Threshold singularities in the XXZ- spin chain.

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Abstract

We calculate the critical exponents of the threshold singularity for the spectral density of the XXZ- spin chain at zero magnetic field for the lower threshold. We show that the corresponding phase shifts are momentum - independent and coincide with predictions of the effective mobile impurity Hamiltonian approach.

1. Introduction

The XXZ- spin chain is interesting both from the theoretical and the experimental points of view. The Hamiltonian of the model has the form:

\[ H = \sum_{i=1}^{L} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) + h \sum_i S_i^z, \]  

where the periodic boundary conditions are assumed, \( L \) is the length of the chain, the anisotropy parameter \( \Delta = \cos(\eta) \) and \( h \) is the magnetic field. Recently along with the calculation of the asymptotics of the correlators for the XXZ- spin chain and the other integrable models [1],[2], the calculation of the critical exponents of the threshold singularities of different correlators attracted much interest. The first attempts [3],[4] to calculate these exponents for the model (1) are based on the notion of the effective mobile impurity Hamiltonian [5],[6] combined with the calculation of the parameters with the help of the Bethe Ansatz. However the predictions of this approach contradict the universal behaviour of the phase shifts at small momentum \( k \rightarrow 0 \) [7]. Thus there is an obvious contradiction between the results of ref.[3],[4] and the predictions of the Luttinger liquid Bosonization approach [7],[8] at low momentum. The formfactors of the exactly solvable models were studied in the framework of the rigorous approach [9]. Although in general the formfactors of the XXZ- spin chain corresponding to the long-distance behaviour of the correlation functions were obtained in [9], and the singularities for the 1D Bose gas were obtained in [10] using the formfactor approach, the clear results for the singularities of the XXZ- spin chain at zero magnetic field are still absent. Also in [9],[10] all the critical exponents are expressed through the two-particle dressed phase
shifts [11]. However the calculation of these momentum-dependent phase shifts in the XXZ- spin chain and comparison of the results with the predictions of ref.[3],[4] is a separate problem.

It is the goal of the present paper to obtain the critical exponent of the singularity of the correlator \( \langle S_x^+ S_0^- \rangle \) at the lower threshold in the model (1) at \( h = 0 \) with the help of the rigorous approach [9],[10] and compare the results with the predictions of ref.[3],[4] and the universal phase shifts [7]. Our results confirm the phase shifts [3] for the XXZ- spin chain at zero magnetic field and contradict the predictions of ref.[7],[8] at small momentum.

2. Generalized Cauchy determinant at finite magnetic field.

Let us consider first the particular case of the XX- spin chain (\( \Delta = 0 \)). The solution of the model has the following form [12]. We assume for simplicity \( L \)- to be even and \( M = L/2 \) to be odd (\( S_z^0 = 0 \) for the ground state and \( M - 1 \)- even, we also assume \( L \) to be even so that the ground state is not degenerate). Then each eigenstate in the sector with \( M \) particles (up-spins) is characterized by the set of the momenta \( \{p\} = \{p_1, \ldots p_M\} \) such that \( p_i = 2\pi n_i/L, n_i \in \mathbb{Z} \) and each eigenstate in the sector with \( M - 1 \) particles is characterized by the set of the momenta \( \{q\} = \{q_1, \ldots q_{M-1}\}, q_i = 2\pi(n_i + 1/2)/L, n_i \in \mathbb{Z} \). The ground-state in the sector with \( M \) particles (up-spins) is given by the configuration \( \{p\} = \{p_1, \ldots p_M\}, p_i = 2\pi/L(i - (M + 1)/2), (M- is odd), and the ground state in the sector with \( M - 1 \) particles \( \{q_0\} = \{q_1, \ldots q_{M-1}\}, q_i(0) = 2\pi/L(i - M/2). \) Equivalently one can take the shifted momenta

\[
p_i = (2\pi/L)(i), \quad i = 1, \ldots M, \quad q_j^{(0)} = (2\pi/L)(j + 1/2), \quad j = 1, \ldots M - 1.
\]

In terms of the sets of the momenta \( \{p\} \) and \( \{q\} \) the formfactor \( \langle \{q\}|S_0^-|\{p\} \rangle \) can be represented in the following form [15]:

\[
\langle \{q\}|S_0^-|\{p\} \rangle \sim \frac{\prod_{i<j} \sin((p_i - p_j)/2) \prod_{i<j} \sin((q_i - q_j)/2)}{\prod_{i,j} \sin((p_i - q_j)/2)}.
\]

(2)

Let us note that the expression (2) for the formfactor is exact for an arbitrary state characterized by the momenta \( q_1, \ldots q_{M-1} \).

