

# The Thermodynamics of the XXZ Heisenberg Chain with Impurities

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## Abstract

In this paper, we discuss the effect of the arbitrary spin impurities to the spin-1/2 and spin-1 XXZ model. The effect of ground state, the free energy, the magnetic susceptibility, the specific heat and the Kondo temperature are given by using the thermodynamic Bethe ansatz equation.

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## I. INTRODUCTION

Behavior of a quantum chain will be quite different when impurities embedding in the system. With the method of bosonization and renormalization techniques, Kane and Fisher proved this result when they studied the properties of a potential scattering center in a Luttinger liquid [1]. After their work, many papers have paid their attention to the problems of local perturbation to a Luttinger liquid, especially the Kondo problem in the system [2-5]. It is well known that the spin dynamics of the Kondo problem is equivalent to the dynamics of the spin chain with magnetic impurities [6].

The Heisenberg chain is an important model in the study of integrable system. Firstly, Andrei and Johannesson considered a spin- $s$  ( $s > \frac{1}{2}$ ) impurity embedding in the spin- $\frac{1}{2}$  Heisenberg chain with periodic boundary condition [7]. Then, Lee and Schlottmann generalized the problem to arbitrary spin [8]. However, it is found that the open boundary theory is better to deal with quantum chains with impurities, since the periodic boundary condition would lead to the presence of some unphysical terms in the Hamiltonian to maintain the integrability [9,10]. In recent research, in the frame of the quantum inverse scattering method, Wang studied the exact solution of the spin- $\frac{1}{2}$  XXX open Heisenberg chain with two arbitrary spin impurities [9]. Subsequently, Hu and Pu considered the spin- $\frac{1}{2}$  XXZ chain with two spin- $\frac{1}{2}$  impurities [10]. In the previous paper [11], we obtained the eigenvalues of the Hamiltonian and the Bethe ansatz equations for both the spin- $\frac{1}{2}$  and spin-1 XXZ chains with two arbitrary spin impurities.

The low-temperature thermodynamics was first proposed by Yang and Yang. In their series papers, they studied systematically the ground state, the magnetic susceptibility and the specific heat of the spin- $\frac{1}{2}$  Heisenberg chain [12–14]. Directly, this method was generalized to other models, such as the Hubbard model *etc* [15–17]. In the Ref. [18–22], Babujian, Kirillov and Reshetikhin and others studied thermodynamics of the arbitrary spin XXX and XXZ Heisenberg chain respectively. In the present paper, we study thermal properties of the spin- $\frac{1}{2}$  and spin-1 XXZ chains with two arbitrary spin impurities by using the standard

method at low temperature.

## II. THE MODEL

The integrability of the spin- $\frac{1}{2}$  and spin-1 XXZ Heisenberg chains with two arbitrary spin impurities have been discussed in the Ref. [11]. Hamiltonians of them can be represented by

$$H = \frac{-i}{2\rho^N(0)\rho_d(c_a)\rho_d(c_b)\text{tr}_\tau K^+(0)} \times \left. \frac{d t(u)}{du} \right|_{u=0}, \quad (1)$$

where  $t(u)$  is the transfer matrix,  $\rho(0)$  and  $\rho_d(c_i)$  ( $i = a, b$ ) are constants appearing in unitarity relations of the  $R$ -matrix in the bulk and the boundary respectively,  $K^+$  is the dual reflection matrix, and  $c_i$  are coupling constants.

Applying the Hamiltonians  $H$  on the multi-particle-state Bethe vector  $|\Omega\rangle$ , we obtain the eigenvalues as follows

$$E = E_b + E_i + E_\infty, \quad (2)$$

where  $E_b$ ,  $E_i$  and  $E_\infty$  stand for the energy of boundary, impurities and the bulk respectively.

