Precise estimates by finite-size extrapolations of the $S=1$ Haldane-gapped system

Hiroki Nakano
Graduate School of Material Science, University of Hyogo, Kouto, Kamigori, Ako 678-1297, Japan
E-mail: hnakano@sci.u-hyogo.ac.jp

Abstract. We carry out finite-size extrapolations of numerical-diagonalization data of the $S=1$ Heisenberg chain having a nonzero energy gap between the unique singlet ground state and the first excited state, namely the Haldane gap. Very precise estimates of the ground-state energy per site $E_g/N = -1.4014840447(39)$ and the staggered component of the magnetic structure factor $S_\pi = 3.864356(31)$ at $T=0$ are successfully obtained from the finite-size data of system sizes up to $N = 24$ under the twisted boundary condition by the sequence interval squeeze method, which was applied to a precise estimation of the Haldane gap by Nakano and Terai [J. Phys. Soc. Jpn. 78 (2009) 014003]. The present estimates are compared with other estimates in previous studies from various methods including the quantum Monte Carlo simulation and the density matrix renormalization group calculation.

Extrapolation is a fundamental technique that is often used in the condensed matter physics in order to capture the physical properties of a system with the infinite size from several data of finite-size systems. However, to obtain a very precise extrapolated value with a reliable error is generally difficult. Under circumstances, a recent study[1] proposed a way to estimate such an error for the extrapolation based on the convergence acceleration applied to an initial sequence obtained numerically. The method was immediately applied to the estimation of the $S=1$ Haldane gap. The Haldane gap is the nonzero energy gap between the unique ground state and the first excited state of the integer-spin one-dimensional (1D) Heisenberg antiferromagnet.[2, 3].

The purpose of this study is to examine the validity of the proposed method in the extrapolation of other physical quantities. We focus our attention on the 1D $S=1$ Heisenberg antiferromagnet. We present successful applications of the ground-state energy per site and the staggered component of the magnetic structure factor at $T=0$. Its Hamiltonian is given by

$$\mathcal{H} = \sum_{m=1}^{N} J \mathbf{S}_m \cdot \mathbf{S}_{m+1}, \quad (1)$$

where $\mathbf{S}_m$ is the $S=1$ spin operator at the $m$-th site, $J$ is the interaction constant to be unity as the unit of energy, and $N$, being assumed to be an even integer, denotes the number of spin sites. We impose the twisted boundary condition (TBC) given by $S^x_{N+1} = -S^x_1$, $S^y_{N+1} = -S^y_1$, and $S^z_{N+1} = S^z_1$, as long as we particularly mention the boundary condition. Note here that the superiority of the TBC in the quantum spin systems was shown in the studies of the Haldane gap estimation in [1] and the precise estimation of the gapless transition points of the bond-alternating chain in [4]. By means of the numerical-diagonalization (ND) method
based on the Lanczos algorithm, we have calculated the ground-state energy \( E_g(N) \) and the spin correlation function \( \langle S_i^x S_j^x \rangle \) at \( T=0 \). From these quantities, we have studied the ground-state energy per site \( e_g(N) = \bar{E}_g(N)/N \) and the staggered component of the magnetic structure factor \( S_\pi(N) = \sum_{m=0}^{N-1} (-1)^m \langle S_i^z S_{i+m}^z \rangle \). Note here that \( \langle S_i^z S_{i+1}^z \rangle = \langle S_i^z S_{i+N-m}^z \rangle \).

Before our results are presented, we briefly explain the procedure of the proposed method in [1]. Suppose first that there is a sequence \( A_N^{(0)} \) which converges to a certain limit \( A_N^{(0)} \) monotonically with respect to \( N \). What we would like to do is to estimate \( A_N^{(0)} \) precisely from a finite part of the sequence \( A_N^{(0)} \). The superscript (0) means that the sequence \( A_N^{(0)} \) works as an initial sequence for higher-level sequences. We construct the higher-level sequences by the convergence-acceleration transformation given by

\[
1/[A_{N}^{(k+1)} - A_{N-2}^{(k)}] = 1/[A_{N-4}^{(k)} - A_{N-2}^{(k)}] + 1/[A_{N}^{(k)} - A_{N-2}^{(k)}] + \alpha_k/[A_{N-4}^{(k)} - A_{N-2}^{(k)}],
\]

