Magnetic susceptibility and low-temperature specific heat of the integrable one-dimensional Hubbard model under open-boundary conditions

1997 J. Phys. A: Math. Gen. 30 8129

(http://iopscience.iop.org/0305-4470/30/23/013)

J. Phys. A: Math. Gen. **30** (1997) 8129–8138. Printed in the UK PII: S0305-4470(97)84415-0

Magnetic susceptibility and low-temperature specific heat of the integrable one-dimensional Hubbard model under open-boundary conditions

Ruihong Yue† and Tetsuo Deguchi‡

Department of Physics, Faculty of Science, Ochanomizu University, 2-1-1 Ohtsuka, Bunkyo-Ku, Tokyo 112, Japan
Graduate School of Humanities and Sciences, Ochanomizu University, 2-1-1 Ohtsuka, Bunkyo-Ku, Tokyo 112, Japan

Received 22 May 1997

Abstract. The magnetic susceptibility and the low-temperature specific heat of the one-dimensional Hubbard model under the integrable open-boundary conditions are discussed through the Bethe ansatz with the string hypothesis. The contributions of the boundary fields to both the susceptibility and the specific heat are obtained, and their exact expressions are analytically derived.

1. Introduction

The problem of a quantum impurity in three-dimensional (3d) electrons has been a fascinating topic in condensed matter physics. It is related to many nontrivial phenemena such as the Kondo problem. The low-temperature behaviours of the Kondo and the Anderson models are rigorously obtained by the Bethe-ansatz method [1, 2]. Recently, some aspects of the impurity problem in one-dimensional (1d) systems have attracted renewed interest from different branches of physics [3–7]. The motivation of this paper is to investigate the impurity effect in the 1d interacting electrons under integrable boundary conditions.

Generally, it is expected that at low temperature the quantum impurity Hamiltonians are renormalized to critical points which correspond to conformal invariant boundary conditions [4, 5]. In fact, the impurity effects have been discussed from the analysis of the different boundary conditions [6, 8–10]. During the last decade the Bethe-ansatz techniques for integrable open chains have been developed [11–15]. In [9], the magnetization of an anisotropic Heisenberg model with open-boundary conditions was derived. The result is generalized to the supersymmetric t-J model with open boundaries and the bulk and surface magnetizations are obtained [10]. We can also discuss the Bethe-ansatz equations for the 1d Hubbard model under some open-boundary conditions [16–19].

However, the thermodynamic properties of the t–J or Hubbard models have not yet been discussed under the open-boundary condition. It seems that under open boundaries the free energy becomes divergent due to an infinite number of zero modes.

† E-mail address: yue@phys.ocha.ac.jp
‡ E-mail address: deguchi@phys.ocha.ac.jp

Let us discuss one of the most different properties of the 1d impurity effect. In the Kondo problem the Wilson ratio plays an important role [20]. Based on the local Fermi-liquid theory, the local impurity effect in the 3d free electrons is fully characterized by the single parameter which is related to the ratio of the specific heat and the magnetic susceptibility due to the impurity [21]. For the 1d Hubbard model, however, the local impurity effect could not be described by one parameter and it should be highly nontrivial. The low-energy spectrum is given by the Tomonaga–Luttinger liquid, which is completely different from the Fermi liquid. Furthermore, the impurity effect also depends on the Coulomb interaction among the conduction electrons. In this paper, we will evaluate the boundary effects to the magnetic susceptibility and specific heat of the 1d Hubbard model under the open-boundary conditions, which should characterize the impurity effect in the 1d interacting electronic system in the same way as the Wilson ratio does for the Kondo problem.

Let us first review the Hamiltonian on the 1d lattice with L sites [18]

$$\mathcal{H} = -\sum_{j=1}^{L-1}\sum_{\sigma=\uparrow,\downarrow}\left(c^\dagger_{j\sigma}c_{j+1\sigma} + c^\dagger_{j+1\sigma}c_{j\sigma}\right) + U\sum_{j=1}^{L} n_{j\uparrow}n_{j\downarrow} + \mu\sum_{j=1}^{L}(n_{j\uparrow}+n_{j\downarrow})$$
$$-\frac{h}{2}\sum_{j=1}^{L}(n_{j\uparrow}-n_{j\downarrow}) + \sum_{\sigma=\uparrow,\downarrow}(p_{1\sigma}n_{1\sigma} + p_{L\sigma}n_{L\sigma}). \tag{1}$$

Here the symbols $-\mu$ and $-p_{j\sigma}$ ($j = 1$, or L) correspond to the chemical potential and boundary fields, respectively. The symbol U denotes the Coulomb interaction. When $p_{j\uparrow} = p_{j\downarrow}$ (boundary chemical potential) or $p_{j\uparrow} = -p_{j\downarrow}$ (boundary magnetic field) for $j = 1$ and L, we can solve the above Hamiltonian by the Bethe-ansatz method. The solution of N electrons with M down-spins has wavenumbers k_j for $j = 1, \ldots N$ and rapidities v_m for $m = 1 \ldots M$. The Bethe-ansatz equations for it are given in the following [18].

$$\frac{(\mathrm{e}^{-\mathrm{i}k_j}p_{1\uparrow}+1)(\mathrm{e}^{\mathrm{i}k_j}+p_{L\uparrow})}{(\mathrm{e}^{\mathrm{i}k_j}p_{1\uparrow}+1)(\mathrm{e}^{-\mathrm{i}k_j}+p_{L\uparrow})}\mathrm{e}^{\mathrm{i}2k_jL} = \prod_{m=1}^{M}\frac{(\sin k_j - v_m + \mathrm{i}U/4)(\sin k_j + v_m + \mathrm{i}U/4)}{(\sin k_j - v_m - \mathrm{i}U/4)(\sin k_j + v_m - \mathrm{i}U/4)} \tag{2}$$