Now let us consider the general case of the XXZ- spin chain in the finite magnetic field \( h \neq 0 \). Let \( \{t\} = t_1, \ldots t_M \) and \( \{\lambda\} = \lambda_1, \ldots \lambda_{M-1} \) to be the spectral parameters (rapidities) of the ground state \( \{|\{t\}\rangle \} \) and the excited state \( \{|\{\lambda\}\rangle \} \), where the number of roots \( M \) is connected with the magnetic field \( h \). We are interested in the formfactor of the local operator \( S_0^- \) of the form \( \langle \{\lambda\}|S_0^-|\{t\} \rangle \). Suppose the state \( \{|\{\lambda\}\rangle \} \) contains the hole with the rapidity \( t_0 \) corresponding to the momentum \( k \). Then the part of the formfactor which contains the information about the low-energy particle-hole excitations
in the state $|\{\lambda\}\rangle$ has the form of the generalized Cauchy determinant
\[ \langle \{\lambda\}|S_0^{-1}|\{t\}\rangle \sim \frac{\prod_{i<j} \text{sh}(t_i - t_j) \prod_{i<j} \text{sh}(\lambda_i - \lambda_j)}{\prod_{i,j} \text{sh}(t_i - \lambda_j)}. \] (3)
The other factors depend on $k$ but not on the quantum numbers of the low-energy excitations in the state $|\lambda\rangle$. One can present the following arguments in favor of (3). First, one can see that in the XX- limit the determinant (3) reproduce the exact result (2) which follows from the formula $e^{\pi t/\eta} = \text{tg}(p/2 + \pi/4)$, which connects the rapidity $t$ with the corresponding momentum $p$. Second, this statement was proved by means of the complicated analysis in [9]. Third, in fact the results obtained from (3) do not depend on the specific form of the function which enters (3), so this equation can be considered as a natural hypothesis confirmed by the example of the XX- spin chain. Let us stress that we can use the expression (3) only at $h \neq 0$, while the corresponding expression at $h = 0$ is not known. Thus in the present paper we will perform all calculations for $h \neq 0$ and take the limit $h \to 0$ only in the final expressions for the phase shifts.

3. Singularity at the lower threshold.

Here we calculate the phase shifts for the XXZ- spin chain at $h = 0$ starting from the expression (3) for the formfactors. We perform the calculations at $h \neq 0$, or at finite cutoff $\Lambda$ for the rapidities $t_\alpha$, $t_\alpha \in (-\Lambda, \Lambda)$, and take the limit $\Lambda \to \infty$ only at the end of the calculations. We consider the configuration $\{\lambda\}$ obtained from the vacuum configuration of $M - 1$ roots by removing the single root at the position $t_0$ (hole) and adding an extra root $\lambda_M$ at the right end of the interval $(-\Lambda, \Lambda)$. Near the right end of this interval the values of the roots and their difference have the form:
\[ t_i \simeq t_M - \frac{1}{LR(\Lambda)} i, \quad \lambda_j \simeq \lambda_M - \frac{1}{LR(\Lambda)} j, \quad t_i - \lambda_j \simeq \frac{1}{LR(\Lambda)} (i - j + LR(\Lambda)(t_M - \lambda_M)), \] (4)
where $t_M$ and $\lambda_M$ are the maximal roots and $R(t)$ is the density of roots at $t \in (-\Lambda, \Lambda)$. The calculation of the Cauchy determinant (3) corresponding to a given configuration of particles and holes at the right (left) Fermi- points is quite simple and gives the known expression [9],[13],[14] with the phase shift parameter:
\[ \delta_1 = LR(\Lambda)(t_M - \lambda_M) = RW(\Lambda), \] (5)
where the function $W(t)$ is defined as $W(t_\alpha) = L(t_\alpha - \lambda_\alpha)$, where $t_\alpha$ and $\lambda_\alpha$ - are the corresponding roots from the sets $\{t\}$ and $\{\lambda\}$ starting from the roots $t_M$, $\lambda_M$. The equation for the function $RW(t) = R(t)W(t)$ is obtained by the subtraction of the corresponding Bethe Ansatz equations for $t_\alpha$ and $\lambda_\alpha$ and takes the form:
\[ 2\pi RW(t) + \int_{-\Lambda}^{\Lambda} dt' \phi'_2(t - t') RW(t') = -\pi + \phi_2(t - t_0), \] (6)
where the function \( \phi_2(t) = -(1/i) \ln((t - i\eta)/(t + i\eta)) \). Clearly, for the vacuum case (\( \{\lambda\} \)- does not contain a hole) we obtain the same equation (6) with the right-hand side equal to \( \pi + \phi_2(t + \Lambda) \). The solution of the equation (6) is quite standard and is given by the following simple formulas. First, for the term \(-\pi\) at the right-hand side of (6) the solution is given by the dressed charge function \( Z(t) \) defined by the equation