To the spin- $\frac{1}{2}$  chain, we have

$$\begin{aligned} E_b &= -\frac{i \sinh(\xi^+ - \xi)}{2 \sinh \xi^+ \sinh \xi} + \frac{i}{2 \sinh(2\eta)}, \\ E_i &= -\frac{i}{2} \sum_{r=\pm 1} \sum_{k=a,b} \coth(rc_k + s_i \eta + \frac{\eta}{2}), \\ E_\infty &= -N \frac{i \cosh \eta}{\sinh \eta} - \sum_{j=1}^M \frac{2i \sinh \eta}{\cosh(2v_j) - \cosh \eta}, \end{aligned} \quad (3)$$

where  $s_i$  is the arbitrary spin of impurities; to spin-1 chain case, we have

$$\begin{aligned} E_b &= -\frac{i \sinh(2\eta)}{2 \sinh(\xi^+ + \frac{\eta}{2}) \sinh(\xi^+ - \frac{3\eta}{2})} + 2 \frac{i \cosh \eta}{\sinh(3\eta)}, \\ E_i &= -\sum_{r=\pm 1} \sum_{k=a,b} \frac{i \sinh(2rc_k + 2s_i \eta + \eta)}{2 \sinh(rc_k + s_i \eta) \sinh(rc_k + s_i \eta + \eta)}, \\ E_\infty &= -N \frac{i \sinh(3\eta)}{\sinh \eta \sinh(2\eta)} - 2N \frac{i \cosh(2\eta)}{\sinh(2\eta)} - \sum_{j=1}^M \frac{2i \sinh(2\eta)}{\cosh(2v_j) - \cosh(2\eta)}, \end{aligned} \quad (4)$$

where  $\xi^+$ ,  $\xi$  and  $\eta$  are some free parameters and  $v_j$  satisfies the Bethe ansatz equation

$$\frac{\sinh(v_j - \xi^+ - \frac{\eta}{2}) \sinh(v_j + \xi - \frac{\eta}{2}) \sinh(v_j + \frac{\eta}{2}) \cosh(v_j + \frac{\eta}{2}) \sinh^{2N}(v_j + s\eta)}{\sinh(v_j + \xi^+ + \frac{\eta}{2}) \sinh(v_j - \xi + \frac{\eta}{2}) \sinh(v_j - \frac{\eta}{2}) \cosh(v_j - \frac{\eta}{2}) \sinh^{2N}(v_j - s\eta)} \times \prod_{r=\pm 1} \prod_{k=a,b} \frac{\sinh(v_j + rc_k + s_i\eta)}{\sinh(v_j + rc_k - s_i\eta)} = - \prod_{i=1}^M \frac{\sinh(v_j - v_i + \eta) \sinh(v_j + v_i + \eta)}{\sinh(v_j - v_i - \eta) \sinh(v_j + v_i - \eta)}, \quad (5)$$

where  $j = 1, 2, \dots, M$  with  $M$  being the number of down spins.

With the Bethe vector  $|\Omega\rangle$ , according the Ref. [18,19], we can also obtain the eigenvalue of the total spin  $z$ -projection

$$s^z = Ns + 2s_i - M \quad (6)$$

### III. THE GROUND STATE

To obtain precise forms of the eigenvalues of Hamiltonians, denoting

$$\Phi_\gamma(v_j) = 2 \tan^{-1} \left[ \cot \frac{\gamma}{2} \tanh v_j \right], \quad (7)$$

and taking logarithm of the Bethe ansatz equation (5), we have

$$-\Phi_{2\xi^+ + \gamma}(v_j) + \Phi_{2\xi - \gamma}(v_j) + \Phi_\gamma(v_j) - \Phi_{\pi + \gamma}(v_j) + 2N\Phi_{2s\gamma}(v_j) + \sum_{k=a,b} \sum_{r=\pm 1} \Phi_{2s_i\gamma}(v_j + rc_k) = 2\pi I_j + \sum_{i=1}^M \{ \Phi_\gamma(v_j - v_i) + \Phi_\gamma(v_j + v_i) \}, \quad (8)$$

where the transformations  $\eta \rightarrow i\gamma$ ,  $\xi \rightarrow i\xi$  and  $\xi^+ \rightarrow i\xi^+$  have been used, and  $I_j$  is an integer. Taking the thermodynamic limit ( $N \rightarrow \infty$ ), the distribution function of particles can be considered as continuous one. So the Bethe ansatz equation can be written as

$$\rho(v) = \frac{1}{2\pi} \left[ \Phi'_{2s\gamma}(v) + \frac{1}{2N} \theta'(v) \right] - \frac{1}{2\pi} \int_{-\infty}^{\infty} dv \Phi'_{2\gamma}(v - \nu) \rho(\nu) \quad (9)$$

where the distribution function is defined by [12]

$$\rho(v) = \frac{dI_j(v)}{dv}, \quad (10)$$

and

$$\theta(v) \equiv -\Phi_{2\xi^++\gamma}(v) + \Phi_{2\xi-\gamma}(v) + \Phi_\gamma(v) + \Phi_{\pi+\gamma}(v_j) + \sum_{k=a,b} \sum_{r=\pm 1} \Phi_{2s_i\gamma}(v + rc_k).$$

Here the  $\theta(v)$  stands for the effects of open boundary condition and magnetic impurities.