$$\frac{(\zeta_+ - v_m - \mathrm{i}U/4)(\zeta_- - v_m - \mathrm{i}U/4)}{(\zeta_+ + v_m - \mathrm{i}U/4)(\zeta_- + v_m - \mathrm{i}U/4)}\prod_{n=1,n\neq m}^{M}\frac{(v_m - v_n + \mathrm{i}U/2)(v_m + v_n + \mathrm{i}U/2)}{(v_m - v_n - \mathrm{i}U/2)(v_m + v_n - \mathrm{i}U/2)}$$
$$= \prod_{j=1}^{N}\frac{(v_m - \sin k_j + \mathrm{i}U/4)(v_m + \sin k_j + \mathrm{i}U/4)}{(v_m - \sin k_j - \mathrm{i}U/4)(v_m + \sin k_j - \mathrm{i}U/4)} \tag{3}$$

where

$$\zeta_+ = \begin{cases} \infty & \text{for } p_{1\uparrow} = p_{1\downarrow} \\ -\dfrac{1-p_{1\uparrow}^2}{2\mathrm{i}p_{1\uparrow}} & \text{for } p_{1\uparrow} = -p_{1\uparrow} \end{cases} \qquad \zeta_- = \begin{cases} \infty & \text{for } p_{L\uparrow} = p_{L\downarrow} \\ -\dfrac{1-p_{L\uparrow}^2}{2\mathrm{i}p_{L\uparrow}} & \text{for } p_{L\uparrow} = -p_{L\uparrow}. \end{cases} \tag{4}$$

In [18] the Bethe-ansatz equations (2) and (3) are systematically derived by using the reflection equations.

2. The magnetic susceptiblity

Now, we discuss the derivation of the magnetic susceptibility of the Hamiltonian (1) at zero temperature. We shall evaluate the boundary contributions to the susceptibility using the method of [22] where the susceptibility is derived under periodic boundary condition. For the evaluation of the susceptibility we assume that the electron density $n = N/L$ is less than half-filling ($0 < n < 1$).

Let us consider the ground states of the open-boundary Hubbard model for the repulsive ($U > 0$) and attractive ($U < 0$) cases. The equations (2) and (3) hold for positive and negative values of U. However, the ground-state solutions of the Bethe-ansatz equations are different for the two cases. For $U > 0$, we may consider only the case when the ground state is characterized by real k_j's and real v_m's†. For $U < 0$, we may assume that the electrons may form singlet bound pairs in the ground state; the ground-state solution of the Bethe-ansatz equations consists of real k_j's, real v_m's and pairs of complex momenta $k_n^{\pm}$

$$\sin(k_n^{\pm}) = v_n \pm \mathrm{i}u \tag{5}$$

where $u = |U|/4$.

We solve the Bethe-ansatz equations based on the assumptions of the ground state. Hereafter, a subscript $r =$ '$>$' ($r =$ '$<$') stands for the positive (negative) U case. For the positive U case, let $\rho_{>,L}(k)_1$ and $\rho_{>,L}(v)_2$ denote the densities of electron momenta k_j and that of down-spin rapidities v_m, respectively. For the negative U case, we denote by $\rho_{<,L}(k)_1$ and $\rho_{<,L}(v)_2$, the densities of real momenta k_j and that of the string centres v_m, respectively [22]. We denote by $\boldsymbol{\rho}_{r,L}$ the vector of the densities $\boldsymbol{\rho}_{r,L} = (\rho_{r,L}(k)_1, \rho_{r,L}(v)_2)$ for $r =>, <$. We now take the asymptotic expansion with respect to $1/L$. Then, we have the following integral equation

$$\boldsymbol{\rho}_{r,L}(k, v) = \boldsymbol{\rho}^0_{r,L}(k, v) + \boldsymbol{K}_r(k, v|k', v')\boldsymbol{\rho}_{r,L}(k', v'). \tag{6}$$

Here the initial values of the densities $\boldsymbol{\rho}^0_{r,L}(k, v) = \boldsymbol{\rho}^0_{r,\infty}(k, v) + \boldsymbol{\tau}^0_r/L$ are given by

$$\boldsymbol{\rho}^0_{>,\infty}(k, v) = \begin{pmatrix} \frac{1}{\pi} \\ 0 \end{pmatrix} \qquad \boldsymbol{\tau}^0_{>}(k, v) = \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}k} P_{>,0}(k) \\ \frac{\mathrm{d}}{\mathrm{d}v} Q_{>,0}(v) \end{pmatrix} \tag{7}$$

$$\boldsymbol{\rho}^0_{<,\infty}(k, v) = \begin{pmatrix} \frac{1}{\pi} \\ \frac{2}{\pi}\,\mathrm{Re}\,\frac{1}{\sqrt{1-(v-\mathrm{i}u)^2}} \end{pmatrix} \qquad \boldsymbol{\tau}^0_{<}(k, v) = \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}k} P_{<,0}(k) \\ \frac{\mathrm{d}}{\mathrm{d}v} Q_{<,0}(v) \end{pmatrix}. \tag{8}$$

The definitions of $\mathrm{d}/\mathrm{d}k\, P_{r,0}(\mathrm{k})$ and $\mathrm{d}/\mathrm{d}v\, Q_{r,0}(v)$ will be given in equation (20) for $r =>$‡, while for $r =<$ they are given in the following:

$$\begin{aligned} 2\pi \frac{\mathrm{d}}{\mathrm{d}k} P_{<,0}(k) &= \frac{2(1 + p_{L\uparrow} \cos k)}{1 + p_{L\uparrow}^2 + 2p_{L\uparrow} \cos k} - \frac{2p_{1\uparrow}(p_{1\uparrow} + \cos k)}{1 + p_{1\uparrow}^2 + 2p_{1\uparrow} \cos k} + \frac{2u \cos k}{\sin^2 k + u^2} \\ 2\pi \frac{\mathrm{d}}{\mathrm{d}v} Q_{<,0}(v) &= \mathrm{Re}\left(\frac{1 + p_{L\uparrow}\sqrt{1 - (v - \mathrm{i}u)^2}}{1 + p_{L\uparrow}^2 + 2p_{L\uparrow}\sqrt{1 - (v - \mathrm{i}u)^2}} \frac{2}{\sqrt{1 - (v - \mathrm{i}u)^2}} \right) \\ &\quad - \mathrm{Re}\left(\frac{p_{1\uparrow} + \sqrt{1 - (v - \mathrm{i}u)^2}}{1 + p_{1\uparrow}^2 + 2p_{1\uparrow}\sqrt{1 - (v - \mathrm{i}u)^2}} \frac{2p_{1\uparrow}}{\sqrt{1 - (v - \mathrm{i}u)^2}} \right) \\ &\quad + \frac{4u}{v^2 + 4u^2} + \frac{2(u + \mathrm{i}\zeta_+)}{v^2 + (u + \mathrm{i}\zeta_+)^2} + \frac{2(u + \mathrm{i}\zeta_-)}{v^2 + (u + \mathrm{i}\zeta_-)^2}. \end{aligned} \tag{9}$$

