

Effect of the Haldane gap on quasi-one-dimensional systems

Tôru Sakai and Minoru Takahashi

Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo 106

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A quasi-one-dimensional $S=1$ Heisenberg antiferromagnet with a single-ion anisotropy $D \sum_j (S_j^z)^2$ is investigated. By treatment of interchain interactions with coupling constant J as a mean field, this system has been revealed to have a disordered ground state due to an effect of the Haldane gap, if J is small enough. By use of this approximation and application of the finite-size-scaling technique to a chain, the ground-state phase diagram in the JD plane is presented. This analysis leads to the prediction that $\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2(\text{ClO}_4)$ has no Néel order even at $T=0$. In addition it is found that the phase transition with respect to $D (<0)$ for a chain belongs to the two-dimensional Ising-model universality class, which agrees with Haldane's conjecture.

I. INTRODUCTION

Since Haldane¹ predicted that an antiferromagnetic Heisenberg chain has an energy gap and a massive ground state for integral S , while not for half-integral S , this prediction has been supported by many theoretical studies, especially for $S=1$. The approaches used in those are, for example, finite-size scaling,² numerical diagonalizations,³ Monte Carlo calculations,⁴ analyses of an exactly solvable model,⁵ a variational method,⁶ etc. In addition, some recent experimental studies gave evidence of the Haldane gap for CsNiCl_3 (Ref. 7) and $\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2(\text{ClO}_4)$,⁸⁻¹¹ abbreviated NENP.

Real materials taken as one-dimensional systems must have small interchain interactions. Such a quasi-one-dimensional system usually has three-dimensional long-range order at sufficiently low temperature. Actually CsNiCl_3 has Néel order below $T_N (\cong 4.9 \text{ K})$.⁷ But NENP has no Néel order, at least down to 1.2 K.⁸ This property of NENP suggests that, if interchain interactions are small enough, the system has no Néel order even at $T=0$, owing to large quantum fluctuations. It may be strange that a three-dimensional system has such a disordered ground state characteristic of one dimension, in spite of topological differences. However, the absence of Néel order even at $T=0$ has been supported by some theoretical studies, which are the perturbative approach,¹² the field theoretical analysis,¹³ the mean-field approximation for interchain couplings,¹⁴ and the rigorous proof in the reduced Hilbert space.¹⁵ Such a disordered ground state is one of the interesting quantum effects attributed to the Haldane gap. Of course, it does not appear for half-integral- S quasi-one-dimensional antiferromagnets, because the correlation length of the ground state is infinite even for a chain and even infinitesimal interchain interactions may produce the long-range order.¹⁴

In this paper we investigate the $S=1$ quasi-one-dimensional Heisenberg antiferromagnet with single-ion anisotropy, which exists in real materials such as CsNiCl_3 and NENP. The Hamiltonian is

$$H = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + D \sum_j (S_j^z)^2 + J \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where $\langle i,j \rangle$ denotes an intrachain nearest-neighbor pair and (i,j) denotes an interchain one, and the second term describes a single-ion anisotropy. J is the ratio of interchain and intrachain coupling constants and $J \ll 1$. Now J_c denotes the critical value of J , such that the system has no Néel order even at $T=0$ for $J \leq J_c$. Treating interchain interactions which are represented by the third term of (1) as a mean field, J_c is estimated for each value of D to accomplish the phase diagram in the JD plane for the ground state. A single-ion anisotropy is also important from a theoretical point of view, because a phase transition occurs at some values of D for a one-dimensional system.^{1,2} These transitions are also mentioned.

II. MEAN-FIELD APPROXIMATION FOR INTERCHAIN INTERACTIONS

We briefly review the mean-field approximation for interchain interactions^{14,16} we use in order to estimate J_c , which is the largest value of an interchain coupling constant such that the system has a disordered ground state. We restrict lattices to bipartite configurations of chains. First the case of Ising-like anisotropy ($D < 0$) is considered. In this case, Néel order is along the z axis if it exists. When a staggered mean field is substituted for the spin operators of adjacent chains, the reduced Hamiltonian describing a chain in question is

$$H_C = \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} + D \sum_j (S_j^z)^2 - h \sum_j (-1)^j S_j^z, \quad (2)$$