Applying the Fourier transformation on eq.(9), we have

$$\begin{aligned} \hat{\rho}(\omega) = & \frac{\sinh(\pi\omega - 2s\gamma\omega)}{2 \sinh(\pi\omega - \gamma\omega) \cosh(\gamma\omega)} + \frac{1}{2N} \left\{ \frac{\cosh(\frac{\pi}{2}\omega - \gamma\omega) \sinh(\frac{\pi}{2}\omega)}{\sinh(\pi\omega - \gamma\omega) \cosh(\gamma\omega)} \right. \\ & + \frac{\cosh[(\pi - \xi - \xi^+)\omega] \sinh[(\xi^+ - \xi + \gamma)\omega]}{\sinh(\pi\omega - \gamma\omega) \cosh(\gamma\omega)} \\ & \left. + B(\omega) \frac{\sinh(\pi\omega - 2s_i\gamma\omega)}{2 \sinh(\pi\omega - \gamma\omega) \cosh(\gamma\omega)} \right\}, \end{aligned} \quad (11)$$

where the  $B(\omega) = 4 \cos[c_a + c_b]\omega \cos[(c_a - c_b)\omega]$ .

The distribution function  $\rho(v)$  can be obtained by

$$\rho(v) = \int_{-\infty}^{\infty} \hat{\rho}(\omega) e^{-2iv\omega} d\omega. \quad (12)$$

The ground state energy per site for our systems can be written as

$$\frac{E}{N} = \frac{E_i}{N} + \frac{E_b}{N} + \frac{E_\infty}{N}. \quad (13)$$

(i). when  $s = \frac{1}{2}$ , after some calculation, we have the ground state energy of the bulk term

$$E_\infty = -N \frac{\cosh \gamma}{\sinh \gamma} + N \int_{-\infty}^{\infty} dv \frac{\sin(\gamma)}{\cosh(2s\gamma) - \cos(2v)} \quad (14)$$

It is exactly same as one in the periodic case [12]. The contributions of the boundary ( $E_b$ ) and the impurities ( $E_i$ ) are

$$\begin{aligned} E_b = & -\frac{\sinh(\xi^+ - \xi)}{2 \sinh \xi^+ \sinh \xi} + \frac{1}{2 \sinh(2\eta)} \\ & - \int_{-\infty}^{\infty} d\omega \frac{\sinh[(\xi^+ - \xi + \gamma)\omega] \cosh[(\pi - \xi^+ - \xi)\omega]}{\sinh(\pi\omega) \cosh(\gamma\omega)} \\ & - \int_{-\infty}^{\infty} d\omega \frac{\cosh(\pi\omega/2 - \gamma\omega) \sinh(\pi\omega/2)}{\sinh(\pi\omega) \cosh(\gamma\omega)} \end{aligned} \quad (15)$$

$$\begin{aligned} E_i = & \frac{i}{2} \sum_{r=\pm 1} \sum_{k=a,b} \coth(rc_k + is_i\gamma + \frac{i\gamma}{2}) \\ & - \int_{-\infty}^{\infty} d\omega \frac{4 \sinh[(\pi - 2s_i\gamma)\omega] \cos[(c_a + c_b)\omega] \cos[(c_a - c_b)\omega]}{\sinh(\pi\omega) \cosh(\gamma\omega)}; \end{aligned} \quad (16)$$

(ii). when  $s = 1$ , similarly, we have

$$\begin{aligned}
E_\infty &= -N \frac{\sinh(3\gamma)}{\sinh \gamma \sinh(2\gamma)} - 2N \frac{\cosh(2\gamma)}{\sinh(2\gamma)} \\
&\quad - N \int_{-\infty}^{\infty} d\omega \frac{\sinh(\pi\omega - 2\gamma\omega)}{2 \sinh(\pi\omega) \cosh(\gamma\omega)}, \\
E_b &= -\frac{\sinh(2\gamma)}{2 \sinh(\xi^+ + \frac{\gamma}{2}) \sinh(\xi^+ - \frac{3\gamma}{2})} + \frac{2 \cosh \gamma}{\sinh(3\gamma)} \\
&\quad - \int_{-\infty}^{\infty} d\omega \frac{\sinh[(\xi^+ - \xi + \gamma)\omega] \cosh[(\pi - \xi^+ - \xi)\omega]}{\sinh(\pi\omega) \cosh(\gamma\omega)} \\
&\quad - \int_{-\infty}^{\infty} d\omega \frac{\cosh(\pi\omega/2 - \gamma\omega) \sinh(\pi\omega/2)}{\sinh(\pi\omega) \cosh(\gamma\omega)} \tag{17}
\end{aligned}$$