We note that the kernel $\boldsymbol{K}_>$ was given in [18] and $\boldsymbol{K}_< = \sigma^3 \boldsymbol{K}_> \sigma^3$ [22]. The parameters Q and B [18] for the upper or lower bounds of the integral intervals have the following

† For some values of the boundary fields, the Bethe-ansatz equations may have pure imaginary solutions (boundary bound states) for the ground state.

‡ $\mathrm{d}/\mathrm{d}v\, Q_{>,0}(v)$ is given by $\mathrm{d}/\mathrm{d}v\, Q_0^n(v)$ of $n = 1$ in equation (20).

constraints

$$\int_{-Q}^{Q} \rho_{>,L}(k)_1\,\mathrm{d}k = 2n + \frac{1}{L} \qquad \int_{-B}^{B} \rho_{>,L}(v)_2\,\mathrm{d}v = n - 2s + \frac{1}{L}$$
$$\int_{-Q}^{Q} \rho_{<,L}(k)_1\,\mathrm{d}k = 4s + \frac{1}{L} \qquad \int_{-B}^{B} \rho_{<,L}(v)_2\,\mathrm{d}v = n - 2s + \frac{1}{L} \tag{10}$$

where s has been defined by $s = (N - 2M)/2L$. The ground-state energy E_r for $r =>, <$ is given by

$$\frac{E_>}{L} = \frac{1}{L}[1 - \mu_s - h/2] + (\boldsymbol{e}^0_>, \boldsymbol{\rho}_{>,L})$$
$$\frac{E_<}{L} = \frac{1}{L}[1 - \mu_s - \mu + 2\sqrt{1+u^2}] + (\boldsymbol{e}^0_<, \boldsymbol{\rho}_{<,L}) \tag{11}$$

where $\mu_s = \mu/2 - h/4$. The dressed energy $\boldsymbol{e}_r$ satisfies $\boldsymbol{e}_r = \boldsymbol{e}^0_r + \boldsymbol{K}^T_r \boldsymbol{e}_r$ with the initial values

$$\boldsymbol{e}^0_> = \begin{pmatrix} \mu_s - \cos k \\ h/2 \end{pmatrix} \qquad \boldsymbol{e}^0_< = \begin{pmatrix} \mu_s - \cos k \\ -2\,\mathrm{Re}\sqrt{1 - (v - \mathrm{i}u)^2} \end{pmatrix}. \tag{12}$$

By minimizing the ground-state energy with respect to the variable s, we have the following functional relation between s and h through the constraints (10).

$$h = 2\frac{\epsilon_r(Q)_1\zeta_r(B)_2 - \epsilon_r(B)_2\zeta_r(Q)_1}{\det \xi_r(Q, B)} \qquad \text{for } r =>, < . \tag{13}$$

The dressed charge matrix $\boldsymbol{\xi}_r$ is defined by the relation $\boldsymbol{\xi}_r(k, v) = \mathbf{1} + \boldsymbol{K}^T_r(k, v|k', v')\boldsymbol{\xi}_r(k', v')$, and the symbols $\zeta_{r,j}$ are given by the matrix elements of the dressed charge $\boldsymbol{\xi}_r$ as follows; when $r =>$ $\zeta_{>,j} = (\xi_>)_{j1}$ for $j = 1, 2$, and when $r =<$ $\zeta_{<,j} = (\xi_<)_{j1} + 2(\xi_<)_{j2}$ for $j = 1, 2$. The symbols $\boldsymbol{\epsilon}_r$ are defined by

$$\boldsymbol{\epsilon}^0_> = \boldsymbol{e}^0_> + \begin{pmatrix} h/4 \\ -h/2 \end{pmatrix} \qquad \boldsymbol{\epsilon}^0_< = \boldsymbol{e}^0_< + \begin{pmatrix} h/4 \\ 0 \end{pmatrix}. \tag{14}$$

We can calculate the magnetization s through equations (13) and (10). We thus derive the magnetic susceptibility $\chi_{r,L}$ of the finite lattice of L sites, for the $r =>$ and $r =<$ cases. Here L is a large but finite number.

$$\chi_{r,L} = \left\{ \frac{\partial h}{\partial Q}\frac{\partial Q}{\partial S} + \frac{\partial h}{\partial B}\frac{\partial B}{\partial S} \right\}^{-1} = \left\{ \frac{2v_{r,1}(Q)}{\rho_{r,L}(Q)_1}\frac{\zeta^2_{r,2}(B)}{\det^2 \boldsymbol{\xi}_r(Q, B)} + \frac{2v_{r,2}(B)}{\rho_{r,L}(B)_2}\frac{\zeta^2_{r,1}(Q)}{\det^2 \boldsymbol{\xi}_r(Q, B)} \right\}^{-1}$$
$$\text{for } r =>, < . \tag{15}$$

The Fermi velocities $v_{r,j}$ are given by the jth component of $\boldsymbol{v}_r$ defined by $\boldsymbol{v}_r = \boldsymbol{e}'^0_r + \boldsymbol{K}_r\boldsymbol{v}_r$, where $\boldsymbol{e}'^0_r$ denote the vector whose first and second components are $\mathrm{d}/\mathrm{d}k\, e_r(k)_1$ and $\mathrm{d}/\mathrm{d}v\, e_r(v)_2$, respectively. We note that if we specify the density n and magnetization s, then the parameters Q and B in equation (15) are defined by (10).