$$h = zJM_{\text{st}}, \quad (3)$$

where z is the number of adjacent chains, and M_{st} is a staggered magnetization defined by

$$M_{\text{st}} = \frac{1}{N} \sum_j (-1)^j \langle S_j^z \rangle. \quad (4)$$

$\langle \cdots \rangle$ denotes the ground-state expectation value of a chain described by (2). These self-consistent equations have a nonzero solution for M_{st} , if

$$zJ\chi_{\text{st}}^{\text{zz}} > 1, \quad (5)$$

where $\chi_{\text{st}}^{\text{zz}}$ is the staggered susceptibility along z axis for a chain, which is defined by

$$\chi_{\text{st}}^{\text{zz}} = \left(\frac{\partial M_{\text{st}}}{\partial h} \right)_{h=0}. \quad (6)$$

Therefore, J_c is given by

$$J_c = \frac{1}{z\chi_{\text{st}}^{\text{zz}}}. \quad (7)$$

Thus, we have only to estimate the staggered susceptibility for a one-dimensional system at $T=0$.

In order to estimate $\chi_{\text{st}}^{\text{zz}}$, we calculate numerically $\chi_{\text{st}}^{\text{zz}}(D, N)$ which denotes the staggered susceptibility of a finite ring with N sites, and extrapolate to an infinite chain. $\chi_{\text{st}}^{\text{zz}}(D, N)$ is calculated as follows. We consider an N -site ring subject to a staggered magnetic field, which is described by the Hamiltonian (2). The Lanczos algorithm is used in the reduced Hilbert space where $\sum_j S_j^z = 0$ and $k=0$ or π , to calculate the wave function of the ground state for this system, and M_{st} is estimated. $\chi_{\text{st}}^{\text{zz}}(D, N)$ is derived from the numerical differentiation of M_{st} with respect to h . Now we use Shanks' transformation¹⁷ to extrapolate to an infinite chain. The algorithm of applying this transformation to a sequence $\{P_n\}$ is

$$P'_n = \frac{P_{n-1}P_{n+1} - P_n^2}{P_{n-1} + P_{n+1} - 2P_n}. \quad (8)$$

This is useful to estimate the limit P_∞ when $\{P_n\}$ has the asymptotic form

$$P_n \sim P_\infty + O[\exp(-\Gamma n)] \quad (n \rightarrow \infty), \quad (9)$$

where Γ is a positive constant. Thus, this transformation can be used to estimate $\chi_{\text{st}}^{\text{zz}}$ at the thermodynamic limit when the system is far from a critical point D_c . D_c is the point where an energy gap disappears and $\chi_{\text{st}}^{\text{zz}}$ diverges. In order to estimate $\chi_{\text{st}}^{\text{zz}}$ at each value of D , we apply Shanks' transformation twice to $\chi_{\text{st}}^{\text{zz}}(D, N)$ calculated for $N=6, 8, 10, 12, 14$. For example, the result for $D=-0.02$ is shown in Table I. It leads to $\chi_{\text{st}}^{\text{zz}}=21 \pm 1$ at $D=-0.02$. This extrapolation cannot be performed for $D < -0.1$ because (9) is not satisfied.

Next the case of XY -like anisotropy ($D > 0$) is considered. In this case, the Néel order of a quasi-one-dimensional system would appear in the xy plane. Thus, J_c is given by

$$J_c = \frac{1}{z\chi_{\text{st}}^{\text{xx}}}, \quad (10)$$

where $\chi_{\text{st}}^{\text{xx}}$ is the staggered susceptibility along the x axis for a chain. In order to estimate $\chi_{\text{st}}^{\text{xx}}$, we have to treat rings subject to a staggered magnetic field described by $-\hbar \sum_j (-1)^j S_j^x$, instead of the third term of (2). This

TABLE I. Result of Shanks' transformation applied to $\chi_{\text{st}}^{\text{zz}}(D, N)$ for $D = -0.02$.