$$\begin{aligned}
E_i &= - \sum_{r=\pm 1} \sum_{k=a,b} \frac{i \sinh(2rc_k + 2is_i\gamma + i\gamma)}{2 \sinh(rc_k + is_i\gamma) \sinh(rc_k + is_i\gamma + i\gamma)} \\
&\quad - \int_{-\infty}^{\infty} d\omega \frac{4 \sinh[(\pi - 2s_i\gamma)\omega] \cos[(c_a + c_b)\omega] \cos[(c_a - c_b)\omega]}{\sinh(\pi\omega) \cosh(\gamma\omega)}. \tag{18}
\end{aligned}$$

#### IV. TBA AND PHYSICAL PROPERTIES

It is well known that that the general solution of Bethe ansatz equation (5) in the thermodynamic limit lies in the complex plane and forms strings with the length  $n$  [14,23]:

$$v_j \equiv \lambda_{\alpha,j}^n = \lambda_\alpha^n + i\frac{\gamma}{2}(n+1-2j) \quad (j = 1, 2, \dots, n), \tag{19}$$

where  $n = 1, 2, \dots, \infty$ , and  $\alpha = 1, 2, \dots, M^{(n)}$ . Here the number of  $n$ -strings  $M^{(n)}$  satisfies  $\sum_{n=1}^{\infty} nM^{(n)} = M$ . Substituting the above string solution into eq.(5), we have

$$2N\psi_n^s(\lambda_\alpha^n) + \theta_n(\lambda_\alpha^n) = 2\pi I_\alpha^n + \sum_{m,\beta>0} \left\{ \varphi_{mn}(\lambda_\alpha^n - \lambda_\beta^m) + \varphi_{mn}(\lambda_\alpha^n + \lambda_\beta^m) \right\}. \tag{20}$$

Here,

$$\begin{aligned}
\psi_n^s(\lambda_\alpha^n) &= \begin{cases} \Phi_{n\gamma}(\lambda_\alpha^n) & s = \frac{1}{2} \\ \Phi_{\gamma(n+1)}(\lambda_\alpha^n) + \Phi_{\gamma(n-1)}(\lambda_\alpha^n) & s = 1, \end{cases} \\
\theta_n(\lambda_\alpha^n) &= \Phi_{n\gamma}(\lambda_\alpha^n) - \Phi_{\pi+n\gamma}(\lambda_\alpha^n) - \Phi_{\gamma(n-\frac{2}{\gamma}\xi^+-2j)}(\lambda_\alpha^n) + \Phi_{\gamma(n+\frac{2}{\gamma}\xi-2j)}(\lambda_\alpha^n) \\
&\quad + \sum_{r,k} \Phi_{\gamma(n+2s_i+1-2j)}(\lambda_\alpha^n + rc_k) \\
\varphi_{mn}(\lambda_\alpha^n \pm \lambda_\beta^m) &= (1 - \delta_{mn})\Phi_{\gamma|m-n|}(\lambda_\alpha^n \pm \lambda_\beta^m) + 2\Phi_{\gamma(|m-n|+2)}(\lambda_\alpha^n \pm \lambda_\beta^m) \\
&\quad + \dots + 2\Phi_{\gamma(|m+n|-2)}(\lambda_\alpha^n \pm \lambda_\beta^m) + \Phi_{\gamma(m-n)}(\lambda_\alpha^n \pm \lambda_\beta^m)
\end{aligned}$$

Under the thermodynamic limit, according to [14], we obtain the following equation

$$\rho_n^h(\lambda) = \frac{1}{2\pi}[(\psi_n^s)'(\lambda) + \frac{1}{2N}\theta_n'(\lambda)] - \sum_{m \geq 1} \int_{-\infty}^{\infty} d\mu A_{nm}(\lambda - \mu)\rho_n(\mu), \quad (21)$$

where  $\rho_n$  and  $\rho_n^h$  are the distribution functions of the particle and the hole respectively, and

$$A_{nm}(\lambda - \mu) = \frac{1}{2\pi}[\varphi'_{nm} + 2\pi\delta_{nm}\delta(\lambda - \mu)].$$

