Thermodynamic Bethe ansatz equations of one-dimensional Hubbard model and high-temperature expansion

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A numerical method to calculate thermodynmic Bethe ansatz equations is proposed based on Newton's method. Thermodynamic quantities of the one-dimensional Hubbard model are numerically calculated and compared with high-temperature expansion and numerical results of the quantum transfer matrix method by Jüttner, Klümper, and Suzuki. The coincidence is surprisingly good. We obtain the high-temperature expansion of the grand potential up to β^6.

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I. INTRODUCTION

Many years ago, one of the authors (M.T.) proposed thermodynamic Bethe ansatz (TBA) equations for the one-dimensional (1D) Hubbard model.[2] In this theory several kinds of strings are assumed and it is widely believed that this set of equations gives the exact thermodynamic quantities of this model. Low-temperature thermodynamics were investigated by MT,[3] and actual numerical calculations at finite temperature were done by Kawakami, Usuki, and Okiji.[4] Essler, Korepin, and Schoutens[5] counted the number of states by single-k excitations, Λ strings, and k-Λ strings. They found that total number of these Bethe ansatz states and their relatives is 4^{N_a}, where N_a is the length of the systems. This implies that the Bethe ansatz can give all eienstates and eigenvalues. However, some physicists are still skeptical about this theory.[6] Recently Charret *et al.*[7] did a numerical calculation of this equation and concluded that it does not coincide with the high-temperature expansion (HTE) and the quantum transfer matrix (QTM) method by Jüttner, Klümper, and Suzuki.[8] In this paper we give a practical method to calculate numerically the TBA equations which has infinite unknown functions. Numerical results completely coincide with those of the QTM and the HTE methods. The numerical calculation of the TBA equations of Charret *et al.* is wrong. The Hubbard Hamiltonian is

$$\mathcal{H}(t,U,A,h)=-t\sum_{\langle ij\rangle}\sum_{\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})+U\sum_{i=1}^{N_a}c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow}-A\sum_{i=1}^{N_a}(c_{i\uparrow}^{\dagger}c_{i\uparrow}+c_{i\downarrow}^{\dagger}c_{i\downarrow})-h\sum_{i=1}^{N_a}(c_{i\uparrow}^{\dagger}c_{i\uparrow}-c_{i\downarrow}^{\dagger}c_{i\downarrow}). \quad (1)$$

Here $c_{j\sigma}^{\dagger}$ and $c_{j\sigma}$ are creation and annihilation operators of an electron at site j. $\langle ij\rangle$ means that sites i and j are nearest neighbors. N_a is the number of atoms. We put $t>0, U>0$. The thermodynamic potential per site g at temperature T is determined by

$$g=e_0-A-T\left\{\int_{-\pi}^{\pi}\rho_0(k)\ln[1+\zeta(k)]dk+\int_{-\infty}^{\infty}\sigma_0(\Lambda)\ln[1+\eta_1(\Lambda)]d\Lambda\right\}. \quad (2)$$

Here e_0, $\rho_0(k)$, and $\sigma_0(\Lambda)$ are energy per site and distribution functions of k's and Λ's at $T=h=U/2-A=0$ (half-filled, zero-field ground state),

$$e_0=-4t\int_0^{\infty}\frac{J_0(\omega)J_1(\omega)d\omega}{\omega[1+\exp(2U'\omega)]}, \quad (3)$$

$$\sigma_0(\Lambda)=\int_{-\pi}^{\pi}s(\Lambda-\sin k)\frac{dk}{2\pi}, \quad (4)$$

$$\rho_0(k)=\frac{1}{2\pi}+\cos k\int_{-\infty}^{\infty}a_1(\Lambda-\sin k)\sigma_0(\Lambda)d\Lambda, \quad (5)$$

and

$$a_1(x)\equiv\frac{U'}{\pi(U'^2+x^2)},\quad s(x)\equiv\frac{1}{4U'}\mathrm{sech}\frac{\pi x}{2U'},\quad U'\equiv\frac{U}{4t}. \quad (6)$$

$\zeta(k)$ and $\eta_1(\Lambda)$ are hole-particle ratios of k excitations and single-Λ excitations. These are determined by the thermodynamic Bethe ansatz equations for k excitations, Λ strings, and k-Λ strings:

$$\ln\zeta(k)=\frac{\kappa_0(k)}{T}+\int_{-\infty}^{\infty}d\Lambda s(\Lambda-\sin k)\ln\left(\frac{1+\eta_1'(\Lambda)}{1+\eta_1(\Lambda)}\right), \quad (7)$$

$$\ln\eta_1(\Lambda)=s*\ln[1+\eta_2(\Lambda)]-\int_{-\pi}^{\pi}s(\Lambda-\sin k)\times\ln[1+\zeta^{-1}(k)]\cos k dk, \quad (8)$$

$$\ln\eta_1'(\Lambda)=s*\ln[1+\eta_2'(\Lambda)]-\int_{-\pi}^{\pi}s(\Lambda-\sin k)\times\ln[1+\zeta(k)]\cos k dk, \quad (9)$$

$$\ln \eta_j(\Lambda) = s*\ln\{[1+\eta_{j-1}(\Lambda)][1+\eta_{j+1}(\Lambda)]\},\quad j\geqslant 2, \tag{10}$$