N	$\chi_{\text{st}}^{\text{zz}}(D, N)$		
6	7.18167		
8	10.0985	30.1183	
10	12.6444	24.2350	21.3167
12	14.7318	22.2843	
14	16.3672		

term cannot commute with $\sum_j S_j^z$. Thus, the Lanczos method has to be performed in a larger Hilbert space where $k=0$ or π to calculate $\chi_{\text{st}}^{\text{xx}}(D, N)$ for finite rings. To extrapolate to an infinite system, we use the same method as for $D < 0$. Here Shanks' transformation cannot be applied for $0.3 < D < 1.6$ because the system is close to a critical region.

Using the above methods, we estimate J_c for $-0.1 < D < 0.3$ and $D > 1.6$, and give the detailed phase diagram of the quasi-one-dimensional system in the JD plane for $-0.1 < D < 0.3$ in Fig. 8.

III. PHASE BOUNDARIES OF A CHAIN

A. Finite-size scaling and phenomenological renormalization

In order to get the complete phase diagram in the JD plane for the quasi-one-dimensional system (2), we also investigate the behavior of $\chi_{\text{st}}^{\text{zz}}$ and $\chi_{\text{st}}^{\text{xx}}$ of a chain for regions close to critical points. The behavior of an energy gap of a chain is sketched in Fig. 1, which has been given by Botet, Jullien, and Kolb,² using the phenomenological renormalization-group method and the finite-size-scaling technique¹⁸ up to $N=12$. But the critical behavior at D_{c2} is altered to be adapted to the result presented later in this paper. There are three critical points at most, as shown in Fig. 1. Glaus and Schneider¹⁹ conjectured $D_{c2}=D_{c3}$ with different critical exponents between the right- and left-hand sides using the similar method up to $N=14$. In order to estimate more precise values of D_c

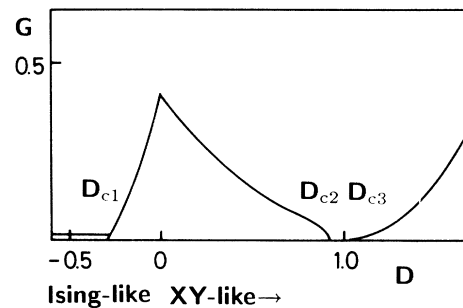


FIG. 1. Variation of an energy gap with a single-ion anisotropy parameter D for an infinite chain. D_{c1} , D_{c2} , and D_{c3} are critical points. It is noted that ν is smaller than 1 according to the present analysis by the phenomenological renormalization-group method up to $N=16$.

and a critical exponent γ , which is defined by

$$\chi_{\text{st}}(D, \infty) \sim |D - D_c|^{-\gamma}, \quad (11)$$

at each critical point, we perform the phenomenological renormalization-group and the finite-size-scaling methods again, up to $N=16$.

Then we review those techniques briefly as follows. Now $G(D, N)$ denotes an energy gap of an N -site ring. According to the theory of conformal invariance,²⁰ the behavior of an energy gap at a critical point has the asymptotic form

$$G(D_c, N) \sim \frac{1}{N} \quad (N \rightarrow \infty). \quad (12)$$

Based on the property (12), the phenomenological renormalization-group equation is constructed as follows:

$$(N+2)G(D', N+2) = NG(D, N). \quad (13)$$

$D_c(N, N+2)$ denotes the N -dependent fixed point and it is extrapolated to the thermodynamic limit, in order to estimate D_c . Next, to estimate a critical exponent ν , determined by

$$G(D, \infty) \sim |D - D_c|^\nu, \quad (14)$$

we define

$$\nu(N, N+2) = \ln \left[\frac{N+2}{N} \right] / \ln \left[\frac{(N+2)G'(N+2)}{NG'(N)} \right], \quad (15)$$

where $G'(N)$ denotes the derivative of $G(D, N)$ with respect to D , at $D = D_c(N, N+2)$. The form (15) is derived from linearizing Eq. (13) near the fixed point $D_c(N, N+2)$. Further, we define an exponent ω by

$$\chi_{\text{st}}(D_c, N) \sim N^\omega \quad (N \rightarrow \infty). \quad (16)$$

If ω is known, γ is determined by the relation

$$\gamma = \nu\omega, \quad (17)$$

which is derived from the finite-size-scaling hypothesis.²¹ In addition, η is defined by

$$\langle S_0^z S_r^z \rangle \sim (-1)^r r^{-\eta} \quad (r \rightarrow \infty), \quad (18)$$

at $D = D_c$ and $N \rightarrow \infty$. Since it is difficult to estimate η accurately by an analysis of correlation functions of small systems, we make use of the relation

$$\left\langle \left[\frac{1}{N} \sum_j (-1)^j S_j^z \right]^2 \right\rangle \sim N^{-\eta} \quad (N \rightarrow \infty), \quad (19)$$

at $D = D_c$, instead. This is derived from (18) approximately if $\eta < 1$.