\[
2\pi Z(t) + \int_{-\Lambda}^{\Lambda} dt' \phi_2'(t - t') Z(t') = 2\pi.
\]

It is known that \( Z(\Lambda) = 1/\sqrt{\xi} \), where \( \xi = 2(\pi - \eta)/\pi \) is the standard Luttinger liquid parameter for the XXZ spin chain. Second, to obtain the solution for the second term \( RW_1(t) \), for the right-hand side, we rewrite the equation (6) in the form:

\[
\chi(t) = f(t) + \int_0^\infty dt' F(t - t') \chi(t'),
\]

where \( \chi(t) = RW_1(t + \Lambda) \), the Fourier transform \( F(\omega) = \phi_2'(\omega)/(2\pi + \phi_2(\omega)) \) and the function \( f(t) = \tilde{F}(t + \Lambda - t_0) \), where the function \( \tilde{F}(t) \) is defined by the equation \( \tilde{F}'(t) = F(t) \). The general solution of the equation (7) is

\[
\chi^+(\omega) = G^+(\omega) \int \frac{d\omega'}{2\pi i (\omega' - \omega - i0)} G^-(\omega') f(\omega'),
\]

where \( \chi^+(\omega) = \int_0^\infty dt e^{i\omega t} \chi(t) \), the functions \( G^+(\omega) \) holomorphic at the upper (lower) half-plane of the variable \( \omega \) are defined by the equation \( F(\omega) = 1 - 1/G^+(\omega)G^-(\omega) \) (for example, see [16]) and in our case \( f(\omega) = e^{-i\omega(\Lambda - t_0)} \tilde{F}(\omega) \). Taking the limit \( \omega \to \infty \) in the equation (8) we obtain the contribution to the phase shift:

\[
RW_1(\Lambda) = \chi(0) = \int \frac{d\omega}{2\pi} e^{-i\omega(\Lambda - t_0)} G^-(\omega) \tilde{F}(\omega).
\]

To obtain the Fourier transform \( \tilde{F}(\omega) \) one can use the following identity:

\[
\phi_2(\omega) = \frac{i}{\omega + i} \phi'_2(\omega) - 2\pi(\pi - 2\eta)\delta(\omega).
\]

Thus the corresponding contribution to the phase shift (9) is found. To calculate (9) at \( (\Lambda - t_0) \gg 1 \) one should consider the integration contour at the lower half-plane of the complex variable \( \omega \). The leading \( \sim O(1) \) is given by the residue of the pole at \( \omega = -i0 \). Thus taking into account the contribution of the first term in (6) we obtain the phase shift for the right Fermi-point at \( (\Lambda - t_0) \gg 1 \):

\[
\delta_1 = \frac{1}{2\sqrt{\xi}} + \frac{1}{2}\sqrt{\frac{\xi}{2}}(1 - 1/\xi) = \frac{\sqrt{\xi}}{2} - \frac{1}{\sqrt{\xi}}.
\]

At the same time at the left Fermi-point the phase shift \( \delta_2 \) is equal to its “vacuum” value \( \delta_2 = \sqrt{\xi}/2 \).
One can easily verify that these values of the phase shifts $\delta_1, \delta_2$ coincide with the predictions of the mobile impurity Hamiltonian method [3]. At the same time at $(\Lambda - t_0) \gg 1$ the result for $\delta_1$ does not coincide with the prediction of the Luttinger liquid Bosonization approach $\delta_1 = 1 - \sqrt{\xi}/2$.