The energy of per cite can be written as

$$\frac{E}{N} = \frac{1}{N}E_f^s - \sum_{n \geq 1} \int_{-\infty}^{\infty} d\lambda (\psi_n^s)'(\lambda)\rho_n(\lambda), \quad (22)$$

where

$$E_f^s = E_b^s + E_i^s + \begin{cases} N \cosh \eta & s = \frac{1}{2} \\ N \frac{\sinh(3\eta)}{\sinh} \eta + 2N \cosh(2\eta) & s = 1 \end{cases}$$

The entropy of per cite can be obtained after we analysis the distributions of particles and holes. It reads

$$\frac{S}{N} = \sum_{n \geq 1} \int_{-\infty}^{\infty} d\lambda \{(\rho_n(\lambda) + \rho_n^h(\lambda)) \ln(\rho_n(\lambda) + \rho_n^h(\lambda)) - \rho_n(\lambda) \ln \rho_n(\lambda) - \rho_n^h(\lambda) \ln \rho_n^h(\lambda)\}. \quad (23)$$

The eigenvalue of the spin z-projection can be obtained with the so-called Bethe vector.

With the distribution function, we have

$$\frac{s^z}{N} = s + \frac{2}{N}s_i - \sum_{n \geq 1} n \int_{-\infty}^{\infty} \rho_n(\lambda) d\lambda \quad (24)$$

In order to find the equilibrium distribution functions at the finite temperature  $T$ , we must minimize the free energy

$$F = E - TS - HS^z \quad (25)$$

with  $\delta F = 0$  subject to the constrain eq. (22). Then we obtain the thermodynamic Bethe ansatz (TBA) equation

$$\ln\left(1 + \frac{\hat{\rho}_n^h(\omega)}{\hat{\rho}_n(\omega)}\right) = \frac{1}{T}(Hn - \frac{1}{2}(\psi_n^s)'(\omega)) + \sum_{m \geq 1} \hat{A}_{nm} \ln\left(1 + \frac{\hat{\rho}_n(\omega)}{\hat{\rho}_n^h(\omega)}\right), \quad (26)$$

where symbols with a hat are results after Fourier transformation on them, and

$$\hat{A}_{nm}(\omega) = \frac{2 \coth(\gamma\omega) \sinh[\min(m, n)\gamma\omega] \sinh[\pi\omega - \max(m, n)\gamma\omega]}{\sinh(\pi\omega)}, \quad (27)$$

$$\hat{A}_{nm}^{-1}(\omega) = \delta_{nm} - \frac{1}{2 \cosh(\gamma\omega)} (\delta_{n,m+1} + \delta_{n,m-1}). \quad (28)$$

Define

$$\hat{\varepsilon}_n(\omega) = T \ln \frac{\hat{\rho}_n^h(\omega)}{\hat{\rho}_n(\omega)}. \quad (29)$$

Then, the above TBA equation can be rewritten as

$$\ln(1 + e^{\hat{\varepsilon}_n(\omega)/T}) = \frac{1}{T} (Hn - \frac{1}{2}(\psi_n^s)'(\omega)) + \sum_{m \geq 1} \hat{A}_{nm} \ln(1 + e^{-\hat{\varepsilon}_n(\omega)/T}) \quad (30)$$

Solving the  $\hat{\varepsilon}_n(\omega)$  from the above equation, we have

$$\hat{\varepsilon}_1(\omega) = T\hat{p} \ln(1 + e^{\hat{\varepsilon}_{n+1}(\omega)/T}) \quad (31)$$

$$\hat{\varepsilon}_n(\omega) = T\hat{p} \ln[(1 + e^{\hat{\varepsilon}_{n+1}(\omega)/T})(1 + e^{\hat{\varepsilon}_{n-1}(\omega)/T})] - \pi\hat{p}\delta_{n,2s} \quad (32)$$

where  $\hat{p} \equiv \frac{1}{2 \cosh(\gamma\omega)}$ . From eq. (28), it is easy to find that

$$\lim_{n \rightarrow \infty} \frac{\varepsilon_n}{n} = H. \quad (33)$$

Taking into account (26) and (27), the free energy per site at equilibrium state is given by