$$\ln \eta'_j(\Lambda) = s*\ln\{[1+\eta'_{j-1}(\Lambda)][1+\eta'_{j+1}(\Lambda)]\},\quad j\geqslant 2, \tag{11}$$

$$\lim_{n\to\infty}\frac{\ln \eta_n(\Lambda)}{n} = \frac{2h}{T}, \tag{12}$$

$$\lim_{n\to\infty}\frac{\ln \eta'_n(\Lambda)}{n} = \frac{U-2A}{T}. \tag{13}$$

Here $s*f(\Lambda)\equiv\int_{-\infty}^{\infty}s(\Lambda-\Lambda')f(\Lambda')d\Lambda'$ and $\kappa_0(k)$ is defined by

$$\kappa_0(k)\equiv -2t\cos k - 4t\int_{-\infty}^{\infty}d\Lambda s(\Lambda-\sin k)\times \mathrm{Re}\sqrt{1-(\Lambda-U'i)^2}. \tag{14}$$

Details of the derivation are given in Refs. 1, 2, 9, and 10. Noting that $\ln(1+\zeta^{-1})=\ln(1+\zeta)-\ln\zeta$ in Eq. (8) and substituting Eq. (7) we have

$$\ln \eta_1(\Lambda) = \frac{s_1(\Lambda)}{T} + s*\ln[1+\eta_2(\Lambda)] - \int_{-\pi}^{\pi}s(\Lambda-\sin k)\ln[1+\zeta(k)]\cos k dk,$$

$$s_1(\Lambda)\equiv -2t\int_{-\pi}^{\pi}\cos^2 k s(\Lambda-\sin k)dk. \tag{15}$$

In Ref. 2 this set of equations was solved analytically in the limits $T\to 0$, $t\to 0$, and $U\to 0$ and coincided with known exact results. In a recent paper Charret *et al.*[7] solved numerically this set of equations at high temperature and argued that there is a discrepancy from the high-temperature expansion and the numerical results of the Jüttner-Klümper-Suzuki (JKS) equations.[8] We recalculate the same quantities in this region and find that the results coincide with the high-temperature expansion and the JKS equations to high accuracy. In Sec. III we review the t expansion for the one-dimensional Hubbard model by the conventional linked cluster expansion. From the t expansion, we can derive the β expansion of $-g\beta$ for the 1D Hubbard model up to β^6. Expansions of the susceptibility and specific heat are obtained. In the Appendix, we can perform a t expansion of the TBA equations. The results coincide with the cluster expansion up to second order. We expect that the higher terms also coincide.

II. TRUNCATION OF THE TBA EQUATIONS TO FINITE UNKNOWN FUNCTIONS

As an approximation we replace $s(\Lambda)$ by $\frac{1}{2}\delta(\Lambda)$ at $j>n_c$ in Eqs. (10) and (11). Then we get the difference equations

$$\eta_j(\Lambda)^2 = [1+\eta_{j-1}(\Lambda)][1+\eta_{j+1}(\Lambda)],$$
$$\eta'_j(\Lambda)^2 = [1+\eta'_{j-1}(\Lambda)][1+\eta'_{j+1}(\Lambda)],\quad j>n_c. \tag{16}$$

This approximation is reasonable because the functions $\eta_j(\Lambda)$ and $\eta'_j(\Lambda)$ vary very slowly at sufficiently large j and $\int_{-\infty}^{\infty}s(\Lambda)d\Lambda=1/2$. General solutions of these difference equations are

$$\eta_j(\Lambda) = \left(\frac{\sinh[f(\Lambda)+j]a}{\sinh a}\right)^2 - 1,$$

$$\eta'_j(\Lambda) = \left(\frac{\sinh[g(\Lambda)+j]b}{\sinh b}\right)^2 - 1,\quad j\geqslant n_c. \tag{17}$$

From the conditions (12) and (13), the parameters a and b must be h/T and $(U/2-A)/T$. Then $1+\eta_{n_c+1}(\Lambda)$ and $1+\eta'_{n_c+1}(\Lambda)$ are represented by

$$\left(\cosh\frac{h}{T}\sqrt{1+\eta_{n_c}(\Lambda)}+\sqrt{1+\sinh^2\frac{h}{T}[1+\eta_{n_c}(\Lambda)]}\right)^2,$$

$$\left(\cosh\frac{h'}{T}\sqrt{1+\eta'_{n_c}(\Lambda)}+\sqrt{1+\sinh^2\frac{h'}{T}[1+\eta'_{n_c}(\Lambda)]}\right)^2,$$

$$h'\equiv U/2-A. \tag{18}$$

Thus integral equations with infinite unknown functions are approximated by those with $2n_c+1$ unknowns $\ln\eta'_{n_c}(\Lambda),\dots,\ln\eta'_1(\Lambda),\ln\zeta(k),\ln\eta_1(\Lambda),\dots,\ln\eta_{n_c}(\Lambda)$. Then the equations to be solved are

$$z_1 = s*\ln\{(1+\exp z_2)[\cosh u_2\sqrt{1+\exp z_1}+\sqrt{1+\sinh^2 u_2(1+\exp z_1)}]^2\}, \tag{19}$$

$$z_j = s*\ln(1+\exp z_{j-1})(1+\exp z_{j+1}),\quad j=2,\dots,n_c-1,$$

$$z_{n_c} = s*\ln(1+\exp z_{n_c-1}) - \int_{-\pi}^{\pi}s(\Lambda-\sin k)\ln(1+\exp z_{n_c+1})\cos k dk,$$