Let us discuss the boundary contribution $\delta\chi_r$ to the susceptibility for both the repuslive and attractive cases. We assume that the finite and infinite systems have the same n and s. Then we may formally define $\delta\chi_r$ by the following

$$\delta\chi_r = \chi_{r,L}(Q, B) - \chi_{r,\infty}(Q_\infty, B_\infty) \qquad \text{for } r =>, < . \tag{16}$$

Here Q_∞ and B_∞ are the interval parameters for the infinite system, which are given by eq. (10) after taking the infinite limit: $L \to \infty$. For the case of nonzero magnetic field

($B_\infty \neq \infty$), we may evaluate $\delta B = B - B_\infty$ by taking the derivatives of eq. (10). In terms of the dressed charge we have

$$\begin{pmatrix} \delta Q \\ \delta B \end{pmatrix} = \frac{1}{L} \begin{pmatrix} \xi_{r,22} & -\xi_{r,21} \\ -\xi_{r,12} & \xi_{r,11} \end{pmatrix} \begin{pmatrix} 1 - \int_{-Q_\infty}^{Q_\infty} \tau_r(k)_1 \, \mathrm{d}k \\ 1 - \int_{-B_\infty}^{B_\infty} \tau_r(v)_2 \, \mathrm{d}v \end{pmatrix} \frac{1}{\det \boldsymbol{\xi}_r} \qquad \text{for } r =>, < . \tag{17}$$

Here the matrix elements of the dressed charge are evaluated at Q_∞ and B_∞. For $U > 0$, by the Wiener–Hopf method we can show that under zero magnetic field B is as large as $\log L$. We also note that for some values of the boundary fields, the magnetization s of the finite system can take a nonzero value under zero magnetic field: $h = 0$, in general.

We find that the boundary contribution $\delta\chi_r$ to the magnetic suceptibility contains both the charge and spin parts. We recall that the densities of the rapidities contain the $1/L$-terms, which come from the open-boundary condition. We note that under the periodic boundary condition, the finite-size corrections of the densities do not have $1/L$-terms; the first nonzero order is given by $1/L^2$-terms. Therefore, the $1/L$-term together with δQ and δB will reflect the effect of the open-boundary conditions. It seems that the result is different from the perturbative calculation of the $\delta\chi$ in [7]. However, the $\delta\chi$ in [7] is obtained by using the bosonization method, where some limiting procedures are employed. Thus, it is not easy to point out the most important reason why they are different. We shall discuss this possible discrepancy in later publications.

3. The specific heat

In the rest of the paper, we show how to calculate the low-temperature specific heat of the open-boundary Hubbard model. We consider only the repulsive case ($U > 0$). For the negative U case, we can derive similar results making use of the particle–hole transformation. Under the zero boundary fields case, the Bethe-ansatz equations (2) and (3) are equivalent to those of the periodic case. Thus, the solutions of the Bethe-ansatz equations have the same structure such as in the periodic Hubbard model [23]. There are both real and complex solutions for the momentum k_j and rapility v_m. They can be classified into three groups: real momenta k, n-λ strings and n-λ-k strings. The n-λ string solution for the rapidity v is given by

$$\lambda_m^{n,j} = \lambda_m + \mathrm{i}u(n + 1 - 2j) \qquad j = 1, \ldots, n. \tag{18}$$

The n-λ-k string solutions for the momentum k and the rapidity v are defined by

$$\begin{aligned} &\lambda_m^{\prime n,j} = \lambda'_m + \mathrm{i}u(n + 1 - 2j) \qquad j = 1, \ldots, n \\ &k_m^{n,2j+1} = \pi - \sin^{-1}(\lambda'_m + \mathrm{i}u(n - 2j)) \qquad 0 \leqslant j \leqslant n - 1 \\ &k_m^{n,2j} = \sin^{-1}(\lambda'_m + \mathrm{i}u(n - 2j)) \qquad 1 \leqslant j \leqslant n - 1 \\ &k_m^{n,2n} = \pi - \sin^{-1}(\lambda'_m - \mathrm{i}un). \end{aligned} \tag{19}$$

Here λ_n and λ'_n are the centres of an n-λ string and an n-λ-k string, respectively. The symbols M_n, M'_n and M' are the numbers of n-λ strings, n-λ-k strings and the all λ-k strings, respectively. The k_j's form real momenta for $j = 1, \ldots, N - 2M'$. We note $M' = \sum_n nM'_n$. We recall $u = U/4$. In this paper, we only consider the case where all solutions are given by the three groups with the strings.

Taking the asymptotic expansion (up to the order of $1/L$), we can derive the following integral equations of the densities of particles and holes from the Bethe-ansatz equations

(2) and (3).

$$
\begin{aligned}
\rho^h(k) &= -\rho(k) + \frac{1}{\pi} + \frac{1}{L}\frac{\mathrm{d}}{\mathrm{d}k}P_0(k) + \sum_{n=1}^{\infty}\int \theta_n'(\sin k - \lambda)\cos k(\sigma_n(\lambda) + \tilde{\sigma}_n(\lambda))\,\mathrm{d}\lambda \\
\sigma_n^h(\lambda) &= \frac{1}{L}\frac{\mathrm{d}}{\mathrm{d}\lambda}Q_0^n(\lambda) + \int \theta_n'(\sin k - \lambda)\rho(k)\,\mathrm{d}k - \sum_{m=1}^{\infty} A_{nm}\sigma_m(\lambda) \\
\tilde{\sigma}_n^h(\lambda) &= \frac{2}{\pi}\,\mathrm{Re}\left(\frac{1}{\sqrt{1-(\lambda - \mathrm{i}nu)^2}}\right) + \frac{1}{L}\frac{\mathrm{d}}{\mathrm{d}\lambda}\tilde{Q}_0^n(\lambda) \\
&\quad + \int \theta_n'(\sin k - \lambda)\rho(k)\,\mathrm{d}k - \sum_{m=1}^{\infty} A_{nm}\tilde{\sigma}_m(\lambda) \\
P_0(k) &= \frac{1}{2\pi\mathrm{i}}\log\frac{(1+p_{1\uparrow}\mathrm{e}^{-\mathrm{i}k})(p_{L\uparrow}+\mathrm{e}^{\mathrm{i}k})}{(1+p_{1\uparrow}\mathrm{e}^{\mathrm{i}k})(p_{L\uparrow}+\mathrm{e}^{-\mathrm{i}k})} - \sum_{m=1}^{\infty}\theta_m(\sin k)(2-\delta(M_m,0)-\delta(M_m',0))
\end{aligned} \tag{20}
$$