B. Calculations and results

1. Ising-like region ($D < 0$)

Independent of a sign of D , the ground state of a chain without an external field belongs to the space where

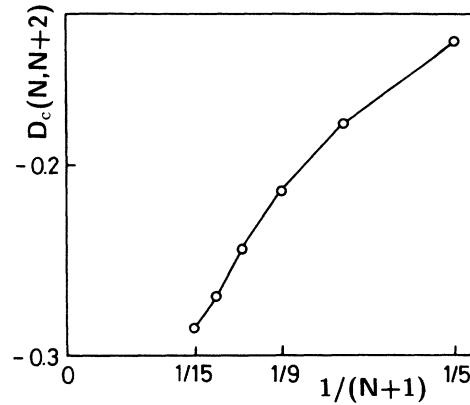


FIG. 2. Fixed point $D_{c1}(N, N+2)$ of the phenomenological renormalization-group equation for an energy gap, plotted vs $1/(N+1)$.

$\sum_j S_j^z = 0$ and $k=0$. For $D < 0$, the first excited state is the lowest-energy state in the space where $\sum_j S_j^z = 0$ and $k = \pi$. Thus, $G(D, N)$ can be obtained, calculating the lowest energy in each space by the Lanczos method. We apply the phenomenological renormalization to $G(D, N)$ up to $N=16$. The results of $D_{c1}(N, N+2)$ and $\nu(N, N+2)$ are plotted versus $1/(N+1)$ in Figs. 2 and 3, respectively. $D_{c1}(N, N+2)$ does not converge well, but ν rapidly converges to 1.03 at $N=14$. This behavior of $\nu(N, N+2)$ suggests that the finite-size correction decays faster than it does algebraically, but it vanishes so suddenly that it is difficult to perform a precise extrapolation from smaller-size data. In fact, the curve of $D_{c1}(N, N+2)$ bends only slightly at $N=14$, but maybe it converges at the next point, if we get it. Thus, we regard the largest-size result as the best value we can get, and we think that its error is about the difference from the next-largest-size result, that is, $D_{c1} = -0.29 \pm 0.01$. Next we calculate ω , applying relation (16) to $\chi_{\text{st}}^{zz}(-0.29, N)$ and $\chi_{\text{st}}^{zz}(-0.29, N+2)$. The results are shown in Table II. η is also calculated, using (19), as shown in Table III. Further, γ is obtained by (17). By the same analysis as D_{c1} ,

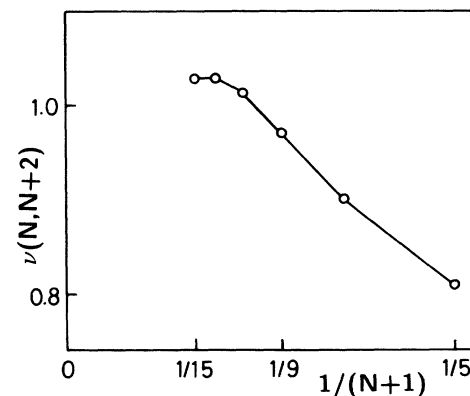


FIG. 3. Exponent $\nu(N, N+2)$ of the phenomenological renormalization-group equation for an energy gap at D_{c1} , plotted vs $1/(N+1)$. It converges at $N=14$ and gives $\nu \cong 1.03$.

TABLE II. Exponent ω estimated by applying the asymptotic form (16) to $\chi_{st}(D, N)$ calculated at $D = -0.29, 0.93,$ and $1.01,$ which are critical points $D_{c1}, D_{c2},$ and D_{c3} estimated by the phenomenological renormalization-group method.