$$z_{n_c+1} = u_1\kappa_0 + \int_{-\infty}^{\infty}d\Lambda s(\Lambda-\sin k)\ln\left(\frac{1+\exp z_{n_c}}{1+\exp z_{n_c+2}}\right),$$

$$z_{n_c+2}=u_1s_1+s*\ln(1+\exp z_{n_c+3})-\int_{-\pi}^{\pi}s(\Lambda-\sin k)\ln(1+\exp z_{n_c+1})\cos k dk,$$

$$z_j=s*\ln(1+\exp z_{j-1})(1+\exp z_{j+1}),\quad j=n_c+3,\ldots,2n_c,$$

$$z_{2n_c+1}=s*\ln\{(1+\exp z_{2n_c})[\cosh u_3\sqrt{1+\exp z_{2n_c+1}}+\sqrt{1+\sinh^2 u_3(1+\exp z_{2n_c+1})}]^2\}.$$

We introduce three thermodynamic parameters

$$u_1\equiv 1/T,\quad u_2\equiv(U/2-A)/T,\quad u_3\equiv h/T.$$

For actual numerical calculations we choose L discrete points of k and Λ as follows:

$$k_j=\pi(j-1/2)/L,\quad \Lambda_j=\sin q_j\sqrt{1+\frac{U'^2}{\cos^2 q_j}},$$

$$q_j=\pi(j-1/2)/(2L),\quad j=1,\ldots,L. \tag{20}$$

Here the function $\Lambda=\sin q\sqrt{1+(U'/\cos q)^2}$ is the inverse function of $\int^{\Lambda}\mathrm{Re}[1-(t-U'i)^2]^{-1/2}dt$. We think that this change of parameters is reasonable because the change of functions is very slow at large Λ. For very big U' this function behaves as $U'\tan q$ and for small U' it behaves as $\sin q$. Unknown functions are represented by vectors with length L and integration kernels are represented by $L\times L$ matrices.

Usually this kind of nonlinear equation is calculated by successive iterations, which is called Kepler's method. In the solution of the TBA equations we need to repeat several tens or several hundreds times of iterations to get a good convergence.

So here we propose to use Newton's method. Consider coupled nonlinear equations

$$X_j-F_j(X_1,X_2,\ldots,X_N)=0,\quad j=1,\ldots,N. \tag{21}$$

For approximate vectors $X_j^{(l)}$ assume that we have deviations Δ_j:

$$X_j^{(l)}-F_j(X_1^{(l)},X_2^{(l)},\ldots,X_N^{(l)})=\Delta_j. \tag{22}$$

In Kepler's method the next approximation is

$$X_j^{(l+1)}=X_j^{(l)}+\Delta_j. \tag{23}$$

In Newton's method we put

$$X_j^{(l+1)}=X_j^{(l)}+\xi_j, \tag{24}$$

where ξ_j is a solution of the linear equation

$$\sum_j\left(\delta_{i,j}-\frac{\partial F_i(X_1^{(l)},X_2^{(l)},\ldots,X_N^{(l)})}{\partial X_j}\right)\xi_j=\Delta_i. \tag{25}$$

This method is much faster than Kepler's method. But we must solve linear equations with an $N\times N$ matrix. In our TBA problem, N is $(2n_c+1)L$. This large matrix is block tridiagonal. Regarding $L\times L$ blocks as a number, we can solve this set of linear equations. We need only 5–6 times of iterations at most to get sufficient convergence $\Sigma_j|\Delta_j|<10^{-8}$. We can get the thermodynamic potential through Eq. (2):

$$\frac{g}{T}=\left(e_0-\frac{U}{2}\right)u_1+u_2-\int\rho_0(k)\ln[1+\exp z_{n_c+1}(k)]dk$$
$$-\int\sigma_0(\Lambda)\ln[1+\exp z_{n_c+2}(\Lambda)]d\Lambda. \tag{26}$$

To get the first-order thermodynamic quantities like magnetization (m), electron density (n), and entropy we need to calculate $\partial(g/T)/\partial u_1$, $\partial(g/T)/\partial u_2$, and $\partial(g/T)/\partial u_3$:

$$\partial_i\frac{g}{T}=\left(e_0-\frac{U}{2}\right)\delta_{1i}+\delta_{2i}-\int\rho_0(k)\frac{\partial_i z_{n_c+1}(k)}{1+\exp[-z_{n_c+1}(k)]}dk$$
$$-\int\sigma_0(\Lambda)\frac{\partial_i z_{n_c+2}(\Lambda)}{1+\exp[-z_{n_c+2}(\Lambda)]}d\Lambda. \tag{27}$$

The equation for $\partial_i z_\alpha$ is a linear equation which has the same homogeneous term with that in Newton's method. Inhomogeneous terms are calculated from z_α. Therefore we can calculate these quantities by one operation of linear calculation:

$$e=\partial_1(g/T)+A\partial_2(g/T),$$

$$n=\partial_2(g/T),\quad m=\partial_3(g/T),$$

$$\text{entropy}=u_1(e-g)-u_3m+(u_2-Uu_1/2)n. \tag{28}$$

To calculate the second-order thermodynamic quantities such as specific heat, susceptibility, and compressibility we need the 3×3 tensor $\partial_i\partial_j(g/T)$. As this is a symmetric tensor, we need to calculate six components. We consider equations for

$$f_\alpha^{(ij)}=\partial_i\partial_j z_\alpha+\frac{1}{1+\exp z_\alpha}(\partial_i z_\alpha)(\partial_j z_\alpha),\quad i\leqslant j. \tag{29}$$

