Abstract

We study the exact solution of the anisotropic spin-1/2 Heisenberg chain with a boundary magnetic field in the region where the bulk excitations are gapless. It is shown that near the boundary a bound state is created which is underscreened when $\gamma < \pi/3$ and which at low temperatures behaves like a single spin weakly coupled to the bulk. The IR fixed point in this case belongs to the universality class of the underscreened anisotropic Kondo model. We argue that the same fixed point appears in the boundary sine-Gordon model when the scaling dimension of the boundary term $2/3 < \Delta < 1$.

Problems about the influence of impurities and imperfections on the behaviour of one dimensional strongly correlated systems are attracting growing attention. So far the main interest has been concentrated on effects of potential scattering on the behaviour of electrons in Luttinger liquids\textsuperscript{1,2}. It is widely believed that there the conductance of a one-dimensional chain vanishes at $T = 0$ even if only a single impurity is present, provided the electron-electron interaction is repulsive\textsuperscript{1}. The best studied model deals with spinless interacting electrons and in the continuous limit is equivalent to the so-called boundary sine-Gordon (BSG) model. There are strong reasons to believe that this model is related to the problem of the spin-1/2 Heisenberg chain with a boundary magnetic field\textsuperscript{3}:

$$H = \frac{J}{2} \sum_{n=1}^{N-1} \left[ \frac{1}{2} (-\sigma^+_n \sigma^-_{n+1} - \sigma^+_n \sigma^-_{n+1}) + \cos \gamma \sigma^z_n \sigma^z_{n+1} \right] - \frac{1}{2} h_1 \sigma^z_1 - \frac{1}{2} h_2 \sigma^z_N$$

(1)
We shall discuss this relation below. The model (1), however, is interesting in its own right. At $h_{1,2} = 0$ it describes an experimentally accessible situation of a one-dimensional magnet where some spins are replaced by non-magnetic ions.

The model (1) is exactly solvable by the Bethe ansatz\textsuperscript{4,5}. The Bethe ansatz equations are

\[ [e_1(u_a)]^{2N} e_{2S_1}(u_a) e_{2S_2}(u_a) = \prod_{b=1, b \neq a}^{M} e_2(u_a - u_b) e_2(u_a + u_b) \]  

\[ e_n(u) = \frac{\sinh[\gamma(u - in/2)]}{\sinh[\gamma(u + in/2)]} \]  

\[ \exp(2i \gamma S_j) = e_1 \left[ \frac{1}{2 \gamma} \ln \left( \frac{h_j}{J} + \cos \gamma \right) \right] \]  

and the energy is given by

\[ E = \overline{J} \sum_{a=1}^{M} \frac{1}{2i\pi} \frac{1}{du_a} \ln e_1(u_a) - \frac{1}{2}(h_1 + h_2) \]  

where

\[ \overline{J} = \frac{2\pi \sin \gamma}{\gamma} J \]

The quantities $S_{1,2}$ are defined in such a way that at $h = 0$ $2S = \pi/\gamma - 1$ and $S = 2\pi/\gamma - 1$ at $h \to \infty$. Solutions $u_a$ and $-u_a$ describe the same eigenstate.

Since we are interested in boundary effects we have to compare the free energy of the open chain with that of a chain with periodic boundary conditions. In order to make this comparison we shall rewrite the Bethe ansatz equations in a form where they are maximally similar to the equations for the XXZ model with the periodic boundary conditions. Following Ref. 3, we define a new set of rapidities $v_a$ such that

\[ v_a = \begin{cases} u_a, & a = 1, 2, \ldots M \\ -u_{2M-a+1}, & a = M + 1, \ldots 2M \end{cases} \]

Then Eqs.(2) become

\[ [e_1(v_a)]^{2N} e_{2S_1}(v_a) e_{2S_2}(v_a) \frac{\sinh[2\gamma(v_a - i/2)]}{\sinh[2\gamma(v_a + i/2)]} = \prod_{b=1}^{2M} e_2(v_a - v_b) \]

The last term on the left hand side is introduced to compensate the term with $v_b = -v_a$ now present on the right hand side. This term can be rewritten as

\[ \frac{\sinh[2\gamma(v_a - i/2)]}{\sinh[2\gamma(v_a + i/2)]} = e_1(v_a) e_{1-\gamma}(v_a) \]
The term $e_1(v)$ can be included into the bulk part. Finally, we get the following Bethe ansatz equations:

$$[e_1(v_a)]^{2N+1}[e_2S_1(v_a)e_2S_2(v_a)e_1-\pi/\gamma(v_a)] = \prod_{b=1}^{2M} e_2(v_a - v_b)$$  \hspace{1cm} (8)

with the energy equal to

$$E = -\frac{1}{2} J\sum_{a=1}^{2M} \frac{1}{2i\pi} d\ln e_1(v_a) - \frac{1}{2}(h_1 + h_2)$$  \hspace{1cm} (9)