N	ω		
	$D = -0.29$	$D = 0.93$	$D = 1.01$
4			
6	2.017	1.724	1.713
8	2.031	1.611	1.654
10	1.988	1.638	1.634
12	1.912	1.629	1.626
14	1.828	1.625	1.623
16	1.761		

we estimate these exponents at the thermodynamic limit. The results about this phase transition are as follows:

$$\begin{aligned}
 D_{c1} &= -0.29 \pm 0.01, \\
 \nu &= 1.03, \\
 \omega &= 1.76 \pm 0.06, \\
 \gamma &= 1.81 \pm 0.06, \\
 \eta &= 0.26 \pm 0.02.
 \end{aligned}$$

The scaling relation

$$\gamma = \nu(2 - \eta) \tag{20}$$

holds within the errors. Based on these results, it is reasonable to determine that this transition belongs to the

TABLE III. Exponent η estimated by applying the asymptotic form (19) to $\langle (1/N \sum_j (-1)^j S_j^2)^2 \rangle$ calculated at $D = -0.29, 0.93,$ and $1.01,$ which are critical points $D_{c1}, D_{c2},$ and D_{c3} estimated by the phenomenological renormalization-group method.

N	η		
	$D = -0.29$	$D = 0.93$	$D = 1.01$
4			
6	0.209	0.321	0.325
8	0.195	0.338	0.341
10	0.203	0.347	0.349
12	0.221	0.351	0.353
14	0.241	0.354	0.356
16	0.260		

same universality class as the two-dimensional Ising model, whose critical exponents are $\nu=1, \gamma=1.75,$ and $\eta=0.25.$ This statement agrees with Haldane's conjecture. We think that the small difference of ν from 1 is attributed to the logarithmic correction for (12), predicted by conformal invariance.²² Thus, we use $\nu=1$ and $\gamma=1.75$ for later analyses.

2. XY-like region ($D > 0$)

For $D > 0,$ the first excited state exists in the space where $\sum_j S_j^z = \pm 1.$ Thus, the Lanczos algorithm is executed there to calculate $G(D, N)$ up to $N=16,$ but $\chi_{st}^{xx}(D, N)$ can only be calculated up to $N=14$ owing to the memory limit of a computer because $\sum_j S_j^z$ does not conserve under a staggered magnetic field along the x axis. Now the same analysis is applied to critical points D_{c2} and $D_{c3},$ as the Ising-like case. The results are shown in Figs. 4 and 5 and Tables II and III. Then our estimations are as follows:

$$\begin{aligned}
 D_{c2} &= 0.93 \pm 0.02, \\
 \nu &= 0.16 \pm 0.04, \\
 \omega &= 1.625 \pm 0.004, \\
 \gamma &= 0.26 \pm 0.07, \\
 \eta &= 0.354 \pm 0.003,
 \end{aligned}$$

and

$$\begin{aligned}
 D_{c3} &= 1.01 \pm 0.01, \\
 \nu &= 1.29 \pm 0.04, \\
 \omega &= 1.623 \pm 0.003, \\
 \gamma &= 2.09 \pm 0.07, \\
 \eta &= 0.356 \pm 0.003.
 \end{aligned}$$

As shown in Fig. 5, ν is likely to converge to a finite limit

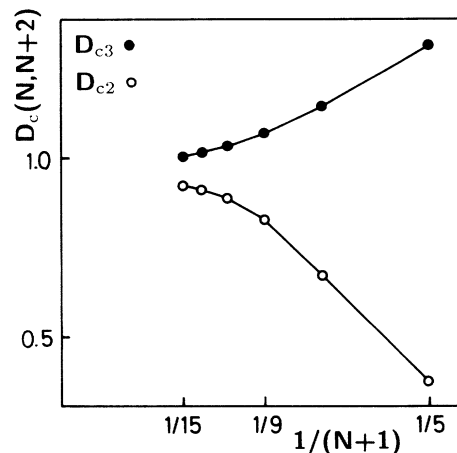


FIG. 4. Fixed points $D_{c2}(N, N+2)$ and $D_{c3}(N, N+2)$ of the phenomenological renormalization-group equation for an energy gap, plotted vs $1/(N+1).$ It cannot be determined definitely whether $D_{c2} = D_{c3}$ is true or not.