$$
\begin{aligned}
Q_0^n(\lambda) &= \sum_{m=1}^{\infty}\Theta_{nm}(\lambda)(1-\delta(M_m,0)) \\
&\quad - \frac{1}{2\pi\mathrm{i}}\sum_{j=1}^{n}\log\frac{(\lambda+\zeta_+ + \mathrm{i}u(n-2j))(\lambda+\zeta_- + \mathrm{i}u(n-2j))}{(\lambda-\zeta_+ - \mathrm{i}u(n-2j))(\lambda+\zeta_- - \mathrm{i}u(n-2j))} \\
\tilde{Q}_0^n(\lambda) &= \sum_{m=1}^{\infty}\Theta_{nm}(\lambda)(1-\delta(M_m',0)) - \frac{1}{2\pi\mathrm{i}}\sum_{j=1}^{2n}\log\frac{(1+p_{1\uparrow}\mathrm{e}^{-\mathrm{i}k^{n,j}})(p_{L\uparrow}+\mathrm{e}^{\mathrm{i}k^{n,j}})}{(1+p_{1\uparrow}\mathrm{e}^{\mathrm{i}k^{n,j}})(p_{L\uparrow}+\mathrm{e}^{-\mathrm{i}k^{n,j}})} \\
&\quad + \frac{1}{2\pi\mathrm{i}}\sum_{j=1}^{n}\log\frac{(\lambda+\zeta_+ + \mathrm{i}u(n-2j))(\lambda+\zeta_- + \mathrm{i}u(n-2j))}{(\lambda-\zeta_+ - \mathrm{i}u(n-2j))(\lambda+\zeta_- - \mathrm{i}u(n-2j))} \\
A_{nm}f(x) &= \delta_{nm}f(x) + \frac{\partial}{\partial x}\int \Theta_{nm}(x-x')f(x')\,\mathrm{d}x'
\end{aligned}
$$

where $\theta_n(x) = 2\tan^{-1}(x/nu)/2\pi$ and $\Theta_{nm}(x) = (1-\delta_{nm})\theta_{|n-m|}(x) + 2\theta_{|n-m|+2}(x) + \cdots + 2\theta_{n+m-2}(x) + \theta_{n+m}(x)$. The symbol $\delta(j,k)$ denotes the Kronecker delta. We note that ρ, σ_n and $\tilde{\sigma}_n$ are the particle densities of the real momenta k_j's, the centres of the n-Λ strings, and the centres of the n-Λ-k strings, respectively; ρ^h, σ_n^h and $\tilde{\sigma}_n^h$ are the hole densities of them, respectively. It is remarked that in the derivation of the Bethe-ansatz equations (20), we have assumed that the string solutions for the finite system could have small deviations from those of the infinite system given in (19).

The total energy E of the system is given by

$$
\begin{aligned}
\frac{E}{L} &= \frac{1}{L}\left((1-\mu_s)(1-\delta(N,2M')) - \frac{h}{2}\sum_{n=1}^{\infty}n(1-\delta(M_n,0))\right) \\
&\quad - \frac{1}{L}\sum_{n=1}^{\infty}\left(2\sqrt{1+(nu)^2}+n\mu\right)(1-\delta(M_n',0)) + \int_{-\pi}^{\pi}(\mu_s - \cos k)\rho(k)\,\mathrm{d}k \\
&\quad + \frac{h}{2}\sum_{n=1}^{\infty}n\int_{-\infty}^{\infty}\sigma_n(\lambda)\,\mathrm{d}\lambda + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty}2\,\mathrm{Re}\left(\sqrt{1-(\lambda-\mathrm{i}nu)^2}+n\mu\right)\tilde{\sigma}_n(\lambda)\,\mathrm{d}\lambda.
\end{aligned} \tag{21}
$$

It should be emphasized that the sums for the zero modes in (21) do not become infinite because we take L a large but finite number.

Minimizing the thermodynamic potential $\Omega = E - TS$, we can show the following thermal Bethe-ansatz equations for the ratios of the particle and hole densities $\zeta = \rho^h/\rho$, $\eta_n = \sigma_n^h/\sigma_n$, and $\tilde{\eta}_n = \tilde{\sigma}_n^h/\tilde{\sigma}_n$:

$$\begin{aligned}
\ln\zeta(k) &= -\frac{2\cos k}{T} + \int_{-\infty}^{\infty} \operatorname{sech}\left(\frac{\pi(\lambda - \sin k)}{2u}\right)\left(\ln\frac{1+\tilde{\eta}_1}{1+\eta_1} - \frac{4\,\mathrm{Re}(\sqrt{1-(\lambda - \mathrm{i}u)^2}}{T}\right)\frac{\mathrm{d}\lambda}{4u} \\
\ln\eta_1(\lambda) &= s * \left(\ln(1+\eta_2(\lambda)) - \int_{-\pi}^{\pi} \ln(1+\zeta^{-1}(k)\cos k\,\delta(\lambda - \sin k)\,\mathrm{d}k\right) \\
\ln\tilde{\eta}_1(\lambda) &= s * \left(\ln(1+\tilde{\eta}_2(\lambda)) - \int_{-\pi}^{\pi} \ln(1+\zeta(k)\cos k\,\delta(\lambda - \sin k)\,\mathrm{d}k\right) \\
\ln\eta_n(\lambda) &= s * (\ln(1+\eta_{n+1}(\lambda)) + \ln(1+\zeta_{n-1}(\lambda))) \\
\ln\tilde{\eta}_n(\lambda) &= s * (\ln(1+\tilde{\eta}_{n+1}(\lambda)) + \ln(1+\tilde{\zeta}_{n-1}(\lambda))) \\
\ln\eta_n(\lambda) &\overset{n\to\infty}{=} n\frac{h}{T} \\
\ln\tilde{\eta}_n(\lambda) &\overset{n\to\infty}{=} n\frac{4u+2\mu}{T}
\end{aligned} \tag{22}$$