In these notations the Bethe ansatz equations look similar to the equations for the periodic XXZ spin-1/2 Heisenberg chain with an inserted impurity spin\(^6\) or the equations for an anisotropic Kondo model with the large coupling constant (see, for example, Ref. 7). The analogy becomes complete when one of the boundaries is free ($h_2 = 0, 2S_2 = \pi/\gamma - 1$). Then the two phases on the left hand side of Eq.(8) cancel and the resulting Bethe ansatz equation is the same as that for the Kondo model with impurity spin $S_1$. Except for the special case $h_1 \to \infty$ this spin is never equal to 1/2. Since the XXZ Heisenberg chain with an impurity spin is very similar to the Kondo problem\(^6\), where the singlet ground state is guaranteed to exist only if the impurity spin is equal to 1/2, one can expect here non-analytic contributions from the boundary. As we shall see later, this does occur when $0 < \gamma < \pi/2$ when the IR fixed point of the model (1) coincides with the fixed point of the underscreened Kondo model. At $\pi/2 < \gamma < \pi$ the boundary spins are completely screened at $T \to 0$.

Below we shall consider the thermodynamical properties of the model (1). In order to simplify the calculations we shall do it at the special points (a) $\gamma = \pi/\nu$ and (b) $\gamma = \pi(1 - \nu^{-1})$, where the solutions of Eqs.(8) have especially simple classification\(^8\). The equations for the distribution functions of rapidities coincide for the both cases, but the energy has different signs. Since the results for a finite boundary magnetic field do not differ qualitatively from those for the open boundary conditions and the latter case is more physical, we shall concentrate on the problem with open boundary conditions and make only few remarks about the general case when it will be appropriate.

We emphasise that we are interested in boundary effects, but not in finite size effects. The latter ones disappear when the length of the chain becomes infinite. Neglecting finite size effects we get the following thermodynamic equations for the open boundary conditions:

$$\epsilon_n = -\frac{1}{2}\tilde{J}\eta s(v)\delta_{n,1} + Ts \ast \ln \left(1 + e^{\epsilon_{n-1}/T}\right) \left(1 + e^{\epsilon_{n+1}/T}\right)$$
\[+T\delta_{n,\nu-2}s* \ln \left(1 + e^{\epsilon_{\nu-1}/T}\right), \ n = 1, \ldots \nu - 2 \quad (10)\]

\[\epsilon_{\nu-1} = Ts* \ln \left(1 + e^{\epsilon_{\nu-2}/T}\right) + \frac{\nu}{2}H \quad (11)\]

\[\epsilon_0 = Ts* \ln \left(1 + e^{\epsilon_{\nu-2}/T}\right) - \frac{\nu}{2}H \quad (12)\]

\[F_{\text{bulk}} = -2NT \int_{0}^{\infty} dv s(v) \ln \left(1 + e^{\epsilon_{1}/T}\right) \quad (13)\]

\[F_{\text{boundary}} = F_1 + F_2 \]

\[F_1 = -T \int_{0}^{\infty} dv s(v) \ln \left(1 + e^{\epsilon_{\nu-1}/T}\right) \left(1 + e^{\epsilon_0/T}\right) \]

\[F_2 = -T \int_{0}^{\infty} dv s(v) \ln \left(1 + e^{\epsilon_{1}/T}\right) \]

(14)

where \(\eta = 1\) for \(\gamma < \pi/2\) and \(\eta = -1\) for \(\gamma > \pi/2\) and \(H\) is the magnetic field in the bulk. The sign \(*\) stands for convolution

\[f * g(v) = \int_{-\infty}^{\infty} f(v - v')g(v')dv'\]

and \(s(v) = \left[4 \cosh(\pi v/2)\right]^{-1}\).

As we have said, one can expect these equations to be similar to the equations for the Kondo problem. There is one important difference, however: the non-trivial part of the boundary free energy \(F_2\) (14) is equal to 1/2 of the free energy of the Kondo impurity. This is, of course, due to the restriction that only symmetric distribution of rapidities are allowed. Eqs.(10-14) are also similar to the thermodynamic equations for BSG problem derived in Refs. (9, 10) from the bootstrap solution of Ref. 11. The anisotropy parameter \(\gamma\) is related to the scaling dimension of the boundary term in BSG problem:

\[\Delta = 1 - \gamma/\pi \quad (15)\]

Here the differences are more important. The least important one is that the BSG equations contain the boundary energy scale \(T_B\). This difference by setting \(T_B\) equal to the ultraviolet cut-off \(\Lambda \approx J\). What is more important, however, is the fact that the boundary free energy in BSG model has a different form:

\[F_{\text{BSG}} = -T \int_{-\infty}^{\infty} dv s[v - \frac{2}{\pi} \ln(\Lambda/T_B)] \ln \left(1 + e^{\epsilon_{\nu-1}/T}\right) \]

(16)

At \(H = 0\) when \(\epsilon_{\nu-1} = \epsilon_0\) and \(\Lambda = T_B\) these two expressions are equivalent, but at \(H \neq 0\) one can expect differences. These differences are due to the asymmetry between solitons and antisolitons in BSG.