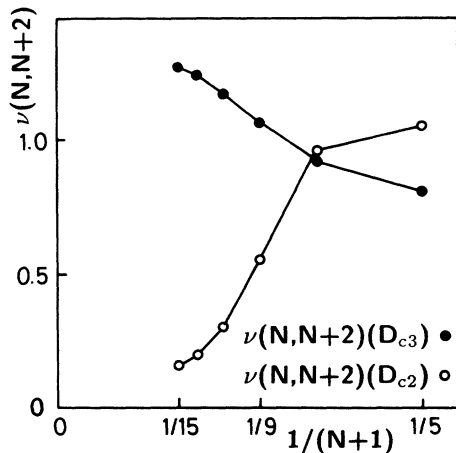


FIG. 5. Exponent $\nu(N, N+2)$ of the phenomenological renormalization-group equation for an energy gap at D_{c2} and D_{c3} , plotted vs $1/(N+1)$.

in each case. Further, the scaling relation (20) is also satisfied. Thus, both are algebraic phase transitions. It corresponds with Glaus and Schneider's conclusion.¹⁹ However, our estimation leads to $D_{c2} \neq D_{c3}$, which is against their conjecture. Therefore, whether $D_{c2} = D_{c3}$ is true, is still an unsolved problem.

IV. PHASE DIAGRAM IN THE JD PLANE

Having determined the values of χ_{st}^{zz} and χ_{st}^{xx} for D far from critical points, and a critical exponent γ , we give the whole behavior of $\chi_{st}^{zz}(D < 0)$ and $\chi_{st}^{xx}(D > 0)$ for a chain, which is a solid line in Fig. 6. For $-0.1 < D < 0.3$ and $D > 1.6$, we use the values extrapolated from finite rings up to $N=14$, and for other region the line is so extrapolated as to give the estimated critical exponent at each critical point. The dashed curves are the results for finite rings up to $N=12$. Now we can get the entire phase diagram in the JD plane for the quasi-one-dimensional system described by the Hamiltonian (1), us-

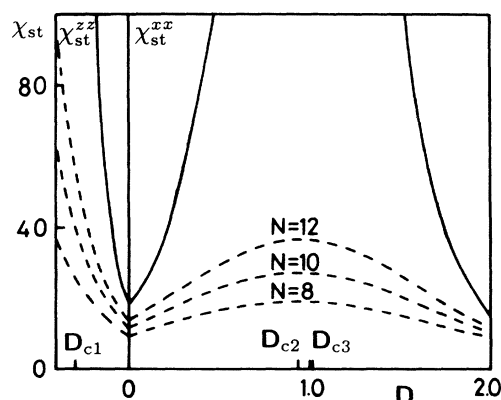


FIG. 6. Variation of the staggered susceptibilities $\chi_{st}^{zz}(D < 0)$ and $\chi_{st}^{xx}(D > 0)$ for a chain. The solid and dashed curves represent those of an infinite chain and N -site rings, respectively.

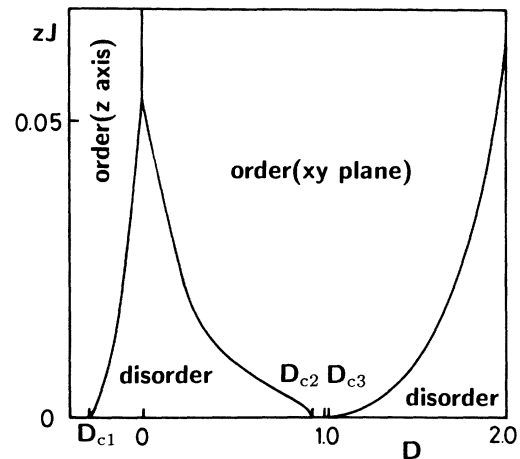


FIG. 7. Outlined phase diagram in the JD plane for the ground state of a quasi-one-dimensional system. z is the number of adjacent chains.

ing the formulas (7) and (10). It is shown in Fig. 7, where z is the number of adjacent chains. We explicitly distinguish D_{c2} from D_{c3} , but the two points are possibly identical. For a later discussion, it is convenient to show a magnified phase diagram for $-0.1 < D < 0.3$, in Fig. 8. An error attributed to extrapolation is a few percent at most, for each point. Thus, we do not draw an error bar explicitly.

