Takahashi Integral Equation
and High-Temperature Expansion of the Heisenberg Chain

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(Dated:)

Recently a new integral equation describing the thermodynamics of the 1D Heisenberg model was discovered by Takahashi. Using the integral equation we have succeeded in obtaining the high temperature expansion of the specific heat and the magnetic susceptibility up to $O((J/T)^{100})$. This is much higher than those obtained so far by the standard methods such as the linked-cluster algorithm. Our results will be useful to examine various approximation methods to extrapolate the high temperature expansion to the low temperature region.

PACS numbers: 75.10.Jm, 75.40.Cx, 05.30.-d

The Hamiltonian of the spin-1/2 Heisenberg $XXX$ chain is defined by

$$H = -J \sum_{j=1}^{N} \left[ S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + S_j^z S_{j+1}^z - \frac{1}{4} \right]$$

$$- 2h \sum_{j=1}^{N} S_j^z,$$

(1)

where $S^x, y, z_j$ are the local spin-1/2 operators acting on the site $j$. We assume the periodic boundary conditions $S_{N+1} = S_1$. Note that in our definition, the coupling constant $J$ is positive for the ferromagnetic case and negative for the antiferromagnetic case.

Takahashi’s integral equation for the isotropic $XXX$ case is given by

$$u(x) = 2 \cosh h/T$$

$$+ \oint_C \left\{ \frac{1}{x - y - 2i} \exp \left[ - \frac{2J/T}{(y + 1)^2 + 1} \right] \right\} \frac{1}{u(y)} \frac{dy}{2\pi i}$$

$$f = -T \ln u(0),$$

(2)

where the contour $C$ is a loop surrounding the origin in a counterclockwise manner. The equation can be solved numerically.

In the following we derive the HTE of $u(x)$. Actually what we have to do is only to assume $u(x)$ in the form

$$u(x) = \exp \left[ \sum_{n=0}^{\infty} a_n(x) (J/T)^n \right]$$

$$= e^{a_0(x)} \left\{ 1 + a_1(x) J/T + \left( a_2(x) + \frac{1}{2} a_1(x)^2 \right) (J/T)^2 \right.$$}

$$+ \left( a_3(x) + a_2(x) a_1(x) + \frac{1}{6} a_1(x)^3 \right) (J/T)^3 + \cdots \}.$$
and substitute it into the equation \(^2\). Then by comparing the same order of \(J/T\) in the LHS and the RHS, we can get the equations, which, to our surprise, determine the functions \(a_n(x)\) recursively. For example, from the 0-th order, we get immediately

\[
a_0(x) = \ln \left(2 \cosh \frac{h}{T} \right).
\]

Similarly by comparing the 1-st order, we have an equation,

\[
a_1(x) = \frac{1}{4 \cosh^2 \frac{h}{T}} \left\{ \oint_C \left\{ \frac{-2}{y(y+2i)(x-y-2i)} + \frac{2}{y(y-2i)(x+y+2i)} \right\} \frac{dy}{2\pi i} \right\}
\]

\[
- \oint_C \left\{ \frac{1}{x-y-2i} + \frac{1}{x+y+2i} \right\} a_1(y) \frac{dy}{2\pi i}.
\]

Noting that the second term in the RHS vanishes because the integrand is regular at \(y = 0\), we can calculate \(a_1(x)\) explicitly as

\[
a_1(x) = -\frac{1}{\cosh^2 \frac{h}{T} x^2 + 4}.
\]

Repeating the similar procedures we can derive each \(a_n(x)\) successively. For example, we have found

\[
a_2(x) = \frac{1}{4 \cosh^2 \frac{h}{T} (x^2 + 4)^2} \left[ x^2 + 12 \right.
\]

\[
- \frac{1}{4 \cosh^4 \frac{h}{T} (x^2 + 4)^2} x^2 + 6 \left. \right]\]

\[
+ \frac{1}{24 \cosh^2 \frac{h}{T} (x^2 + 4)^3} 3x^4 + 36x^2 + 160
\]

\[
+ \frac{1}{4 \cosh^4 \frac{h}{T} (x^2 + 4)^3} x^4 + 11x^2 + 36
\]

\[
- \frac{1}{24 \cosh^6 \frac{h}{T} (x^2 + 4)^3} 3x^4 + 30x^2 + 80 \right\} d(x).
\]

Some of the lower terms are given as

\[
f/T = -\ln(2 \cosh(h/T)) + \frac{J}{4T} (1 - B^2)
\]

\[
- \frac{3J^2}{32T^2} (1 - B^4)
\]

\[
+ \frac{J^3}{192T^3} (1 - B^2)(3 + 7B^2 + 10B^4)
\]

\[
+ \frac{5J^4}{3072T^4} (1 - B^2)(3 - B^2 - 9B^4 - 21B^6)
\]

\[
- \frac{J^5}{5120T^5} (1 - B^2)(1 + 2B^2)
\]

\[
\times (15 - B^2 + 21B^4 - 63B^6)
\]

\[
- \frac{7J^6}{122880T^6} (1 - B^2)
\]

\[
\times (3 - 35B^2 - 85B^4 - 95B^6 - 30B^8 + 330B^{10})
\]

\[
+ \ldots.
\]

where we have set \(B = \tanh(h/T)\). From the expansion \(^2\), one can get the HTE for other physical quantities.