where the convolution $s*$ is given by $s * f(x) = \int(\operatorname{sech}(\pi(x-x')/2u)/4u)\,f(x')\,\mathrm{d}x'$. The last two limits in (22) should be understood as the asymptotic limit of n consistent with that of $1/L$; the notation $n \to \infty$ means that n should be taken a very large but finite number. We should note that the variation of the particle and hole densities should be taken over all the positive values of rapidities since they are even functions; we have such as $\rho(k) = \rho(-k)$, and so on: $\sigma(v) = \sigma(-v)$, and $\tilde{\sigma}(v) = \tilde{\sigma}(-v)$, $\rho^h(k) = \rho^h(-k)$, $\sigma^h(v) = \sigma^h(-v)$, and $\tilde{\sigma}^h(v) = \tilde{\sigma}^h(-v)$.

Substituting (20) into Ω we have the asymptotic expansion of the thermodynamic potential $\omega_L = \Omega/L$ with respect to $1/L$

$$\begin{aligned}
\omega_L = \frac{1}{L}&\left((1-\mu_s)(1-\delta(N,2M')) - \frac{h}{2}\sum_{n=1}^{\infty}(1-\delta(M_n,0))\right) \\
&- \frac{1}{L}\sum_{n=1}^{\infty}\left(2\sqrt{1+(nu)^2} + n\mu\right)(1-\delta(M_n',0)) \\
&- \int_{-\pi}^{\pi}\left(\frac{1}{2\pi} + \frac{1}{2L}\frac{\mathrm{d}P_0(k)}{\mathrm{d}k}\right) T\ln(1+\zeta^{-1}(k))\,\mathrm{d}k \\
&- \sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\frac{1}{2L}\frac{\mathrm{d}Q_0^n(\lambda)}{\mathrm{d}\lambda} T\ln(1+\eta_n^{-1}(\lambda))\,\mathrm{d}\lambda \\
&- \sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\left(\frac{1}{\pi}\,\mathrm{Re}(\frac{1}{\sqrt{1-(\lambda - \mathrm{i}nu)^2}} + \frac{1}{2L}\frac{\mathrm{d}\tilde{Q}_0^n(\lambda)}{\mathrm{d}\lambda}\right) \\
&\times T\ln(1+\tilde{\eta}_n^{-1})\,\mathrm{d}\lambda + \mathrm{o}\left(\frac{1}{L}\right).
\end{aligned} \tag{23}$$

We now introduce $\kappa = T\ln\zeta$ and $\epsilon_1 = T\ln\eta_1$. We denote the zero-temperature limits of κ and ϵ_1 by $\kappa^{(0)}$ and $\epsilon_1^{(0)}$, respectively. Hereafter we assume $h \gg T$. We can calculate the specific heat C_L through $C_L = -T\partial^2\omega_L/\partial T^2$. We give the final results:

(a) $-\mu \leqslant -2 - h/2$.

$$\omega_L(T,h,\mu) = \omega_L(0,h,\mu) - \frac{T^{3/2}}{\pi}\left(1+\frac{\delta_f}{L}\right)\int_0^\infty \ln\left(1+\mathrm{e}^{-x^2}\exp\left\{\frac{2+h/2-\mu}{T}\right\}\right)\mathrm{d}x \tag{24}$$

where

$$\delta_f = \begin{cases} 1/(1+p_{L\uparrow}) & p_{L\uparrow} \neq -1 \\ 1/2 & p_{L\uparrow} = -1 \end{cases} - \left\{\begin{pmatrix} p_{1\uparrow}/(1+p_{1\uparrow}) & p_{1\uparrow} \neq -1 \\ 1/2 & p_{1\uparrow} = -1 \end{pmatrix}\right\}.$$

Let C_∞ and δC denote the bulk and the boundary specific heats, respectively. Then from (24), we see the following

$$C_L = C_\infty + \delta C = C_\infty\left(1+\frac{1}{L}\delta_f\right). \tag{25}$$

(b) $\epsilon_1^{(0)}(0) \geqslant 0$, $-\mu > -2 - h/2$.

In this region, the thermodynamic potential is given by

$$\begin{aligned}\omega_L(T,h,\mu) = \omega_L(0,h,\mu) &- \frac{\pi^2 T^2}{12\sin Q}\left(\frac{1}{\pi}+\frac{1}{L}\frac{\mathrm{d}}{\mathrm{d}k}P_0(Q)\right)\\ &-2T^{3/2}\left[g(0)+\frac{1}{L}\delta g(0)\right]\sqrt{\frac{2}{\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2}\epsilon_1^{(0)}(0)}}\int_0^\infty \ln(1+\mathrm{e}^{-x^2}\mathrm{e}^{-\epsilon_1^{(0)}(0)/T})\,\mathrm{d}x\\ g(\lambda) &= \frac{1}{2\pi}\int_{-Q}^{Q}\frac{2u}{(\lambda-\sin k)^2+u^2}\frac{\mathrm{d}k}{2\pi}\\ \delta g(\lambda) &= \frac{1}{2}\int_{-Q}^{Q}\frac{2u}{(\lambda-\sin k)^2+u^2}\frac{\mathrm{d}}{\mathrm{d}k}P_0(k)\frac{\mathrm{d}k}{2\pi}+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\lambda}Q_0^1(\lambda).\end{aligned} \tag{26}$$

Here the parameter Q is the zero of $\kappa^{(0)}(k)$. From this expression, we find the ratio $\delta C/C_\infty$

$$\frac{\delta C}{C_\infty} = \frac{\pi}{L}\frac{\mathrm{d}}{\mathrm{d}k}P_0(Q). \tag{27}$$

(c) $h \geqslant 4(\sqrt{1+u^2}-u)$, $-\mu \geqslant 2 - h/2$.