The tensor is given by

$$\partial_i\partial_j\frac{g}{T}=-\int\rho_0(k)\frac{f_{n_c+1}^{(ij)}(k)}{1+\exp[-z_{n_c+1}(k)]}dk$$
$$-\int\sigma_0(\Lambda)\frac{f_{n_c+2}^{(ij)}(\Lambda)}{1+\exp[-z_{n_c+2}(\Lambda)]}d\Lambda. \tag{30}$$

The inhomogeneous terms are calculated from z_α and $\partial_i z_\alpha$. So we can calculate thermodynamic quantities from ten quantities g/T and its derivatives for a given temperature, magnetic field, and chemical potential after several times of linear equation solving. The specific heat c in constant n and m, susceptibility χ in constant n and temperature, compressibility κ in constant temperature, and m/n are given by

$$c=u_1^2\left(D_{11}+\frac{D_{13}^2D_{22}+D_{12}^2D_{33}-2D_{12}D_{13}D_{23}}{D_{23}^2-D_{22}D_{33}}\right), \quad (31)$$

$$\chi=u_1\left(D_{33}-\frac{D_{23}^2}{D_{22}}\right),$$

$$\kappa=u_1\left[D_{22}-\frac{(nD_{13}+mD_{22})D_{23}}{nD_{33}+mD_{13}}\right],$$

$$D_{ij}\equiv\partial_i\partial_j(g/T).$$

If we want to calculate thermodynamic quantities at fixed electron density, we can use Newton's method again. Using the compressibility we reach the target density after few times of iterations.

III. t EXPANSION AND β $(=1/T)$ EXPANSION

The t expansion of thermodynamic potential up to t^4 has been done for the single-band Hubbard model by Kubo[11] and Liu.[12] For the one-dimensional model their expansion becomes

$$-g\beta=\log[\xi]+(\beta t)^2\frac{2}{\xi^2}G_1+(\beta t)^4\left(\frac{2}{\xi^2}G_2+\frac{2}{\xi^3}G_3-\frac{6}{\xi^4}G_1^2\right)+O((\beta t)^6), \quad (32)$$

where

$$\xi\equiv1+2\cosh(\beta h)e^{\beta A}+e^{\beta(2A-U)},$$

$$G_1=\cosh(\beta h)e^{\beta A}(1+e^{\beta(2A-U)})+\frac{2e^{2\beta A}}{\beta U}(1-e^{-\beta U}),$$

$$G_2=\frac{1}{12}\cosh(\beta h)e^{\beta A}(1+e^{\beta(2A-U)})+\frac{4e^{2\beta A}}{(\beta U)^2}(1+e^{-\beta U})-\frac{8e^{2\beta A}}{(\beta U)^3}(1-e^{-\beta U}),$$

$$G_3=\frac{1}{6}\xi e^{\beta A}\cosh(\beta h)(1+e^{\beta(2A-U)})+\frac{3e^{2\beta A}}{\beta U}[1+e^{\beta(2A-U)}-2\cosh(\beta h)e^{\beta(A-U)}]+\frac{2e^{2\beta A}}{(\beta U)^2}[2\cosh(\beta h)e^{\beta A}(1-2e^{-\beta U})$$
$$-(2-e^{-\beta U})(1+e^{\beta(2A-U)})]+\frac{2\xi e^{2\beta A}}{(\beta U)^3}(1-e^{-\beta U}). \quad (33)$$

G_1 term is the second-order term of the t expansion. G_2, G_3, and G_1^2 terms are fourth order. It is expected that $-g\beta$ is expanded by $\beta t,\beta h,\beta h',\beta u'$, where we put $h'\equiv U/2-A$, $u'\equiv U/4$:

$$-g\beta=\sum_{n_1,n_2,n_3,n_4\geqslant0}A_{n_1,n_2,n_3,n_4}(\beta t)^{n_1}(\beta h)^{n_2}(\beta h')^{n_3}(\beta u')^{n_4}. \quad (34)$$

From Eqs. (32) and (33) we can calculate all coefficients A_{n_1,n_2,n_3,n_4} at $n_1<6$. On the other hand, we have

$$-g\beta=\ln4+\frac{(\beta t)^2}{2}-\frac{(\beta t)^4}{16}+\frac{(\beta t)^6}{144}-O((\beta t)^8), \quad (35)$$

when $U=h=h'=0$. Then we have $A_{6,0,0,0}=1/144$ and $A_{7,0,0,0}=0$. In this way, we can determine A_{n_1,n_2,n_3,n_4} at $n_1+n_2+n_3+n_4\leqslant7$ and obtain the β expansion of the grand potential:

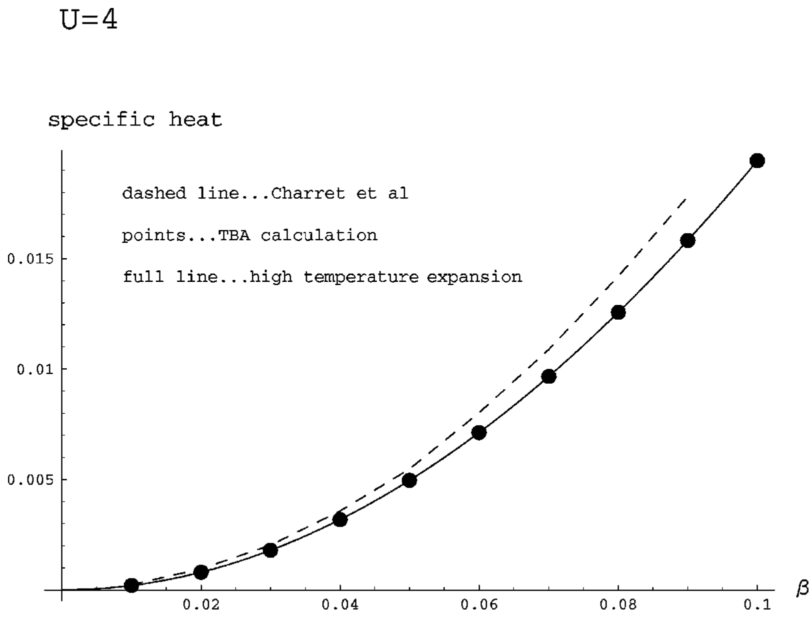

FIG. 1. Specific heat at $U=4$, $h=0$, and $U/2-A=0$. Points are our results of TBA calculations and the dashed line is the calculation of Charret *et al.* The solid line is the high-temperature expansion.

$$
\begin{aligned}
g=&-\frac{\ln 4}{\beta}+(h'-u')-\frac{\beta}{4}(2t^2+2u'^2+h^2+h'^2)-\frac{\beta^2}{4}(h^2-h'^2)u'+\frac{\beta^3}{96}(6t^4+12t^2(h^2+h'^2)+32t^2u'^2+8u'^4+h^4\\
&+6h^2h'^2+h'^4)+\frac{\beta^4}{24}u'(h^2-h'^2)(6t^2+2u'^2+h^2+h'^2)-\frac{\beta^5}{1440}\{10t^6+t^4[306u'^2+90(h^2+h'^2)]+t^2[288u'^4\\
&+60u'^2(h^2+h'^2)+30(h^4+6h^2h'^2+h'^4)]+32u'^6-45u'^2(h^4-2h^2h'^2+h'^4)+h^6+h'^6+15(h^4h'^2+h^2h'^4)\}\\
&-\frac{\beta^6}{2880}u'(h^2-h'^2)\{540t^4+t^2[720u'^2+300(h^2+h'^2)]+96u'^4+40(h^2+h'^2)u'^2+17(h^4+h'^4)+62h^2h'^2\}+O(\beta^7),
\end{aligned}
\tag{36}
$$

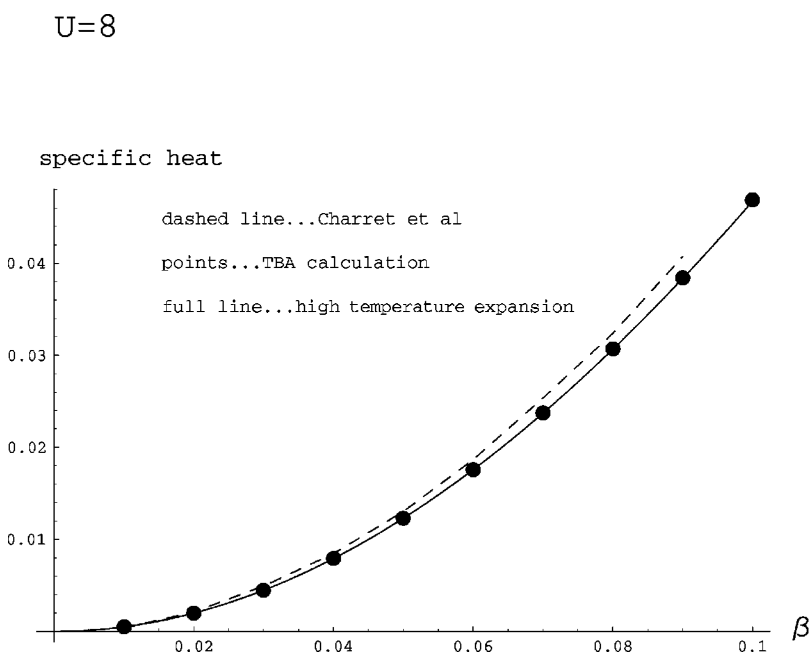

FIG. 2. Specific heat at $U=8$, $h=0$, and $U/2-A=0$.