Since the obtained thermodynamic equations are very similar to those for BSG model and the latter were analysed for \(\eta = -1\) in Refs. (9, 10), we shall...
concentrate on the case $\eta = +1$, $\gamma < \pi/2$. In this case the ground state consists of real $v$'s, i.e. the only non-vanishing energy at $T = 0$ is $\epsilon_1$.

Analytical solutions are available for asymptotics of $\epsilon_n(x)$ at $v \to 0, \infty$ (see, for example, Refs.(7, 8)). At large temperatures $T >> J$ the free energy is determined by the asymptotics at $v \to +\infty$ where

\[
\left(1 + e^{\epsilon_0/T}\right) \left(1 + e^{\epsilon_{\nu-1}/T}\right) = \left[\frac{\sinh \nu H/2T}{\sinh H/2T}\right]^2
\]

such that we have

\[
F_{\text{boundary}} \to -\frac{T}{2} \ln \left[\frac{\sinh \nu H/2T}{\sinh H/2T}\right]
\]

At small temperatures the leading contribution comes from the region $v \to 0$ where $\epsilon_n (\nu \neq 1)$ are again almost constant and $\exp(\epsilon_1/T)$ is small. Then the corrections can be determined from the expansion in $\exp(\epsilon_1/T)$:

\[
g_n(v) \equiv \ln \left(1 + e^{\epsilon_n(v)/T}\right) = g_n^{(0)} + g_n^{(1)}(v) + ...
\]

\[
g_n^{(0)} = 2 \ln \Phi(n) (n = 2, 3, ... \nu - 2),
\]

\[
g_{\nu-1}^{(0)} = \ln[1 + \exp(\nu H/2T)\Phi(\nu - 2)],
\]

\[
g_n^{(1)}(v) = \frac{1}{\Phi(2)\Phi(n)}[\Phi(n + 1)a_n * g_1(v) - \Phi(n - 1)a_{n+2} * g_1(v)]
\]

\[
\Phi(n) = \frac{\sinh n \nu H/2(\nu - 1)T}{\sinh \nu H/2(\nu - 1)T},
\]

\[
a_n(\omega) = \frac{\sinh[(\nu - n)\omega/2]}{\sinh[(\nu - 1)\omega/2]}
\]

Using these expressions we get the following expansion for the free energy:

\[
F_{\text{boundary}} \to -\frac{T}{2} \ln \Phi(\nu - 1) - T \int_0^{\infty} dv f(v) \ln \left(1 + e^{\epsilon_1(v)/T}\right)
\]

where $\Delta = 1 - 1/\nu = 1 - \gamma/\pi$ and

\[
f(\omega) = \frac{\tanh(\omega/2)}{\sinh[(\nu - 1)\omega/2]}
\]

In order to estimate the second term in Eq.(21) we use the crude approximation:

\[
\ln \left(1 + e^{\epsilon_1(v)/T}\right) \approx C\theta \left(v - \frac{2}{\pi} \ln(J/T)\right)
\]

where $C$ is a constant.

The first result is that the ground state has a finite entropy $S(0) = -\frac{1}{2} \ln(\Delta^{-1} - 1)$ which corresponds to the the half of the entropy of the underscreened spin ($S - 1/2$). A careful analysis shows that this entropy disappears at $\Delta \leq 1/2$.  

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The ratio of boundary contributions to the partition functions in the ultraviolet and the infrared limits is
\[ Z_{UV}/Z_{IR} = \Delta^{-1/2} \] (23)

The same expression remains valid at \( \pi > \gamma > \pi/2 \).

From the obtained expression for the free energy we derive the following asymptotics for the specific heat and the magnetic susceptibility at \( \nu > 2, H \to 0 \):
\[ \chi = \frac{(\nu + 1)\nu^2}{24(\nu - 1)T} \left[ 1 + B \left( \frac{T}{J} \right)^{2/(\nu - 1)} + \ldots \right] \] (24)
\[ C_v \sim (T/J)^{2/(\nu - 1)} \] (25)

where \( B \) is a constant.