In this region, we find

$$\begin{aligned}\omega_L(T,h,\mu) = \omega_L(0,h,\mu) &- T^{3/2}\pi^{-1}\left(1+\frac{\pi\frac{\mathrm{d}}{\mathrm{d}k}P_0(\pi)}{L}\right)\int_0^\infty \ln(1+\mathrm{e}^{\alpha}\mathrm{e}^{-x^2})\,\mathrm{d}x\\ &-T^{3/2}4(1+u^2)^{1/4}\pi^{-1}\left(1+\frac{\Gamma}{L}\right)\int_0^\infty \ln(1+\mathrm{e}^{\beta}\mathrm{e}^{-x^2})\,\mathrm{d}x\\ \alpha &= \frac{2+u-h/2}{T} \qquad \beta = -\frac{h-4(\sqrt{1+u^2}-u)}{T}\\ \Gamma &= \frac{\pi\sqrt{1+u^2}}{2}\left[\int_{-\pi}^{\pi}\frac{2u}{\sin^2 k+u^2}\frac{\frac{\mathrm{d}}{\mathrm{d}k}P_0(k)}{2\pi}\,\mathrm{d}k+\frac{\mathrm{d}}{\mathrm{d}\lambda}Q_0^1(0)\right].\end{aligned} \tag{28}$$

(d) $\epsilon_1^{(0)}(0) < 0$, $\kappa^{(0)}(\pi) > 0$.

Let us denote by B the zero of $\epsilon_1^{(0)}(\lambda)$. Then from the thermal Bethe-ansatz equations (23), we obtain

$$\omega_L(T,h,\mu) = \omega_L(0,h,\mu) - \frac{\pi^2 T^2}{6\frac{\mathrm{d}}{\mathrm{d}k}\kappa^{(0)}(Q)}\rho_L^c(Q) - \frac{\pi^2 T^2}{6\frac{\mathrm{d}}{\mathrm{d}\lambda}\epsilon_1^{(0)}(B)}\rho_L^s(B) \tag{29}$$

where the density functions are given by $\rho_L^c(k) = \rho_{>,L}(k)_1$ and $\rho_L^s(v) = \rho_{>,L}(v)_2$, where $\boldsymbol{\rho}_{>,L} = (\rho_{>,L}(k)_1, \rho_{>,L}(v)_2)$ is the density for the ground state of the repulsive case. (See also [18].)

(e) $4\sqrt{1+u^2} - u > h \gg T$, $\kappa^{(0)}(\pi) \leqslant 0$.

In this region, the free energy can be evaluated as

$$\begin{aligned} \omega_L(T,\mu,h) = \omega_L(0,\mu,h) - \frac{\pi^2 T^2}{6\frac{\mathrm{d}}{\mathrm{d}\lambda}\epsilon_1^{(0)}(B)}\sigma_1^{(0)}(B) \\ -T^{3/2}\rho_0(\pi)\sqrt{\frac{2}{-\frac{\mathrm{d}^2}{\mathrm{d}k^2}\kappa^{(0)}(\pi)}}\int_0^\infty \ln(1+\mathrm{e}^{\kappa^{(0)}(\pi)/T}\mathrm{e}^{-x^2})\,\mathrm{d}x \end{aligned} \tag{30}$$

where ρ_0 and $\sigma_1^{(0)}$ are defined by

$$\begin{aligned} \sigma_1^{(0)}(\lambda) &= \sigma_0(\lambda) + \int_{|\lambda'|>B} R(\lambda-\lambda')\sigma_1^{(0)}(\lambda')\,\mathrm{d}\lambda \\ \frac{\mathrm{d}}{\mathrm{d}\lambda}\epsilon_1^{(0)}(\lambda) &= \int_{-\pi}^{\pi} s(\sin k-\lambda)\cos k\,\mathrm{d}k + \int_{|\lambda'|>B} R(\lambda-\lambda')\frac{\mathrm{d}}{\mathrm{d}\lambda'}\epsilon_1^{(0)}(\lambda')\,\mathrm{d}\lambda' \\ \sigma_0(\lambda) &= \int_{-\pi}^{\pi}\frac{1}{\pi}s(\lambda-\sin k)\,\mathrm{d}k + \frac{1}{L}\left(\frac{\mathrm{d}}{\mathrm{d}\lambda}Q_0^1(\lambda) + R*\frac{\mathrm{d}}{\mathrm{d}\lambda}Q_0^1(\lambda)\right) \\ &\quad +\frac{1}{L}\int_{-\pi}^{\pi} s(\lambda-\sin k)\left(\frac{\mathrm{d}}{\mathrm{d}k}P_0(k) - \hat{Q}_0(k)\right)\mathrm{d}k \\ \rho_0(k) &= \frac{1}{\pi} + \frac{1}{L}\left(\frac{\mathrm{d}}{\mathrm{d}k}P_0(k) - \hat{Q}_0(k)\right) + \cos k\int_{-\infty}^{\infty} a_1(\sin k-\lambda) \\ &\quad \times\left(\sigma_0(\lambda) - \frac{1}{L}\left[\frac{\mathrm{d}}{\mathrm{d}\lambda}Q_0^1(\lambda) + R*\frac{\mathrm{d}}{\mathrm{d}\lambda}Q_0^1(\lambda)\right]\right)\mathrm{d}\lambda \end{aligned} \tag{31}$$

and $\hat{Q}(k) = \cos k \int s(\sin k - x)\,\mathrm{d}/\mathrm{d}x\, Q_0^1(x)\,\mathrm{d}x$. Here $f * g(x) = \int f(x-x')g(x')\,\mathrm{d}x'$, $s(x) = \mathrm{sech}(\pi x/2u)/4u$ and $R(x) = s * 2u/(2\pi(x^2+u^2))$.