$$\begin{aligned} \frac{F}{N} &= \frac{1}{N} E_f - 2 \tan(2n\gamma) - H(s + \frac{1}{N} s_i) \\ &\quad - \frac{T}{2\pi} \sum_{n \geq 1} \int_{-\infty}^{\infty} d\lambda (\psi_n^s)'(\lambda) \ln(1 + e^{-\varepsilon_n(\lambda)/T}) \\ &\quad - \frac{1}{N} \frac{T}{2\pi} \sum_{n \geq 1} \int_{-\infty}^{\infty} d\lambda \frac{\theta_n'(\lambda)}{(\psi_n^s)'(\lambda)} (\psi_n^s)'(\lambda) \ln(1 + e^{-\varepsilon_n(\lambda)/T}) \end{aligned} \quad (34)$$

We can now obtain the specific heat in the condition  $T \rightarrow 0$ ,  $H = 0$ , and the magnetic susceptibility at the small magnetic field by using the following formulas

$$C_s = -T \frac{\partial}{\partial T} \left( \frac{S}{N} \right) \Big|_H = -T \frac{\partial^2}{\partial T^2} \left( \frac{F}{N} \right) \Big|_H \quad (35)$$

$$\chi_s = -\frac{\partial^2}{\partial H^2} \left( \frac{F}{N} \right) \Big|_T \quad (36)$$



Substituting eq.(34) into eq.(35) and (36), we find that the former three terms are zero and the fourth term is exactly same as the periodic case which has been discussed in Ref. [15,18–20]. Then, we shall discuss the last term of the eq. (34). As before, the  $\theta_n(\lambda)$  can be divided into the boundary and the impurity terms

$$\theta_n^b(\lambda) = \Phi_{n\gamma}(\lambda_\alpha^n) - \Phi_{\pi+n\gamma}(\lambda_\alpha^n) - \Phi_{\gamma(n-\frac{2}{\gamma}\xi+2j)}(\lambda_\alpha^n) + \Phi_{\gamma(n+\frac{2}{\gamma}\xi-2j)}(\lambda_\alpha^n), \quad (37)$$

$$\theta_n^i(\lambda) = \sum_{r,k} \Phi_{\gamma(n+2s_i+1-2j)}(\lambda_\alpha^n + rc_k). \quad (38)$$

Then, the last term of eq.(34) can be rewritten as

$$\begin{aligned} \frac{\tilde{F}}{N} &= -\frac{1}{N} \frac{T}{2\pi} \sum_{n \geq 1} \int_{-\infty}^{\infty} d\lambda \frac{(\theta_n^b)'(\lambda)}{(\psi_n^s)'(\lambda)} (\psi_n^s)'(\lambda) \ln(1 + e^{-\varepsilon_n(\lambda)/T}) \\ &\quad - \frac{1}{N} \frac{T}{2\pi} \sum_{n \geq 1} \int_{-\infty}^{\infty} d\lambda \frac{(\theta_n^i)'(\lambda)}{(\psi_n^s)'(\lambda)} (\psi_n^s)'(\lambda) \ln(1 + e^{-\varepsilon_n(\lambda)/T}) \\ &= -\frac{1}{N} \frac{T}{2\pi} \sum_{n \geq 1} \int_{-\infty}^{\infty} d\omega \frac{(\hat{\theta}_n^b)'(\omega)}{(\hat{\psi}_n^s)'(\omega)} (\hat{\psi}_n^s)'(\omega) \ln(1 + e^{-\hat{\varepsilon}_n(\omega)/T}) \\ &\quad - \frac{1}{N} \frac{T}{2\pi} \sum_{n \geq 1} \int_{-\infty}^{\infty} d\omega \frac{(\hat{\theta}_n^i)'(\omega)}{(\hat{\psi}_n^s)'(\omega)} (\hat{\psi}_n^s)'(\omega) \ln(1 + e^{-\hat{\varepsilon}_n(\omega)/T}) \end{aligned} \quad (39)$$