V. DISCUSSION

Through the above analysis, it is found that a disordered ground state can exist even in a quasi-one-dimensional system with a single-ion anisotropy if inter-chain interactions are sufficiently small. Then we refer to

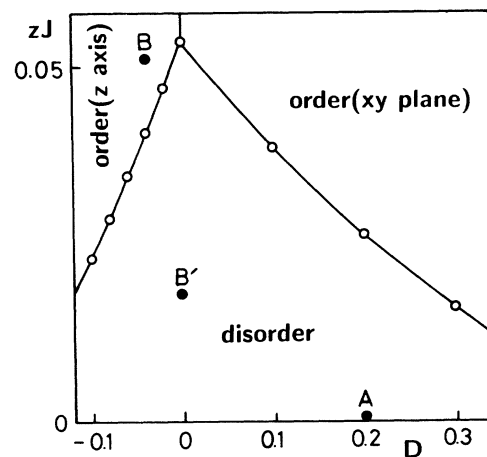


FIG. 8. Phase diagram in the DJ plane for the ground state of a quasi-one-dimensional system, in the region $-0.1 < D < 0.3$. An error due to the extrapolation of χ_{st} is less than a few percent for each point. The result of the neutron-scattering experiment for NENP is located at A . In the case of CsNiCl_3 , the result by Buyers *et al.* is located at B and that by Kakurai *et al.* is located at B' .

consistency with the results of experiments.

NENP has orthorhombic structure. The number of nearest adjacent chains is 2 and that of next-nearest ones is also 2. Thus, we put $z=4$, which leads to smaller estimation of J_c . The neutron-scattering experiments⁹ yielded $J=0.0004$ and $D=0.2$ (*XY* like), which is located at *A* in Fig. 8. NENP is completely included by the disordered region. Apart from this, recent magnetization measurements have given a critical magnetic field along the z axis, which are $g\mu_B H_c^{\parallel} \cong 11$ K by Katsumata *et al.*¹⁰ and 14 K by Ajiro *et al.*¹¹ Since the first excited state has the property $\sum_j S_j^z = \pm 1$, those give an energy gap, and lead to $G \cong 0.23$ and 0.29 , respectively, where we take an intrachain coupling constant as 48 K which was estimated by the susceptibility measurement.²³ To estimate D from these results, a D -versus- G plot for a chain is presented in Fig. 9, where G is an energy gap of an infinite chain estimated by Shanks' transformation from finite rings up to $N=14$, just as χ_{st} . Referring to this plot, the two experimental results lead to $D \cong 0.2$ and 0.3 , respectively. Thus, NENP may be located a little more to the right than *A* in Fig. 8. Nevertheless, NENP is in a disordered region, for J is very small. Therefore, we conclude that NENP has no Néel order even at $T=0$, and it has an energy gap in spite of small interchain interactions. It suggests that NENP is an ideal material to study on the Haldane gap. The present analysis is consistent with no discovery of Néel order down to 1.2 K. We are looking forward to a measurement at lower temperature for NENP.

CsNiCl₃ has been revealed to have Néel order below $T_N (\cong 4.9$ K) by neutron-scattering experiments.⁷ Since chains are arranged in a triangular lattice in CsNiCl₃, sites cannot be divided into two sublattices. Thus, this case is beyond our analysis, but the three-dimensional long-range order measured by experiments has almost a classical 120° structure, at least below $T'_N (\cong 4.4$ K).⁷ When the mean-field approximation for interchain interactions is applied to such a case, we have only to sub-

stitute $M_{st} |\cos 120^\circ|$ for an interaction with each adjacent chain, within the lowest order. Since the number of adjacent chains is six, we may put $z=3$ to refer to the phase diagram in Fig. 8 in this case. Buyers *et al.*⁷ determined $J=0.017$ and $D=-0.038$ (Ising-like) about CsNiCl₃, fitting the spin-wave approximation to the results of neutron-scattering measurements. This is located at *B* in Fig. 8, which is in an ordered region. Thus, the present analysis is also consistent with this experiment. However, Kakurai *et al.*²⁴ have recently found $J=0.006$ and $D=-0.002$ by the polarized neutron-scattering measurement. This result was also derived from fitting the spin-wave approximation, but taking a spin-flip process into consideration. This is located at *B'* in Fig. 8, which is in a disordered region. Thus, it is inconsistent in turn. On the other hand, Affleck¹³ has applied the field theoretical technique to the lattice like CsNiCl₃, and determined $J_c \cong 0.013$ neglecting D . This estimation also does not agree with the result by Kakurai *et al.* In our opinion, CsNiCl₃ has such small interchain interactions that the spin-wave approximation they used is not valid owing to large quantum fluctuations.

