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Energy gap of the $S=1$ antiferromagnetic Heisenberg chain

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The $S=1$ isotropic antiferromagnetic Heisenberg chain is studied by exact diagonalizations using the Lanczös algorithm. Energy gaps, structure factors at $k=\pi$, and staggered susceptibilities at $T=0$ are calculated for finite rings up to $N=16$, and extrapolated to an infinite system using Shanks' transformation. The estimated energy gap is 0.411 ± 0.001, which agrees with the result of Monte Carlo calculations by Nightingale and Blöte. Further, it is found that a finite-size correction decays exponentially and the decay constant corresponds with the correlation length, which is about five.

It was predicted by Haldane[1] that antiferromagnetic Heisenberg chains defined by the Hamiltonian

$$H=\sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z) \tag{1}$$

have a gap in their energy spectrum for integral S, while not for half-integral S. After that, the existence of this gap for $S=1$ was supported by various theoretical approaches, for example, exact diagonalizations[2] of H, Monte Carlo calculations,[3] analyses of an exactly solvable model,[4] variational methods,[5] etc. Haldane's prediction also means that the spin-correlation functions of the ground state decays exponentially for integral S, and it was also supported by some numerical calculations.[6-8] Furthermore, recently experimental evidence of Haldane gap was found for $Ni(C_2H_8N_2)_2NO_2(ClO_4)$,[9-11] which is one of quasi-one-dimensional $S=1$ antiferromagnets.

In this paper, the $S=1$ isotropic antiferromagnetic Heisenberg chain is studied by exact diagonalizations of H using the Lanczös algorithm, for finite rings up to $N=16$, and an accurate value of a gap is given by an extrapolation to an infinite system. In addition, given are values of the staggered susceptibility χ_{st} and the structure factor at wave vector $k=\pi$ defined by

$$S_\pi(N)=\sum_{l=0}^{N}(-1)^l\langle S_0^z S_{0+l}^z\rangle , \tag{2}$$

at $T=0$, which are likely to be finite[12,13] because the system is not critical.

Using the Lanczös method in the reduced Hilbert space, where $\sum_i S_i^z=0$ and $k=0$, we calculated the energy and the wave function of the ground state of H for finite rings up to $N=16$, and obtain spin-correlation functions defined by $\langle S_0^z S_{0+l}^z\rangle$. Those have been calculated by Moreo,[12] but the results for $N=16$ were less precise. The correlation functions for $N=16$ are shown in Table I. Next we calculate the energy of a first excited state by using the same method in the space where $\sum_i S_i^z=0$ and $k=\pi$. The energy gaps of finite rings, which we denote $G(N)$'s are obtained.

A staggered susceptibility at $T=0$ is calculated as follows. We take the system subject to a staggered magnetic field, defined by the Hamiltonian

$$H'=H-h\sum_i^N(-1)^i S_i^z . \tag{3}$$

We calculate the staggered magnetization defined by

$$M_{st}(N)=\frac{1}{N}\sum_i(-1)^i\langle S_i^z\rangle , \tag{4}$$

in the ground state of this system, using the Lanczös method in the space where $\sum_i S_i^z=0$ and $k=0$ or π. Then $\chi_{st}(N)$ is obtained by differentiating M_{st} with respect to h numerically. These results are shown in the first columns of Tables II–IV, respectively.

To extrapolate these results to an infinite chain, we use Shanks' transformation.[14] The algorithm of applying it to a sequence $\{P_n\}$ is

$$P_n^{(m+1)}=\frac{P_{n-1}^{(m)}P_{n+1}^{(m)}-P_n^{(m)2}}{P_{n-1}^{(m)}+P_{n+1}^{(m)}-2P_n^{(m)}} , \tag{5}$$

where $P_n^{(0)}=P_n$. This can be used to estimate the limit P_∞ when $\{P_n\}$ has the asymptotic form

$$P_n\sim P_\infty+A\exp(-\Gamma n) , \tag{6}$$

where A and Γ are constant. The sequences of $G(N)$, $\chi_{st}(N)$, and $S_\pi(N)$ are likely to satisfy (6), because the system is not critical. In Tables II–IV are shown the results of applying Shanks' transformation to them. Only

TABLE I. Spin-correlation functions for $N=16$, calculated by the Lanczös method.

l	$(-1)^l\langle S_0^z S_{0+l}^z\rangle$
1	0.4676418
2	0.2542925
3	0.2002879
4	0.1516994
5	0.1284933
6	0.1101725
7	0.1022869
8	0.0984242

TABLE II. Results of Shanks' transformation applied to energy gaps.

N	$G(N)$	$G^{(1)}(N)$	$G^{(2)}(N)$	$G^{(3)}(N)$
4	1.0000000			
6	0.7206274	0.4875325		
8	0.5935553	0.4437757	0.4126201	
10	0.5248080	0.4255775	0.4112915	0.4107755
12	0.4841965	0.4175743	0.4109199	
14	0.4589653	0.4139409		
16	0.4427956			

TABLE III. Results of Shanks' transformation applied to staggered susceptibilities.

N	$\chi_{st}(N)$	$\chi_{st}^{(1)}(N)$	$\chi_{st}^{(2)}(N)$	$\chi_{st}^{(3)}(N)$
4	4.00000			
6	6.83293	41.91287		
8	9.45418	24.25713	19.74360	
10	11.68110	20.66253	18.67805	18.39722
12	13.46556	19.38393	18.45579	
14	14.83663	18.84616		
16	15.85833			

TABLE IV. Results of the Shanks' transformation applied to structure factors at $k=\pi$.