For example, we list coefficients of the HTE for the specific heat \(C = -T \frac{\partial^2 f}{\partial T^2}\) and the magnetic susceptibility \(\chi = -\frac{\partial f}{\partial h}\) at zero magnetic field in Table 1 and Table 2. Unfortunately due to the lack of space, we can present the coefficients only up to \(O((J/T)^{24})\). The coefficients of higher order will be sent on demand to any interested reader. We remark that the coefficients up to \(O((J/T)^{24})\) completely coincide with those given in \(^1\). Note the differences of the conventions, \(J \leftrightarrow -J\) and \(h \leftrightarrow 2h\).

The terms with the order larger than \(O((J/T)^{25})\) are our new results. It will probably be impossible to get the HTE to such a high order using a conventional method.

![FIG. 1: Specific heat for the antiferromagnetic XXX chain at \(h = 0\).](image)

Usually in order to extrapolate the high temperature expansion series to the low temperature region, some further approximation methods are used. Actually the original series will not converge in the low temperature region \((T \text{ about less than } 0.55)\), because of the existence of the singularities on the complex plane with respect to the inverse temperature.

Here we have applied the standard Padé approximation to our HTE. The results are shown in Fig. 1, Fig. 2, Fig. 3, and Fig. 4.
FIG. 2: Magnetic susceptibility for the antiferromagnetic XXX chain at $h = 0$. $\chi(0)$ is taken from [21].

Since we have obtained the HTE up to $O((J/T)^{100})$, the expressions up to [50, 50] Padé approximant are available. For comparison, we have also plotted the numerical data calculated by the QTM method [11, 15]. (Note that the physical quantities in Fig. 1,...,Fig. 4 were first calculated by the TBA equations. See particularly [6, 7] for the ferromagnetic case.) From Fig. 1,...,Fig. 4, we find that the [50, 50] Padé approximant show good coincidence with data by the QTM to very low temperature region somewhat like $T \sim 0.05$ except for the the magnetic susceptibility for the antiferromagnetic case (Fig. 2.). In that case the logarithmic anomaly around $T \to 0$ is so strong [14, 15, 16] and it probably prevents the good convergence of the Padé approximation [20].

Apart from the very low temperature region, we have found our higher order Padé approximation gives the physical quantities with extremely high precision. For example, we have estimated the peak position of the specific heat and the magnetic susceptibility for the antiferromagnetic case by use of our [50, 50] Padé approximation. The result for the specific heat is

$$C_{\text{max}} = 0.3497121234553176, \quad T_{\text{max}}^{\text{max}}/|J| = 0.4802848685890477,$$

and that for magnetic susceptibility is

$$\chi_{\text{max}} |J| = 0.5877051177413559, \quad T_{\text{max}}^{\text{max}}/|J| = 0.6408510308513831. \quad (11)$$

These values are perfectly identical to the ones in [16], where the non-linear integral equations for the QTM were solved numerically very carefully. (Note that our $\chi_{\text{max}} |J|$ is four times larger than that in [16], because of different normalization factors.) Note also that the peak position of the magnetic susceptibility [11] was first determined in [14].

For comparison we have also estimated the peak position of the specific heat for the ferromagnetic case as

$$C_{\text{max}} = 0.1342441913136996, \quad T_{\text{max}}^{\text{max}}/|J| = 0.3326119630964252. \quad (12)$$

In conclusion, we have shown that the new integral equation by Takahashi is very useful to calculate analytically the HTE for the 1D Heisenberg model. As far as we know, the HTE of such a high order as $O((T/J)^{100})$ has not been achieved for any other models except for free ones. We have seen that our HTE data together with Padé approximation, provide the very accurate numerical data for physical quantities to sufficiently low temperatures. There are several further methods to improve the Padé approximation, for example, to allow for the asymptotic expression as $T \to 0$, etc. (see, for example, [20, 22]). Based on the present results we shall investigate such possibilities in the forthcoming publication.