where we assume \( A_N^{(-1)} = \infty \). If \( \alpha_k \) is fixed to vanish, the transformation is the Aitken-Shanks (AS) acceleration [5]. In the case when \( \alpha_k \) is fixed to be unity, the transformation corresponds to so-called the \( \varepsilon \)-algorithm [6] by Wynn. To know whether the acceleration is successful or not by the transformation (2), we monitor the decay length defined as \( \xi_S(N) = 2/\log \left[ (A_{N-4}^{(k)} - A_{N-2}^{(k)})/(A_{N-2}^{(k)} - A_N^{(k)}) \right] \). One can consider that the convergence of a new sequence \( A_N^{(k)} \) is successfully accelerated when the following conditions hold, (I) \( A_N^{(k)} \) is monotonically increasing with respect to \( N \), (II) \( \xi_S(N) \) increases with \( N \), namely \( \xi_{N+2} > \xi_N \), and (III) \( \xi_S(N) \) decreases with \( k \), namely \( \xi_{(k+1)} < \xi_k \). The next step is the creation of another sequence

\[
B_{N+1}^{(k)} = \left[ A_N^{(k)} A_{N+2}^{(k)} - A_{N+2}^{(k)} A_N^{(k)} \right]/\left[ A_{N+2}^{(k)} - A_N^{(k)} \right] - A_{N+2}^{(k)} + A_N^{(k)}
\]

from \( A_N^{(k)} \) and \( A_N^{(k')} \) that are convergent from the same side, where \( A_N^{(k)} \) is successfully accelerated from \( A_N^{(k')} \), namely \( k > k' \). The new sequence \( B_{N+1}^{(k)} \) is the one that is convergent to \( A_N^{(0)} \) from the side opposite to \( A_N^{(k)} \). If the initial sequence \( A_N^{(0)} \) is monotonically increasing, therefore, \( \max_{k,N}(A_N^{(k)}) \) and \( \min_{k,N}(B_N^{(k)}) \) give a lower bound and an upper one for \( A_N^{(0)} \), respectively; when the direction of \( A_N^{(0)} \) is opposite, \( \min_{k,N}(A_N^{(k)}) \) and \( \max_{k,N}(B_N^{(k)}) \) give an upper bound and a lower one, respectively. Note that if an appropriate acceleration transformation is used, it is easy to obtain a reliable interval including the limit we would like to know and that the interval gets narrower inside as the number of initial data is increased. The present method proposed in [1] is called the sequence interval squeeze (SIS) method in [7]; hereafter, we also use the name.

Nakano and Terai substitute the excitation gap of the finite-size systems under the TBC for \( A_N^{(0)} \). From the numerical data up to \( N = 24 \), the SIS method gives the estimate \( \Delta = 0.4104789(13) \) as the Haldane gap by the acceleration transformation with \( \alpha_k = 1 \). An even more precise estimate of the Haldane gap has been reported quite recently in [7] by using \( \alpha_k = 0.4 \).

Now we present our results; our finite-size ND data are shown in Table 1. We have also carried out ND calculations of the system under the periodic boundary condition (PBC). Our results up to \( N = 22 \) under the PBC agree with those reported in [8] except for the last digit. We have obtained an additional result under the PBC to be \( e_g(N = 24) = -1.401691204590 \). Concerning with the finite-size data, \( e_g(N) \) of TBC seems closer to its thermodynamic limit than that of PBC although the converging directions are opposite with each other. Thus we choose \( e_g(N) \) of TBC to extrapolate. From comparison between \( S_\pi(N) \) of TBC and that of PBC in [9], \( S_\pi(N) \) of TBC is better to extrapolate.

We input finite-size \(-e_g(N)\) under the TBC to \( A_N^{(0)} \) in eq. (2) in order to carry out the SIS method, using \( \alpha_k = \sin(\pi k/2) \) in eq. (2) and \( k' = k - 1 \) in eq. (3). Note that we here employ a
Table 1. Finite-size results from our numerical diagonalizations at $T=0$. The ground-state energy per site $e_g(N)$ under the twisted boundary condition (TBC), the staggered component of the magnetic structure factor $S_\pi(N)$, the spin correlation function $\langle S_z^1 S_z^{1+m} \rangle$ for $N=24$ under the TBC, and $\langle S_z^1 S_z^{1+m} \rangle$ for $N=24$ under the periodic boundary condition (PBC).

| $N$ or $2m$ | $-e_g(N)/$TBC | $S_\pi(N)/$TBC | $\langle S_z^1 S_z^{1+m} \rangle$/TBC | $\langle S_z^1 S_z^{1+m} \rangle$/PBC |
|-----------|----------------|----------------|---------------------------------|-----------------------------------|
| 0         | $-0.6683762389$ | $2/3$          | $-0.4700051650$                 | $-0.4672304015$                   |
| 2         | $-0.4700051650$ | $2/3$          | $-0.1964304043$                 | $-0.1938077876$                   |
| 4         | $3.1927961666$  | $2/3$          | $0.1439777399$                  | $0.141953748$                     |
| 6         | $3.435042397$   | $2/3$          | $0.0917397616$                  | $0.089725476$                     |
| 8         | $3.741766539$   | $2/3$          | $0.0745737260$                  | $0.072532987$                     |
| 10        | $3.584982611$   | $2/3$          | $0.0625117824$                  | $0.060699818$                     |
| 12        | $3.680216983$   | $2/3$          | $0.0546348778$                  | $0.052948778$                     |
| 14        | $3.741766539$   | $2/3$          | $0.0489828207$                  | $0.0473207270$                    |
| 16        | $3.782072510$   | $2/3$          | $0.0448655562$                  | $0.043298447$                     |
| 18        | $3.808747479$   | $2/3$          | $0.0413706379$                  | $0.039828207$                     |
| 20        | $3.826556607$   | $2/3$          | $0.04041358514$                 | $0.0388540447$                    |
| 22        | $3.838534657$   | $2/3$          | $0.039828207$                   | $0.03824038971$                   |
| 24        | $3.846641549$   | $2/3$          | $0.039828207$                   | $0.03824038971$                   |