In the opposite limit $(\Lambda - t_0) \ll 1$ from the equation (9) we obtain exactly this universal value $\delta_1 = 1 - \sqrt{\xi}/2$. However since in this limit $(\Lambda - t_0) \simeq k/2\pi R(\Lambda)$ where $k$ is the momentum of the hole the universal phase shift is reproduced only at the very small momentum $k \ll R(\Lambda) \sim e^{-\pi\Lambda/\eta}$ (note that $\Lambda \to \infty$). Using the formfactors one can easily calculate the threshold singularity for the dynamical structure factor [8]:

$$A(\omega, k) = \sum_x \int dt e^{i\omega t - ikx} \langle S_x^+(t)S_0^-(0) \rangle \sim \frac{1}{(\omega - \epsilon(k))^\mu},$$

where $\epsilon(k)$- is the known excitation energy of the single hole (particle) and the critical exponent is given by the expression:

$$\mu = 1 - \delta_1^2 - \delta_2^2 = 2 - 1/\xi + \xi/2.$$

The reason for the sharp transition from the Luttinger liquid result for $\delta_1$ to the momentum-independent results of ref.[3] is as follows. If $t_0$ is sufficiently close to to the extra root $\lambda_M$ (or $\Lambda$) there is no shift of the roots between $t_0$ and $\Lambda$ and clearly the phase shift $\delta_1 = 1 - \sqrt{\xi}/2$, where $\sqrt{\xi}/2$ is the “vacuum” value of the phase shift. That is what one expects in the framework of the Luttinger liquid. However at $(\Lambda - t_0) \gg 1$ the roots between $t_0$ and $\Lambda$ acquire the additional shift to the left, which is described by the by the equation (6), which makes the naive predictions of the Luttinger liquid (Bosonization) incorrect. At the same time in this case the mobile impurity Hamiltonian approach is still applicable for the formfactors and leads to the results for $\delta_1, \delta_2$ in agreement with the rigorous approach [9],[10] (see (3). The main result of the present letter is that contrary to the naive expectations this shift of the roots is model-dependent and cannot be described in the framework of the Luttinger liquid. Note that the main assumption of mobile impurity Hamiltonian approach is the identification of the Jordan-Wigner fermion $\psi$ with the impurity operator $d$, $\psi^+ \to d^+$. However the similar substitution $\psi^+ \to a^+$, where $a^+$- is the Luttinger liquid fermionic operator, is made in the framework of the Bosonization approach. Summarizing, we have found that for the XXZ- spin chain the matrix element $\langle p, low|S^-|0 \rangle$, where $p$ is the momentum of the hole cannot be calculated in the regime when the momentum $p$ is much larger than the particle-hole momenta $p_i, q_i$ in the state $\langle low \rangle$ (but still much smaller than the Fermi- momentum $\sim 1$) as the matrix element of the exponential operator

$$\langle p, low|e^{i\pi\sqrt{\xi}(\hat{N}_1 - \hat{N}_2)}|0 \rangle,$$

where $\hat{N}_1, \hat{N}_2$ are the rescaled Luttinger liquid fields. The reason for this surprising result is not clear at present time. However let us note that the long-distance asymptotics of the
correlators are reproduced correctly both in the framework of the Bosonization approach and from the formfactors (3).

4. Conclusion.

In conclusion, we obtained the critical exponent of the threshold singularity for the dynamical structure factor in the XXZ- spin chain at zero external magnetic field with the help of the rigorous method. The method is based on the expressions for the formfactors in the form of the generalized Cauchy determinants (3). Our results are in agreement with the predictions of the effective mobile impurity Hamiltonian method [3],[5] and contradict the naive Luttinger liquid theory predictions. Few remarks are in order here. The correct way to calculate the parameters of the effective mobile impurity Hamiltonian $V_L, V_R$ (in the notations of ref.[5]) is to use the results of ref.[17], where the interaction energy of the particle-hole pair in the XXZ- spin chain was calculated. This leads to the values of $V_L, V_R$ which are different from the values found in [3] (the influence of the left and the right densities on the energy of the high-energy particle does not taken into account). However due to the other mistakes (see [18]) the final results for the phase shifts are correct. Finally, we found that the naive application of the Bosonization technique to the calculation of the formfactors does not lead to the correct results even at small energies. At the same time the application of the effective mobile impurity Hamiltonian method gives the correct momentum-independent results for the phase shifts and the critical exponent for the lower threshold singularity of the spectral density. Our main result is that in general the local spin operator cannot be represented as the exponential operator in the effective Luttinger liquid model even at the low energies.

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