Now we shall calculate the boundary contribution to the overall magnetic moment \( M^{\text{boundary}} \) and the average value of spin on the boundary \( \langle S^z_1 \rangle \) at \( T = 0 \).

At zero temperature the only non-vanishing density is the density of real \( v \)'s \( \rho(v) \). From the Bethe ansatz equations (8) we derive the integral equation for \( \rho(v) \):
\[ \int_{-B}^{B} du A_{11}(v-u)\rho(u) = s * A_{11}(v) + \frac{1}{2N} \mu_1(v) \] (26)
\[ E = -\frac{h_1}{2} - JN \int_{-B}^{B} dv s * A_{11}(v)\rho(v) \] (27)

where
\[ A_{11}(\omega) = 1 + \frac{\sinh(\nu - 2\omega)/2}{\sinh \nu \omega/2}, \mu(\omega) = \frac{\sinh(\nu - 2S)\omega/2}{\sinh \nu \omega/2} \]
and the limit \( B \) is determined by the magnetic field in the bulk such that at it is infinite at \( H = 0 \). Let us consider the case \( h = 0 \) first. At \( H << J \) the Fredholm equation (26) can be treated as a Wiener-Hopf equation. The latter can be solved giving the leading asymptotics of the magnetization. The result is
\[ M^{\text{boundary}} = \frac{1}{4\pi} \int_{-\infty}^{\infty} dx \exp \left[ -\frac{2ix}{\pi} \ln(\bar{J}/H) \right] \frac{1}{G^{(-)}(x) \sinh[\Delta x/(1 - \Delta)] \cosh x} \]
\[ \approx \frac{1}{2\sqrt{\pi}} \tan(\pi/\Delta) \frac{\Gamma(1 + 1/\Delta)}{\Gamma(1/\Delta - 1/2)} (H/\bar{J})^{2(\Delta^{-1} - 1)} \]
\[ + \frac{1}{\sqrt{\pi}} \frac{\Gamma[1 + 1/2(1 - \Delta)]}{\Gamma[1 + \Delta/2(1 - \Delta)]} (H/\bar{J}) \] (28)

where \( G^{(\pm)}(x) \) are functions analytical in the upper (lower) half-plane of \( x \):
\[ G^{(+)}(-x) = G^{(-)}(x) = \frac{\Gamma(1 + \frac{ix\Delta}{1-\Delta})\Gamma(1/2 + \frac{ix}{\pi})}{\Gamma(1 + \frac{ix}{\pi(1-\Delta)})\Gamma(1/2)} \] (29)
At $\Delta \geq 2/3 (\nu \geq 3)$ the non-analytic contribution becomes dominant. At $\Delta = 2/3$ there is a double pole and we have a marginal situation with $M_{\text{boundary}} \sim H \ln H$. Comparing Eqs. (28) and (25) we see that $H$ has the same scaling dimension as $T$ which is quite natural since if we have an unscreened spin in our theory.

It is also interesting to know whether the underscreened spins are situated directly on the boundaries. To find this out we calculate the average value of the boundary spin explicitly at $H = 0$, $T = 0$. From Eqs. (26) and (27) we find the $h_1$-dependent part of the ground state energy:

$$E(h) = -\frac{h_1}{2} - J\frac{\nu \sin(\pi/\nu)}{\pi} \int_0^\infty \frac{d\omega}{\sinh \nu \omega \cosh \omega} \sinh[\nu - 2S(h_1)]\omega$$  \hspace{1cm} (30)

Differentiating this expression in $h_1$ and using the definition of $S$ \footnote{[1]} we get

$$\langle S^z_1 \rangle = -\frac{\partial E}{\partial h_1} |_{h_1=0} = \frac{1}{2} - \frac{2}{\pi^2} \int_0^\infty \frac{d\omega}{\sinh \omega} = 0$$  \hspace{1cm} (31)

and

$$\chi_{\text{boundary}} = -\frac{\partial^2 E}{\partial h_1^2} |_{h_1=0} = \frac{4}{\gamma^3 \sin \gamma J} \int_0^\infty \frac{d\omega \omega^2 \tanh \omega}{\sinh(\pi \omega/\gamma)}$$  \hspace{1cm} (32)

Thus we see that the susceptibility of the boundary spins is finite. This means that the boundary spins do not participate in the bound state responsible for the singularities in the free energy.

In conclusion, as we have suggested above, at $\gamma < \pi/3$ the boundary contribution to the free energy is non-analytic in $T$ and $H$ and the boundary free energy is equal to $1/2$ of the free energy of the corresponding underscreened Kondo model. Since the XXZ chain is similar to BSG model, we expect the same type of behaviour for BSG in the area $1/2 < \Delta < 1$.

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