N	$S_\pi(N)$	$S_\pi^{(1)}(N)$	$S_\pi^{(2)}(N)$
8	2.852969		
10	3.128230	3.936074	
12	3.333536	3.908087	3.845105
14	3.484793	3.888710	
16	3.594840		

TABLE V. Results of the Shanks' transformation applied to $\{\xi_N^G\}$.

N	ξ_N^G	$\xi_N^{G(1)}$	$\xi_N^{G(2)}$
6	2.53874		
8	8.25565	5.50848	
10	3.79949	5.34724	5.23515
12	4.20192	5.28111	
14	4.49505		

TABLE VI. Results of the Shanks' transformation applied to $\{\xi_N^\chi\}$.

N	ξ_N^χ	$\xi_N^{\chi(1)}$	$\xi_N^{\chi(2)}$
6	25.75286		
8	12.26741	8.00618	
10	9.02936	6.43605	5.47919
12	7.58934	5.84151	
14	6.79981		

for $S_\pi(N)$, the data for $N=4,6$ cannot be used, because this transformation gives misconvergence due to round off or a serious finite-size effect.

Recently the ground-state energy was estimated precisely by Betsuyaku,[15] using Vanden Broech and Schwartz (VBS) method,[16] which is useful when $\{P_n\}$ has the asymptotic form[17]

$$P_n \sim P_\infty + A_1 n^{-\lambda_1} + A_2 n^{-\lambda_2} \quad (\lambda_1 < \lambda_2) . \tag{7}$$

In fact Shanks' transformation and VBS method lead to almost the same results for the ground-state energy, but the former gives a faster convergence at least for $G(N)$ and $\chi_{st}(N)$ according to our check. Thus we use Shanks' transformation. The extrapolated values are

$$G(\infty) = 0.411 \pm 0.001 ,$$

$$\chi_{st}(\infty) = 18.4 \pm 1.3 ,$$

$$S_\pi(\infty) = 3.85 \pm 0.08 .$$

The results of $G(\infty)$ and $S_\pi(\infty)$ show good agreement with estimations by Monte Carlo calculations, which are $G(\infty)=0.41$ by Nightingale and Blöte,[3] and $S_\pi(\infty)=3.9$ by Nomura.[8] To check the validity of the asymptotic form (6) for $G(N)$ and $\chi_{st}(N)$, we plot $\ln|\chi_{st}(N) - \chi_{st}(\infty)|$ and $\ln|G(N)-G(\infty)|$ vs N. Those are shown in Fig. 1. Both plots are almost linear for $N \geq 10$. Thus the form (6) seems valid.

Now we expect $\Gamma \sim 1/\xi$, where ξ is the correlation length of this system at thermodynamic limit. To examine this we take the sequences $\{\xi_N^G\}$ and $\{\xi_N^\chi\}$, defined by $1/\Gamma$ which is estimated by applying (6) to the values of $\{G(N-2), G(N), G(N+2)\}$ and $\{\chi_{st}(N-2), \chi_{st}(N), \chi_{st}(N+2)\}$, respectively. Those are given by

$$\xi_N^Q = -2/\ln\left(\frac{Q_{N+2}-Q_N}{Q_N - Q_{N-2}}\right) , \tag{8}$$

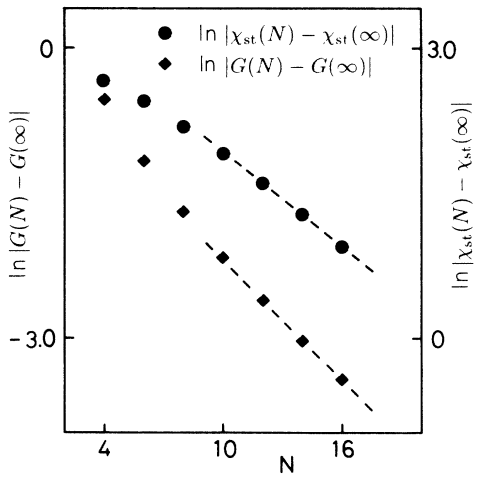

FIG. 1. $\ln|G(N)-G(\infty)|$ and $\ln|\chi_{st}(N)-\chi_{st}(\infty)|$ vs N are plotted. $G(\infty)$ and $\chi_{st}(\infty)$ are estimated by Shanks' transformation. For $N \geq 10$ both plots are almost linear, which shows exponential convergences of $G(N)$ and $\chi_{st}(N)$.

where Q is G or χ_{st}. We use Shanks' transformation again to estimate ξ_∞^G and ξ_∞^χ. The results are shown in Tables V and VI and extrapolated values are

$$\xi_\infty^G = 5.2 \pm 0.3, \quad \xi_\infty^\chi = 5.5 \pm 2.5 .$$

The two values correspond with each other well and therefore the two lines in Fig. 1 will become almost parallel as $N \to \infty$. Further these agree with the correlation length estimated by some Monte Carlo calculations, which are 5.5 ± 2 by Takahashi[7] and 6.3 by Nomura.[8] It suggests that decay constants of finite-size corrections correspond with the correlation length of the system. This consistency supports the validity of our extrapolations and the existence of an energy gap.

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