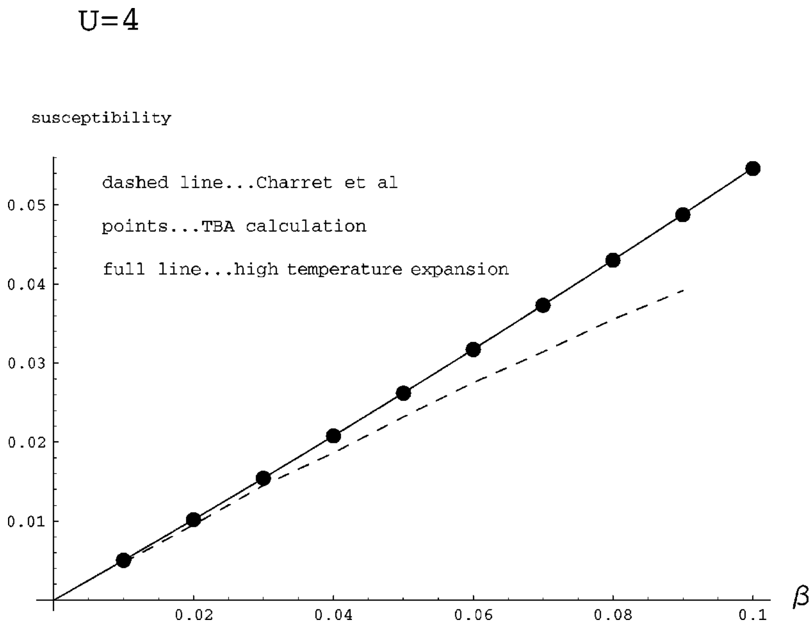

FIG. 3. Magnetic susceptibility at $U=4$, $h=0$, and $U/2-A=0$.

This expansion up to β^4 is equivalent to the one obtained by Charret *et al.* Moreover, we could get two more terms higher than theirs in the high-temperature expansion of the grand potential. From this expansion we get the specific heat and magnetic susceptibility per site in the half-filled and zero-field cases:

$$c=(t^2+u'^2)\beta^2-\left(\frac{3t^4}{4}+4t^2u'^2+u'^4\right)\beta^4+\left(\frac{5t^6}{24}+\frac{51t^4u'^2}{8}+6t^2u'^4+\frac{2u'^6}{3}\right)\beta^6+O(\beta^8), \tag{37}$$

$$\chi=\frac{\beta}{2}+\frac{u'\beta^2}{2}-\frac{t^2\beta^3}{4}-\frac{1}{6}(3t^2+u'^2)u'\beta^4+\frac{1}{24}(3t^2+2u'^2)t^2\beta^5+\left(\frac{3t^4u'}{8}+\frac{t^2u'^3}{2}+\frac{u'^5}{15}\right)\beta^6+O(\beta^7). \tag{38}$$

In Fig. 1 we plot our numerical results of the TBA equations of the specific heat at $U=4$, $h=0$, and $A=U/2$. They agree very well with the high-temperature expansion when $\beta<0.1$. The dashed line is the numerical calculation of the TBA equations by Charret *et al.* Figure 2 is the specific heat at $U=8$. Figure 3 is the susceptibility at $U=4$, $h=0$, and $A=U/2$.

IV. DISCUSSION AND CONCLUSION

In this paper, we show that the TBA equations and QTM formulations by Jüttner *et al.* give completely the same numerical results and coincide also with the high-temperature expansion. The numerical calculation of Charret *et al.* for the TBA equations is not correct. Probably the convergence condition is too generous. Our numerical calculation is done by use of MATHEMATICA 4.1. The source file is available from http://www.issp.u-tokyo.ac.jp/labs/theory/mtaka/index.html.

The calculations of Kawakami *et al.* and Jüttner *et al.* are based on Kepler's method. The TBA equations show a very slow convergence in Kepler's method. One needs several tens or several hundreds of iterations if one takes $n_c=6$. The QTM equation of Jüttner *et al.* is a bit faster but one needs several tens of iterations. The method of Charret *et al.* seems to be based on Kepler's method as they reported that the TBA equations converged after 2–3 times iterations. This is too short and not reliable. We conclude that the discrepancy between the TBA equations with the QTM equations or high-temperature expansion comes from their inappropriate convergence conditions.

We get very fast convergence if we adopt Newton's method. After 5–6 times of iterations we get sufficient convergence. Moreover, in Newton's method the error decreases with acceleration.

We made numerical programs for the TBA and QTM equations. In Table I, we observe the dependence of the numerical results on n_c. As n_c increases they converge to the high-temperature expansion and the QTM calculation of Jüttner *et al.* Both equations give completely the same numerical results. Especially for the grand potential the values coincide within five digits accuracy. We can conclude that both equations are equivalent, although the mathematical equivalence is not yet proved.

About the SO(4) symmetry Ref. 2 did not treat explicitly. But in Ref. 1 the symmetry is treated carefully and the same equations are derived. The thermodynamics may not be sensitive to the SO(4) symmetry. In conclusion we can use the TBA equations for thermodynamic quantities of the 1D Hubbard model. But one needs some numerical technique shown in this paper.

For the XXZ model it is known that the TBA equations

TABLE I. Numerical results of the TBA equations for the grand potential, energy, entropy, specific heat, and susceptibility at $\beta=0.1$, $U=4$, and $h=U/2-A=0$ for various values of n_c. We put $L=64$ and compare with the high-temperature expansion (36) and the QTM equations of Jüttner *et al.* We find that $n_c=6$ is practically sufficient.

	$-g$	e	Entropy	C	χ
$n_c=6$	14.96245182	0.801931104	1.37643829	0.01943355	0.05459858
$n_c=12$	14.96247427	0.801886862	1.37643611	0.01943778	0.05465946
$n_c=24$	14.96247646	0.801882551	1.37643590	0.01943818	0.05467815
$n_c=48$	14.96247660	0.801882261	1.37643588	0.01943821	0.05468324
$n_c=96$	14.96247662	0.801882219	1.37643588	0.01943821	0.05468587
β expt.	14.96246886	0.801890167	1.37643590	0.01943825	0.05468635
JKS	14.96246887	0.801890163	1.37643590	0.01943818	0.05468632

and the QTM method give completely the same results numerically.[13–17] Recently, it is shown that the TBA equations can be derived from the quantum transfer matrix formulations for this model.[18,19] An intriguing simple equation, which has only one unknown function, was also derived both from the TBA and the QTM.[20] In the future, we hope to show the equivalence of the two formulations for the Hubbard model.