The authors are thankful to A. Klümper, Y. Nishiyama and K. Sakai for valuable discussions. This work is supported by Grants-in-Aid for the Scientific Research (B) No. 11440103 from the Ministry of Education, Culture, Sports, Science and Technology, Japan.
TABLE I: Series coefficients $a_n$ for the high temperature expansion of the specific heat $C = \sum_n a_n \left( \frac{\hbar}{\beta T} \right)^n$ at $h = 0$.

| $n$ | $a_n$ | $a_n$ |
|-----|-------|-------|
| 0   | 0     | 0     |
| 1   | 0.26  | 0.26  |
| 2   | -0.27 | -0.27 |
| 3   | 0.28  | 0.28  |
| 4   | -0.30 | -0.30 |
| 5   | 0.31  | 0.31  |
| 6   | 0.32  | 0.32  |
| 7   | 0.33  | 0.33  |
| 8   | 0.34  | 0.34  |
| 9   | 0.35  | 0.35  |
| 10  | 0.36  | 0.36  |
| 11  | 0.37  | 0.37  |
| 12  | 0.38  | 0.38  |
| 13  | 0.39  | 0.39  |
| 14  | 0.40  | 0.40  |
| 15  | 0.41  | 0.41  |
| 16  | 0.42  | 0.42  |
| 17  | 0.43  | 0.43  |
| 18  | 0.44  | 0.44  |
| 19  | 0.45  | 0.45  |
| 20  | 0.46  | 0.46  |
| 21  | 0.47  | 0.47  |
| 22  | 0.48  | 0.48  |
| 23  | 0.49  | 0.49  |
| 24  | 0.50  | 0.50  |
| 25  | 0.51  | 0.51  |
| 26  | 0.52  | 0.52  |
| 27  | 0.53  | 0.53  |
| 28  | 0.54  | 0.54  |
| 29  | 0.55  | 0.55  |
| 30  | 0.56  | 0.56  |
| 31  | 0.57  | 0.57  |
| 32  | 0.58  | 0.58  |
| 33  | 0.59  | 0.59  |
| 34  | 0.60  | 0.60  |
| 35  | 0.61  | 0.61  |
| 36  | 0.62  | 0.62  |
| 37  | 0.63  | 0.63  |
| 38  | 0.64  | 0.64  |
| 39  | 0.65  | 0.65  |
| 40  | 0.66  | 0.66  |
| 41  | 0.67  | 0.67  |
| 42  | 0.68  | 0.68  |
| 43  | 0.69  | 0.69  |
| 44  | 0.70  | 0.70  |
| 45  | 0.71  | 0.71  |
| 46  | 0.72  | 0.72  |
| 47  | 0.73  | 0.73  |
| 48  | 0.74  | 0.74  |
| 49  | 0.75  | 0.75  |
| 50  | 0.76  | 0.76  |

TABLE II: Series coefficients $\beta_n$ for the high temperature expansion of the magnetic susceptibility $\chi = \frac{1}{T} \sum_n \beta_n \left( \frac{\hbar}{\beta T} \right)^n$ at $h = 0$.

| $n$ | $\beta_n$ | $\beta_n$ |
|-----|------|------|
| 0   | 0    | 0    |
| 1   | 1    | 1    |
| 2   | 2    | 2    |
| 3   | 3    | 3    |
| 4   | 4    | 4    |
| 5   | 5    | 5    |
| 6   | 6    | 6    |
| 7   | 7    | 7    |
| 8   | 8    | 8    |
| 9   | 9    | 9    |
| 10  | 10   | 10   |
| 11  | 11   | 11   |
| 12  | 12   | 12   |
| 13  | 13   | 13   |
| 14  | 14   | 14   |
| 15  | 15   | 15   |
| 16  | 16   | 16   |
| 17  | 17   | 17   |
| 18  | 18   | 18   |
| 19  | 19   | 19   |
| 20  | 20   | 20   |
| 21  | 21   | 21   |
| 22  | 22   | 22   |
| 23  | 23   | 23   |
| 24  | 24   | 24   |
| 25  | 25   | 25   |
| 26  | 26   | 26   |
| 27  | 27   | 27   |
| 28  | 28   | 28   |
| 29  | 29   | 29   |
| 30  | 30   | 30   |
| 31  | 31   | 31   |
| 32  | 32   | 32   |
| 33  | 33   | 33   |
| 34  | 34   | 34   |
| 35  | 35   | 35   |
| 36  | 36   | 36   |
| 37  | 37   | 37   |
| 38  | 38   | 38   |
| 39  | 39   | 39   |
| 40  | 40   | 40   |
| 41  | 41   | 41   |
| 42  | 42   | 42   |
| 43  | 43   | 43   |
| 44  | 44   | 44   |
| 45  | 45   | 45   |
| 46  | 46   | 46   |
| 47  | 47   | 47   |
| 48  | 48   | 48   |
| 49  | 49   | 49   |
| 50  | 50   | 50   |

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