From the low-temperature expansion of the thermodynamic potential, we find the boundary contribution to the specific heat at low temperature

$$\frac{\delta C}{C_\infty} = \frac{1}{L}\begin{cases} \delta_f & \text{case (a)} \\ \pi\dfrac{\mathrm{d}}{\mathrm{d}k}P_0(Q) & \text{case (b)} \\ \dfrac{\pi\frac{\mathrm{d}}{\mathrm{d}k}P_0(\pi)C^{\mathrm{c}} + \Gamma C^{\mathrm{s}}}{C^{\mathrm{c}}+C^{\mathrm{s}}} & \text{case (c)} \\ \left(\dfrac{C^{\mathrm{c}}\tau^{\mathrm{c}}(Q)}{\rho_\infty^{\mathrm{c}}(Q)} + \dfrac{C^{\mathrm{s}}\tau^{\mathrm{s}}(B)}{\rho_\infty^{\mathrm{s}}(B)}\right)\Big/(C^{\mathrm{c}}+C^{\mathrm{s}}) & \text{case (d)} \\ \dfrac{\delta\sigma_1^{(0)}(B)}{\sigma_{1,\infty}^{(0)}(B)} & \text{case (e).} \end{cases} \tag{32}$$

Here C_∞ denotes the bulk specific heat, and C^{c} and C^{s} denote the contributions to the bulk specific heat C_∞ from the charge and spin parts, respectively; $C_\infty = C^{\mathrm{c}} + C^{\mathrm{s}}$. The symbols $\sigma_{1,\infty}^{(0)}(B)$ and $\delta\sigma_1^{(0)}(B)$ are the bulk and the $1/L$ parts of $\sigma_1^{(0)}(B)$.

The boundary contributions to the magnetic susceptibility and the specific heat depend on the boundary fields and the electron density. In regions (a), and (c), the specific heat is proportional to $T^{-3/2}\mathrm{e}^{-\alpha/T}$ where α is a positive constant. In regions (b), (d) and (e), the specific heat depends linearly on temperature. For the boundaries of the regions between (a) and (b), (b) and (c), (b) and (d), (c) and (e), and (d) and (e), the specific heat is proportional to $T^{1/2}$. We recall that for some regions of the boundary fields, there may exist other types of solutions (boundary string states) of the Bethe-ansatz equations [24–28]. We can calculate the contribution from the boundary string states simply by modifying the term τ_r^0 in our derivation.

In summary, we have studied the boundary contributions to the magnetic susceptbility and the specific heat for the 1d Hubbard model under the general open-boundary conditions. They are calculated analytically and explicitly. From the results we can discuss exactly the impurity effect in the 1d Hubbard model or in the interacting electrons in 1d.

Acknowledgments

We are grateful to Dr K Kusakaba for helpful discussion on the boundary bound states. RY obtained a grant from the JSPS foundation and the Monbusho Grant-in-Aid of Japanese Government.

References

[1] Andrei N, Furuya K and Lowenstein J H 1983 *Rev. Mod. Phys.* **55** 331
[2] Tsvelik A M and Wiegmann P B 1983 *Adv. Phys.* **32** 453
[3] Kane C L and Fisher M P A 1992 *Phys. Rev. Lett.* **68** 1220
[4] Eggert S and Affleck I 1992 *Phys. Rev.* B **46** 10 866
[5] Sørensen E S, Eggert S and Affleck I 1993 *J. Phys. A: Math. Gen.* **26** 6757
[6] Affleck I and Ludwig A W W 1992 *Phys. Rev. Lett.* **68** 1046
Affleck I and Ludwig A W W 1993 *Phys. Rev.* B **48** 7297
Affleck I and Ludwig A W W 1991 *Nucl. Phys.* B **360** 641
Affleck I and Ludwig A W W 1994 *J. Phys. A: Math. Gen.* **27** 5375
[7] Furusaki A and Nagaosa N 1994 *Phys. Rev. Lett.* **72** 892
[8] Wong E and Affleck I 1994 *Nucl. Phys.* B **417** 403
[9] de Sa P and Tsvelik A 1995 *Phys. Rev.* B **52** 3067
[10] Essler F H L 1996 *J. Phys. A: Math. Gen.* **29** 6183
[11] Sklyanin E K 1988 *J. Phys. A: Math. Gen.* **21** 2375
[12] Mezincescu L and Nepomechie R I 1991 *J. Phys. A: Math. Gen.* **24** L17
Mezincescu L and Nepomechie R I 1992 *J. Phys. A: Math. Gen.* **25** 2533
[13] Förster A and Karowski M 1993 *Nucl. Phys.* B **396** 611
Förster A and Karowski M 1993 *Nucl. Phys.* B **408** 512
[14] de Vega H J and Gonzalez-Ruiz A 1994 *Nucl. Phys.* B **417** 553
[15] Yue R H, Feng H and Hou B Y 1996 *Nucl. Phys.* B **462** 167
[16] Schulz H 1985 *J. Phys. C: Solid State Phys.* **18** 581
[17] Asakawa H and Suzuki M 1995 *J. Phys. A: Math. Gen.* **29** 225
[18] Deguchi T and Yue R H 1996 *Preprint* OCHA-PP-84
Deguchi T and Yue R H 1997 *Preprint* cond-mat/9704138
[19] Shiroishi M and Wadati M 1997 *J. Phys. Soc. Japan* **66** 1
[20] Wilson K G 1975 *Rev. Mod. Phys.* **47** 773
[21] Noziéres P 1974 *J. Low Temp. Phys.* **17** 31
[22] Woynarovich F and Penc K 1991 *Z. Phys.* B **85** 268
[23] Takahashi M 1969 *Prog. Theor. Phys.* **42** 1098
Takahashi M 1972 *Prog. Theor. Phys.* **47** 69
Takahashi M 1974 *Prog. Theor. Phys.* **52** 103
[24] Skorik S and Saleur H 1995 *J. Phys. A: Math. Gen.* **28** 6605
[25] Kapustin A and Skorik S 1996 *J. Phys. A: Math. Gen.* **29** 1629
[26] Tsuchiya O and Yamamoto T 1997 *J. Phys. Soc. Japan* **66** 1950
[27] Bedürftig G and Frahm H 1997 *J. Phys. A: Math. Gen.* **30** 4139
[28] Essler F H L and Frahm H 1997 *Phys. Rev.* B **56** 6631