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APPENDIX: *t* EXPANSION FOR THE TBA EQUATIONS

First, we expand e_0 as a power series of $U'=4t/U$:

$$e_0=-4\left[\left(\frac{1}{2}\right)^2\ln 2\,U'^{-1}-\left(\frac{1\times 3}{2\times 4}\right)^2\frac{\zeta(3)}{3}\left(1-\frac{1}{2^2}\right)\times U'^{-3}+\cdots\right]. \tag{A1}$$

Then we have the t expansion of the constant term of $-g\beta$:

$$(A-e_0)\beta=\beta A+\frac{4\ln 2}{\beta U}(\beta t)^2-\frac{9\zeta(3)}{(\beta U)^3}(\beta t)^4+O(\beta t)^6. \tag{A2}$$

We put $\Lambda=U'x$. σ_0, ρ_0, κ_0, and s_1 are written as follows:

$$\sigma_0(\Lambda)=\frac{t}{U}\text{sech}\frac{\pi}{2}x\left[1+\frac{\pi^2t^2}{U^2}\left(-1+2\tanh^2\frac{\pi}{2}x\right)+O(t^4)\right],$$

$$\rho_0(k)=\frac{1}{2\pi}+\frac{2t\ln 2}{\pi U}\cos k+O(t^3),$$

$$\kappa_0(k)=-2t\cos k-\frac{U}{2}-\frac{4t^2\ln 2}{U}+O(t^3), \tag{A3}$$

$$s_1(\Lambda)=-\frac{2\pi t^2}{U}\text{sech}\frac{\pi x}{2}+O(t^3).$$

The integral $\int_{-\infty}^{\infty}d\Lambda s(\Lambda-\sin k)\cdots$ becomes

$$\int_{-\infty}^{\infty}dx\overline{s}(x)\left[1+\frac{2\pi t}{U}\sin k\tanh\frac{\pi}{2}x+\left(\frac{2\pi t}{U}\sin k\right)^2\times\left(-\frac{1}{2}+\tanh^2\frac{\pi}{2}x\right)+O(t^3)\right],$$

where

$$\overline{s}(x)\equiv\frac{1}{4}\text{sech}\frac{\pi}{2}x.$$

The TBA equations are

$$\ln\zeta(k)=\beta\left(-\frac{U}{2}-2t\cos k-\frac{4t^2\ln 2}{U}\right)+\int_{-\infty}^{\infty}dx\overline{s}(x)\times\left[1+\frac{2\pi t}{U}\sin k\tanh\frac{\pi}{2}x+\left(\frac{2\pi t}{U}\sin k\right)^2\times\left(-\frac{1}{2}+\tanh^2\frac{\pi}{2}x\right)\right]\ln\frac{1+\eta_1'(x)}{1+\eta_1(x)},$$

$$\ln\eta_1(x)=-\frac{8\pi\beta t^2}{U}\overline{s}(x)-\frac{4t}{U}\int_{-\pi}^{\pi}\overline{s}(x)\left(1+\frac{2\pi t}{U}\times\sin k\tanh\frac{\pi}{2}x\right)\ln[1+\zeta(k)]\cos k\,dk+\overline{s}*\ln[1+\eta_2(x)],$$

$$\ln\eta_1'(x)=-\frac{4t}{U}\int_{-\pi}^{\pi}\overline{s}(x)\left(1+\frac{2\pi t}{U}\sin k\tanh\frac{\pi}{2}x\right)\times\ln[1+\zeta(k)]\cos k\,dk+\overline{s}*\ln[1+\eta_2'(x)],$$

$$\ln\eta_j(x)=\overline{s}*\ln\{[1+\eta_{j-1}(x)][1+\eta_{j+1}(x)]\},$$

$$\ln\eta_j'(x)=\overline{s}*\ln\{[1+\eta_{j-1}'(x)][1+\eta_{j+1}'(x)]\}. \tag{A4}$$

$-g\beta$ is given by

$$-g\beta=\beta A+\frac{4\ln 2}{\beta U}(\beta t)^2+\int_{-\pi}^{\pi}\left(\frac{1}{2\pi}+\frac{2\ln 2t}{\pi U}\cos k\right)\times\ln[1+\zeta(k)]dk+\int_{-\infty}^{\infty}\overline{s}(x)\left[1+\frac{\pi^2t^2}{U^2}\left(-1+2\tanh\frac{\pi}{2}x\right)\right]\ln[1+\eta_1(x)]dx. \quad (A5)$$

We expand the functions by a power series of βt:

$$\ln[1+\eta_j(x)]=\ln\frac{\alpha_j}{\alpha_j-1}+(\beta t)f_j^{(1)}(x)+(\beta t)^2f_j^{(2)}(x)+\cdots,$$

$$\ln[1+\eta_j'(x)]=\ln\frac{\alpha_j'}{\alpha_j'-1}+(\beta t)f_j'^{(1)}(x)+(\beta t)^2f_j'^{(2)}(x)+\cdots,$$

$$\ln[1+\zeta(k)]=\ln\frac{z_0}{z_0-1}+(\beta t)z^{(1)}(k)+(\beta t)^2z^{(2)}(k)+\cdots \quad (A6)$$

