagnetic and the entropy is zero.

3.3 The XXZ spin chain

It will be highly desirable if we would be able to obtain the same amount of information about the XXZ spin chain with the hamiltonian

$$\mathcal{H}_{XXZ} = - \sum_{j=-\infty}^{\infty} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z \right)$$

If $\Delta > 1$ the ground-state is ferromagnetic so $S(\rho(n)) = 0$ and in the critical region ($-1 \leq \Delta < 1$) the entropy will scale logarithmically (see 3.4). In the gapped antiferromagnetic case ($\Delta < -1$) we expect that $S(\rho(n))$ will tend to a limiting value $S(\infty)$ but at this moment the analytic evaluation of this constant is missing.

Open problem: For the XXZ spin chain in the antiferromagnetic region ($\Delta < -1$) calculate the limiting value of the entropy of a subsystem when the number of spins in the block is large.

4. Asymptotics of Time and Temperature Dependent Correlation Functions

The last open problem that are we going to present is related to the asymptotic behavior of correlations functions when the space and time separation is large. As in the previous section we are going to present two examples for which we have satisfactory results and which we believe are going to facilitate the understanding of the problem at hand.

Consider the isotropic XY model [32] in transverse magnetic field with the hamiltonian

$$\mathcal{H}_{XY} = - \sum_{j=-\infty}^{\infty} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + h \sigma_j^z \right)$$

where σ are Pauli matrices and h is the magnetic field. We are interested in the asymptotic behavior of the time and temperature correlation function

$$g(n,t) = \frac{\text{Tr} \left\{ \left(e^{-\mathcal{H}_{XY}/T} \right) \sigma_{n_2}^+(t_2) \sigma_{n_1}^-(t_1) \right\}}{\text{Tr} \left(e^{-\mathcal{H}_{XY}/T} \right)} \quad (4.1)$$

when $n = n_2 - n_1$ and $t = t_2 - t_1$ are large and $h \in [0, 2)$. In [35] it was showed that $g(n,t)$ decays exponentially but the rate of decay depends on the direction ϕ defined as $\cot \phi = n/4t$ when $n, t \rightarrow \infty$. The asymptotics in the space-like and time-like regions are:

- Space-like directions $0 \leq \phi < \pi/4$

$$g(n,t) \rightarrow C \exp \left\{ \frac{n}{2\pi} \int_{-\pi}^{\pi} dp \ln \left| \tanh \left[\frac{h - 2 \cos p}{T} \right] \right| \right\} \quad (4.2)$$

- Time-like directions $\pi/4 < \phi \leq \pi/2$

$$g(n,t) \rightarrow C t^{(2v_+^2 + 2v_-^2)} \exp \left\{ \frac{1}{2\pi} \int_{-\pi}^{\pi} dp |n - 4t \sin p| \ln \left| \tanh \left[\frac{h - 2 \cos p}{T} \right] \right| \right\} \quad (4.3)$$

with

$$v_+ = \frac{1}{2\pi} \left| \tanh \left(\frac{h - 2 \cos p_0}{T} \right) \right| \quad v_- = \frac{1}{2\pi} \left| \tanh \left(\frac{h + 2 \cos p_0}{T} \right) \right| \quad \frac{n}{4t} = \sin p_0$$

At zero temperature the asymptotics of the correlation functions were evaluated in [33] and [34] and for $\phi = \pi/2$ the leading factor was computed in [37].

Similar formulae were also obtained for the δ -function Bose gas (N bosons interacting via a repulsive δ -function potential of strength c) which is characterized by the hamiltonian

$$\mathcal{H}_N = - \sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + 2c \sum_{N \geq j > k \geq 1} \delta(x_j - x_k) \quad (4.4)$$

In this case the asymptotic formula ($x, t \rightarrow \infty$) obtained in [36] using the determinant approach to quantum correlation functions [53] is

$$\langle \psi(0,0) \psi^\dagger(x,t) \rangle_T \longrightarrow \exp \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi \rho_t(\lambda)} |x - v(\lambda)t| \ln \left| \tanh \left(\frac{\varepsilon(\lambda)}{2T} \right) \right| \right\} \quad (4.5)$$

where $\varepsilon(\lambda)$, $\rho_t(\lambda)$ and $v(\lambda)$ are the finite temperature dressed energy, pseudoparticle density and Fermi velocity.

4.1 The XXZ Spin Chain

In the last years remarkable progress was made in obtaining multiple integral representation for the correlation functions of the XXZ spin chain. We remind the hamiltonian

$$\mathcal{H}_{XXZ} = - \sum_{j=-\infty}^{\infty} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z + h \sigma_j^z \right)$$

where Δ is the anisotropy and h the magnetic field. Using the q-vertex operator approach and corner transfer matrices, Jimbo, Miki, Miwa and Nakayashiki obtained in 1992 [38] multiple integral representation for the correlation functions in the massive regime ($\Delta < -1$), and a conjecture for the critical regime ($|\Delta| < 1$) was proposed in [39]. The next important steps were made by Kitanine, Maillet, Terras and later Slavnov when they proved the previous results and their extension in the case of a magnetic field in both regimes in 1999 [40, 41]. Their method used the algebraic Bethe Ansatz [53]. Later they were able to obtain representations for the two-point correlations in terms of a multiple integral [42] which they called *master equation*. The generalization of the method for the time-dependent correlations was made in [43] (see [44] for a review of the entire series of papers). The final step was the extension of the multiple integral representation for finite temperatures which was done by Göhmann, Klümper, Seel and Hasenclever in [45, 46]. It should also be mentioned that in the study of the correlation functions in integrable models an important role is played by the quantum Knizhnik-Zamolodchikov equation [48] (see also [49],[51]) and for supersymmetric fermion models determinant representation of the correlations functions were reviewed in [47].

Despite these considerable efforts the asymptotics of time and temperature dependent correlation functions, such as $g(n, t)$ (see 4.1) for the XXZ spin chain, are still out of our reach. We expect that they will decay exponentially like in the previous examples of the isotropic XY spin chain or the δ -function Bose gas but at this moment we do not have such a result.

Open problem: Derive an explicit analytic formula describing the asymptotic exponential decay of time and temperature correlation functions in the critical region ($-1 \leq \Delta < 1$) of the XXZ spin chain.

5. Conclusions

Of course the open problems that we have presented do not exhaust the list of unanswered questions in the field of exactly solvable models. We should mention for example the solving of the time-dependent Schrödinger equation for spin chains which plays an important role in quantum information theory [50]. In the light of the talks given at the conference we can definitely say that Bethe Ansatz is alive and well after 75 years of developments and will carry on into the 21st century.

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