The combination of different acceleration techniques according to the step $k$ because $\alpha_k$ in eq. (2) does not necessarily have to be constant without $k$-dependence. The results are depicted in Figs. 1 and 2. One can observe that the above three conditions for the successful acceleration of convergence are satisfied and confirm that the new sequences $B^{(k)}_N$ converge from the side opposite to $A^{(k)}_N$.

### Figure 1.
System size dependence of $A^{(k)}_N$ for $A^{(0)}_N = -e_g(N)$. Pentagons, double circles, triangles, squares, and pluses denote the cases of $k = 0$, 1, 2, 3, and 4, respectively. The common shift $\xi^{(k)}_N$ is 1.4014840447. Inset depicts the behavior of $\xi^{(k)}_N$; symbols are used in the same as $A^{(k)}_N$.

### Figure 2.
System size dependence of $B^{(k)}_N$ for $A^{(0)}_N = -e_g(N)$. Circles, reversed triangles, diamonds, and crosses denote the cases of $k = 1$, 2, 3, and 4, respectively. The common shift is the same as in Fig. 1. Inset depicts the comparison with estimate $e_g = -1.401484038971(4)$ in [10] denoted by the closed diamond.
Our conclusion for the ground-state energy per site is $E_g = -1.4014840447(39)$. So far, White and Huse[10] reported $E_g = -1.401484038971(4)$ using the density matrix renormalization group method, which looks very precise. This value is very close to our estimate but is a little bit outside the width of our error. It is worth emphasizing that our estimate for the ground-state energy is lower. Our present estimate is within the error of the estimate $E_g = -1.4014841(4)$ from the quantum Monte Carlo (QMC) simulation in [11]. Our estimate agrees with $E_g = -1.401485(2)$ in [8], where the ND data up to $N = 22$ under the PBC were analyzed by the transformation (2) with $k$-independent $\alpha_k$ and the error was obtained from the variance of $\alpha_k$.

Next, we input finite-size $S_{\pi}(N)$ under the TBC to $A^{(0)}_N$ in eq. (2) to carry out the SIS method, using $\alpha_k = 1 - \cos(\pi k/2)$ in eq. (2) and $k' = 0$ in eq. (3); we have confirmed that the above three conditions are successfully satisfied. The results are depicted in Fig. 3. Our conclusion is $S_{\pi} = 3.864356(31)$, which agrees with $S_{\pi} = 3.9$ from the QMC simulation in [12]. Our estimate agrees with $S_{\pi} = 3.85(8)$ from the analysis of the finite-size ND data up to $N = 16$ under the PBC in [9], where the AS transformation was simply applied and the error was determined as the difference between the accelerated result of the data up to $N = 16$ and that of the data up to smaller $N$. The precision of our present estimate is much improved from these previous ones.

In summary, we have clarified the validity of the sequence interval squeeze method in the successful estimations of the ground-state energy per site and the $T=0$ staggered component of the magnetic structure factor of the 1D $S=1$ Heisenberg antiferromagnetic model; our precise estimates are $E_g/N = -1.4014840447(39)$ and $S_{\pi} = 3.864356(31)$. This study indicates that the SIS method is powerful and can contribute for future development in various fields.

The author would like to thank Profs. T. Sakai and Y. Hasegawa for valuable discussions. This work was partly supported by Grants-in-Aid from the Ministry of Education, Culture, Sports, Science and Technology (No. 20340096). A part of computations were performed using facilities of the IIC, Hokkaido Univ. and the Supercomputer Center, ISSP, Univ. of Tokyo.

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Figure 3. The analysis of the SIS method for the staggered component of the magnetic structure factor when $A^{(0)}_N = S_{\pi}(N)$. Double circles, triangles, squares, and pluses denote $A^{(k)}_N$ for $k = 1, 2, 3,$ and 4, respectively; circles, reversed triangles, diamonds, and crosses denote $B^{(k)}_N$ for $k = 1, 2, 3,$ and 4, respectively. The common shift $S_m$ is 3.864356.