In this paper, we mainly discuss the effect of the impurities so here we only give the result about the last term of the eq.(39). For both spin- $\frac{1}{2}$  and spin-1 cases,

$$(\hat{\theta}_n^i)'(\omega) = \begin{cases} 2\pi B(\omega) \frac{\sinh(2s_i\gamma\omega) \sinh(\pi\omega - n\gamma\omega)}{\sinh(\pi\omega) \sinh(\gamma\omega)} & n > 2s_i \\ 2\pi B(\omega) \frac{\sinh(n\gamma\omega) \sinh(\pi\omega - 2s_i\gamma\omega)}{\sinh(\pi\omega) \sinh(\gamma\omega)} & n \leq 2s_i \end{cases}, \quad (40)$$

where  $B(\omega) = 4 \cos[(c_a + c_b)\omega] \cos[(c_a - c_b)\omega]$ . And

$$(\hat{\psi}_n^s)'(\omega) = 2\pi \frac{\sinh(\pi\omega - n\gamma\omega)}{\sinh(\pi\omega)}, \quad (s = \frac{1}{2}) \quad (41)$$

$$(\hat{\psi}_n^s)'(\omega) = 2\pi \frac{2 \cosh(\gamma\omega) \sinh(\pi\omega - n\gamma\omega)}{\sinh(\pi\omega)}. \quad (s = 1) \quad (42)$$

Substituting the results of  $(\hat{\theta}_n^i)'(\omega)$ ,  $(\hat{\psi}_n^s)'(\omega)$  into eq.(39), we can obtain the effect of the impurities to free energy and other physical quantities. However, the calculation is much more complicated than we expected. Fortunately, comparing with the periodic case, we

can obtain the low-temperature specific heat and the magnetic susceptibility contributed by impurities as

$$C_{1/2}^i = \frac{2C_{1/2}^0}{N} \times \cosh \left[ \frac{(c_a + c_b)\pi}{2\gamma} \right] \cosh \left[ \frac{(c_a - c_b)\pi}{2\gamma} \right] \frac{\sin \left[ \pi s_i - \frac{(2K+1)\pi^2}{2\gamma} \right]}{\cos \left( \frac{\pi^2}{2\gamma} \right)}; \quad (43)$$

$$C_1^i = \frac{2C_1^0}{N} \times \cosh \left[ \frac{(c_a + c_b)\pi}{2\gamma} \right] \cosh \left[ \frac{(c_a - c_b)\pi}{2\gamma} \right] \frac{\sin \left[ \pi s_i - \frac{(2K+1)\pi^2}{2\gamma} \right]}{\sin \left( \frac{\pi^2}{2\gamma} \right)}; \quad (44)$$

$$\chi_{1/2}^i = \frac{2\chi_{1/2}^0}{N} \times \cosh \left[ \frac{(c_a + c_b)\pi}{2\gamma} \right] \cosh \left[ \frac{(c_a - c_b)\pi}{2\gamma} \right] \frac{\sin \left[ \pi s_i - \frac{(2K+1)\pi^2}{2\gamma} \right]}{\cos \left( \frac{\pi^2}{2\gamma} \right)}; \quad (45)$$

$$\chi_1^i = \frac{2\chi_1^0}{N} \times \cosh \left[ \frac{(c_a + c_b)\pi}{2\gamma} \right] \cosh \left[ \frac{(c_a - c_b)\pi}{2\gamma} \right] \frac{\sin \left[ \pi s_i - \frac{(2K+1)\pi^2}{2\gamma} \right]}{\sin \left( \frac{\pi^2}{2\gamma} \right)}, \quad (46)$$

therefor, the Kondo temperature can be given by

$$T_{1/2}^k = \cosh^{-1} \left[ \frac{(c_a + c_b)\pi}{2\gamma} \right] \cosh^{-1} \left[ \frac{(c_a - c_b)\pi}{2\gamma} \right] \frac{\cos \left( \frac{\pi^2}{2\gamma} \right)}{2 \sin \left[ \pi s_i - \frac{(2K+1)\pi^2}{2\gamma} \right]}, \quad (47)$$

$$T_1^k = \cosh^{-1} \left[ \frac{(c_a + c_b)\pi}{2\gamma} \right] \cosh^{-1} \left[ \frac{(c_a - c_b)\pi}{2\gamma} \right] \frac{\sin \left( \frac{\pi^2}{2\gamma} \right)}{2 \sin \left[ \pi s_i - \frac{(2K+1)\pi^2}{2\gamma} \right]}, \quad (48)$$