We get

$$\ln\eta_j(x)=\ln\frac{1}{\alpha_j-1}+(\beta t)\alpha_jf_j^{(1)}(x)+(\beta t)^2\left[\alpha_jf_j^{(2)}(x)+\frac{1}{2}(\alpha_j-\alpha_j^2)[f_j^{(1)}(x)]^2\right]+\ldots,$$

$$\ln\eta_j'(x)=\ln\frac{1}{\alpha_j'-1}+(\beta t)\alpha_j'f_j'^{(1)}(x)+(\beta t)^2\left[\alpha_j'f_j'^{(2)}(x)+\frac{1}{2}(\alpha_j'-\alpha_j'^2)[f_j'^{(1)}(x)]^2\right]+\cdots,$$

$$\ln\zeta(k)=\ln\frac{1}{z_0-1}+(\beta t)z_0z^{(1)}(k)+(\beta t)^2\left[z_0z^{(2)}(k)+\frac{1}{2}(z_0-z_0^2)[z^{(1)}(k)]^2\right]+\cdots, \quad (A7)$$

where

$$\alpha_j=\frac{[j+1]^2}{[j][j+2]},\quad \alpha_j'=\frac{[j+1]'^2}{[j]'[j+2]'},\quad z_0=1+e^{\beta U/2}\frac{[2]}{[2]'} \quad (A8)$$

and $[j]$ and $[j]'$ are q integers defined by

$$[j]\equiv\frac{\sinh j\beta h}{\sinh\beta h},\quad [j]'\equiv\frac{\sinh j\beta(U/2-A)}{\sinh\beta(U/2-A)}. \quad (A9)$$

We have

$$f_j^{(1)}(x)=f_j'^{(1)}(x)=0,\quad z^{(1)}(k)=-2z_0^{-1}\cos k. \quad (A10)$$

The equations for $f_j^{(1)}(x)$, $f_j'^{(1)}(x)$, and $z^{(2)}(k)$ are

$$\alpha_1f_1^{(2)}(x)=-\frac{8\pi}{\beta U}(1-z_0^{-1})\overline{s}(x)+\overline{s}*f_2^{(2)}(x),$$

$$\alpha_1'f_1'^{(2)}(x)=\frac{8\pi}{\beta U}z_0^{-1}\overline{s}(x)+\overline{s}*f_2'^{(2)}(x),$$

$$\alpha_jf_j^{(2)}(x)=\overline{s}*[f_{j-1}^{(2)}(x)+f_{j+1}^{(2)}(x)],$$

$$\alpha_j'f_j'^{(2)}(x)=\overline{s}*[f_{j-1}'^{(2)}(x)+f_{j+1}'^{(2)}(x)],$$

$$z_0z^{(2)}(k)=2(1-z_0^{-1})\cos^2k-\frac{4\ln 2}{\beta U}+\int_{-\infty}^{\infty}dx\overline{s}(x)[f_1'^{(2)}(x)-f_1^{(2)}(x)]. \quad (A11)$$

The same kind of equation has appeared in the high-temperature expansion of the XXX model. See pp. 124–126 of Ref. 1 or 13. The solutions of these equations are

$$f_j^{(2)}(x)=-\frac{8\pi}{\beta U}\frac{(1-z_0^{-1})}{[2][j+1]}\{[j+2]\overline{a}_j(x)-[j]\overline{a}_{j+2}(x)\},$$

$$f_j'^{(2)}(x)=\frac{8\pi}{\beta U}\frac{z_0^{-1}}{[2]'[j+1]'}\{[j+2]'\overline{a}_j(x)-[j]'\overline{a}_{j+2}(x)\},$$

$$z^{(2)}(k)=\frac{2(z_0-1)}{z_0^2}\left[\cos^2k-\frac{1}{\beta U[2]^2}\left(1+\frac{[2]}{[2]'}e^{-\beta U/2}\right)\right],$$

$$\overline{a}_j(x)\equiv\frac{j}{\pi(x^2+j^2)}. \quad (A12)$$

Substituting Eqs. (A10) and (A12) into Eqs. (A6) and (A5) we get

$$-g\beta=\beta A-\ln(1-z_0^{-1})+\ln(2\cosh\beta h)+(\beta t)^2\times\left\{\frac{4\ln 2}{\beta U}+\frac{1}{2\pi}\int_{-\pi}^{\pi}\left[z^{(2)}(k)+\frac{4\ln 2}{\beta U}\cos kz^{(1)}(k)\right]dk+\int_{-\infty}^{\infty}\overline{s}(x)\left[f^{(2)}(x)+\ln\frac{\alpha_1}{\alpha_1-1}\frac{\pi^2t^2}{\beta^2U^2}\times\left(-1+2\tanh^2\frac{\pi}{2}x\right)\right]dx\right\}$$
$$=\ln\xi+\frac{2(\beta t)^2}{\xi^2}\left[\cosh(\beta h)e^{\beta A}(1+e^{\beta(2A-U)})+\frac{2}{\beta U}e^{2\beta A}(1-e^{-\beta U})\right], \quad (A13)$$

where ξ is defined in Eq. (33). This coincides with Eq. (32) up to second order. Thus we have proved that the TBA equations give the correct t expansion of $-g\beta$ up to $(t\beta)^2$.

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