Next we consider the nature of the present analysis. The method we use in order to estimate J_c is partly based on a mean-field approximation. Intuitively a mean-field theory tends to overestimate order. In fact, a mean-field approximation for interchain interactions gives an upper bound of T_c at least for the quasi-one-dimensional Ising model.¹⁶ It suggests that the present analysis gives a lower bound of J_c . But this statement is not rigorous and whether it is true or not is too delicate a problem to solve here.

At last we discuss the relation between G and J_c . J_c is plotted versus G in Fig. 10 for $-0.1 < D < 0.3$. The curves for the Ising-like and *XY*-like cases almost coincide with each other. Thus, J_c is determined only by G independently of a sign of D , for a large energy gap. Ac-

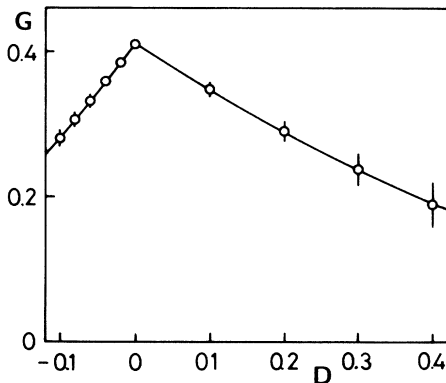


FIG. 9. Variation of an energy gap with a single-ion anisotropy parameter D for an infinite chain, in the region $-0.1 < D < 0.4$. Each point is estimated by Shanks' transformation applied to finite rings for $N=6, 8, 10, 12, 14$. Each error is due to the extrapolation.

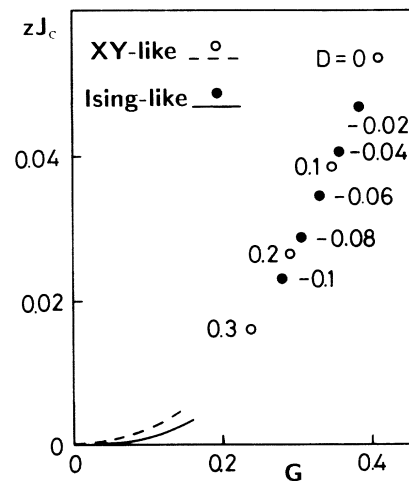


FIG. 10. Plot of zJ_c vs G for $-0.1 < D < 0.3$. The solid and dashed lines represent behaviors of J_c for the Ising-like and *XY*-like cases, respectively, in the small- G region.

ording to the critical behaviors of χ_{st} and G , J_c has the form

$$J_c \sim G^\omega \quad (G \rightarrow 0), \quad (21)$$

where $\omega = 1.75$ for Ising-like case and $\omega \cong 1.6$ for XY -like case. Therefore, in the small-gap region, an energy gap is more effective in destroying Néel order for the XY -like case, within the present analysis.

VI. CONCLUSION

In this paper a quasi-one-dimensional Heisenberg antiferromagnet with a single-ion anisotropy is studied. Treating interchain interactions as a mean field, the largest value of an interchain coupling constant J_c with a disordered ground state is given by $1/(z\chi_{st}^{zz})$ for $D < 0$ and $1/(z\chi_{st}^{xx})$ for $D > 0$, where χ_{st}^{zz} and χ_{st}^{xx} are the stag-

gered susceptibilities of a chain. Then we determine the behavior of χ_{st}^{zz} and χ_{st}^{xx} by the finite-size-scaling technique and present the ground-state phase diagram in the JD plane, as shown in Fig. 8. This result suggests that NENP has no Néel order even at $T=0$.

In addition, it is found that the phase transition of a chain at $D \cong -0.29$ belongs to the same universality class as the two-dimensional Ising model. It agrees with Haldane's conjecture.

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