where  $C_s^0$  and  $\chi_s^0$  are the specific heat and magnetic susceptibility of the infinity size system [18,19], and  $K=0, 1, 2, \dots$  determined by the relation  $0 < 2s_i\gamma - 2K\pi < 2\pi$ . One can check the results eq.(43)-(46) to be sound based on the fact the  $c_i$  and  $\chi_i$  proportion to the shift of the state density at Fermi surface which is proportional to  $\rho_i(v)/\rho_\infty(v)$  ( see eq.(11)and (12) ), where  $\rho_i(v)$  and  $\rho_\infty(v)$  are the density of the impurity and the bulk. If we choose  $c_a = c_b$  and  $s_i = 1/2$ , the results of eq.(43), (45) and (47) can recover those in Ref. [10]. In eq.(47) and (48), when  $c \rightarrow ic$ , the Kondo temperature satisfy the relation  $T_s^k \sim \cos^{-1}[(c_a + c_b)\pi/2\gamma] \cos^{-1}[(c_a - c_b)\pi/2\gamma]$ . The result shows a crossover from an exponential law to a power law as the phenomenon in Ref. [2].

## V. DISCUSSION

In this paper, we obtain the contribution of the boundary arbitrary spin impurities to the susceptibility, the specific heat and the Kondo temperature by using the standard method at

low temperature. The model that XXZ chain coupled with boundary impurities is relevant to the Kondo problem in a Luttinger liquid. And the effect of the impurities to the bulk can be regarded as a perturbation to the bulk. From eq.(43)-(46), we can see that the contribution of impurities strongly depend on the coupling constants  $c_i$  ( $i = a, b$ ) and the spin of the impurities  $s_i$ . Also from these equations, the Wilson ratio can be obtained as  $(C_s^i/C_s^0)/(\xi_s^i/\xi_s^0) = 1$  in this model. This fact can prove that the present model satisfies the theory of the Luttinger liquid. Besides the properties discussed in this paper, other properties of the present model are also worth investigating, such as the critical properties of the present model. And we shall study them in our further papers.

## REFERENCES

- [1] C.L.Kane and M.P.A.Fisher, *Phy.Rev.Lett.* **68**, 1220(1992);
- [2] D.-T. Lee and J.Toner. *Phys.Rev.Lett.***69**. 3378 (1992)
- [3] A.Furusaki and N.Nagaosa, *Phys.Rev.Lett.* **72** 892(1994).
- [4] P.Fröjdh and H.Johannesson, *Phys.Rev.Lett.* **75**, 300(1995).
- [5] Y. Wang and J. Voit. *Phys. Rev.lett.* **77**. 4934 (1996) Y. Wang, J. Dai, Z. Hu and F.-C. Pu *ibid* **79**. 1901
- [6] N.Andrei,K.Furuya,and J.A.Lowenstein, *Rev.Mod.Phy.* **55**, 331(1983).
- [7] N.Andrei,and H.Johannesson, *Phys Lett.* **100A** , 108(1984).
- [8] K.Lee and P.Schlottmann *Phys.Rev.B* **37** 379(1987).
- [9] Y.Wang, *Phys.Rev B* **56** 14045(1997).
- [10] Z.Hu,F.Pu, *Phys.Rev.B* **58** R2925(1998).
- [11] B. Hou, K. Shi, R. Yue and S. Zhao in press.
- [12] C.N. Yang and C.P. Yang *Phys. Rev.* **150** 321 (1966); *Phys. Rev.* **150** 327 (1966)
- [13] C.N. Yang *Phys. Rev. Lett.* **19** 1312 (1967).
- [14] C.N. Yang and C.P. Yang *J. Phys* **A10** 1115 (1969).
- [15] M. Takahashi, *Prog. Theor. Phys.* **46** 401 (1971).
- [16] M. Gaudin *Phys. Rev. Lett.* **26** 1301 (1971).
- [17] J.D. Johnson and B.M. McCoy *Phys. Rev.* **A6** 1613 (1972)
- [18] H.M. Babujian *Nucl. Phys.* **B215** 317 (1983).
- [19] A.N. Kirillov and N.Y. Reshetikhin *J. Phys.* **A20** 1565 (1987)

- [20] L. Mezincescu and R.I. Nepomechie cond-mat 9212124. (1990).
- [21] V. Pasquier and H. Saleur Nucl. Phys. **B330** 523 (1990).
- [22] F.C. Alcaraz, M.N. Barber. M.T. Batchelor. R.T. Baxter and G.R.W. Quispei. J. Phys. **A20** 6397 (1987).
- [23] R.J. Baxter Ann. of Phys. **70** 323 (1972).