Haldane, Large-\(D\) and Intermediate-\(D\) States in an \(S=2\) Quantum Spin Chain with On-Site and \(XXZ\) Anisotropies

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Using mainly numerical methods, we investigate the ground-state phase diagram of the \(S=2\) quantum spin chain described by

\[
\mathcal{H} = \sum_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) + D \sum_j (S_j^z)^2, 
\]

where \(S_j^\alpha (\alpha = x, y, z)\) is the \(\alpha\)-component of the \(S=2\) operator at the \(j\)-th site, and \(\Delta\) and \(D\) are, respectively, the \(XXZ\) anisotropy parameter of the on-site interactions and the on-site anisotropy parameter. Hereafter, we denote the total number of spins in the system by \(N\), assumed to be even, and the \(z\) component of the total spin by \(M(= \sum_j S_j^z)\).

The ground-state phase diagram on the \(\Delta-D\) plane of the same Hamiltonian in the \(S=1\) case was discussed by Schulz\(^3\) and den Nijs and Rommelus\(^4\) and numerically determined by Chen et al.\(^5\). In the present \(S=2\) case, Schulz\(^3\) discussed the ground-state phase diagram with six phases obtained by the bosonization method; the phases are, in our terminology, the ferromagnetic (FM) phase, the Néel phase, the XY1 phase, the XY4 phase, the Haldane phase and the large-\(D\) (LD) phase. The XY1 state is characterized by the power decay of the spin correlation function \(G_{\perp 1}(r)\) and the exponential decay of \(G_{\perp 4}(r)\), whereas the XY4 state by the exponential decay of \(G_{\perp 1}(r)\) and the power decay of \(G_{\perp 4}(r)\). The valence bond pictures of the Haldane state and the LD state are shown in Figs. 1(a) and (c), respectively. About twenty years ago, Oshikawa\(^6\) predicted, in \(S\geq2\) integer quantum spin cases, the existence of the intermediate-\(D\) (ID) phase, the valence bond picture of which is depicted in Fig. 1(b). Figure 2(a) is an interpretation of Oshikawa’s prediction by Aschauer and Schollwöck\(^7\) in the \(S=2\) case.

On the other hand, carrying out the density-matrix renormalization-group (DMRG) calculation, Schollwöck et al.\(^8,9\) and Aschauer and Schollwöck\(^7\) proposed the phase diagram in Fig. 2(b) and concluded the absence of

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On the other hand, carrying out the density-matrix renormalization-group (DMRG) calculation, Schollwöck et al.\(^8,9\) and Aschauer and Schollwöck\(^7\) proposed the phase diagram in Fig. 2(b) and concluded the absence of
the ID phase in the present $S=2$ model. Furthermore, performing the level spectroscopy\cite{10,11} (LS) analysis of the numerical results of exact-diagonalization calculations, Nomura and Kitazawa\cite{11} showed in the case of $\Delta=1$ that, with the increase of $D$ from zero, the ground state changes from the Haldane state to the $XY$ state at $D_{c1}=0.043$ and after that from the $XY$ state to the LD state at $D_{c2}=2.39$. Thus, it has been considered for a long time that the ID phase does not exist in the phase diagram of this model.

The purpose of the present work is to determine as precisely as possible the ground-state phase diagram on the $\Delta-D$ plane of the $S=2$ quantum spin chain described by the Hamiltonian (1). We mainly employ numerical methods based on the exact-diagonalization calculation for finite-spin systems with up to $N=12$, the details of which are described below. For simplicity, we restrict ourselves to the $\Delta \geq 0$ and $D \geq 0$ case. The full phase diagram will be discussed in our future reports.

Figure 3 shows our final result for the ground-state phase diagram. In this phase diagram five states, that is, the $XY1$, LD, ID, Haldane and Néel states, appear as the ground states. As we will discuss later in detail, the Haldane and LD states belong to the same phase, which we denote as the Haldane/large-$D$ (Haldane/LD) phase. Therefore, the phase diagram consists of four phases; they are the $XY1$, LD, Haldane/ID and Néel phases.

In the following discussions for the determination of phase boundary lines, we denote, respectively, by $E_0(N,M;\text{pbc})$ and $E_1(N,M;\text{pbc})$ the lowest and second-lowest energy eigenvalues of the Hamiltonian (1) with periodic boundary conditions within the subspace determined by $N$ and $M$. We also denote by $E_0(N,M,P;\text{tbc})$ the lowest energy eigenvalue of the Hamiltonian (1) with twisted boundary conditions, where an antiferromagnetic bond is twisted, within the subspace determined by $N$, $M$ and $P$. Here, $P(=+1$ or $-1)$ is the eigenvalue of the space inversion operator with respect to the twisted bond.

Both the transition between the Haldane and ID states and that between the LD and ID states are the Gaussian transition, and those between the $XY1$ state to one of the above three states are the Berezinskii-Kosterlitz-Thouless transition.\cite{12,13} Following the LS method\cite{10,11}, we should compare three excitation energies, $E_0(N,0,+1;\text{tbc}) - E_0(N,0;\text{pbc})$, $E_0(N,0,-1;\text{tbc}) - E_0(N,0;\text{pbc})$ and $E_0(N,2;\text{pbc}) - E_0(N,0;\text{pbc})$ in the $N \to \infty$ limit. Namely, the ground state is one of the Haldane/LD, ID and $XY1$ states, depending on whether the first, second or third excitation energy is the lowest among them. A physical and intuitive explanation for this method is given in our recent paper.\cite{14}

From the above arguments, for a fixed $D$, the critical value of the Haldane-ID transition, $\Delta_c^{(H,\text{ID})}$, and that of the ID-LD transition, $\Delta_c^{(\text{ID},\text{LD})}$, can be evaluated by the $N \to \infty$ extrapolation of $\Delta_c^{(H,\text{ID})}(N)$ and $\Delta_c^{(\text{ID},\text{LD})}(N)$, respectively, determined from the equation (\ref{eq1},\ref{eq2})

\begin{equation}
E_0(N,0,+1;\text{tbc}) = E_0(N,0,-1;\text{tbc}) < E_0(N,2;\text{pbc}).\tag{2}
\end{equation}

Our calculations show that eq. (2) has two solutions $\Delta_c^{(H,\text{ID})}(N)$ and $\Delta_c^{(\text{ID},\text{LD})}(N)$ for $N=8$, 10 and 12 in the region of $1.0 \leq D \leq 2.05$, where $\Delta_c^{(H,\text{ID})}(N) > \Delta_c^{(\text{ID},\text{LD})}(N)$. In this region of $D$, we have estimated $\Delta_c^{(H,\text{ID})}(N)$ and $\Delta_c^{(\text{ID},\text{LD})}(N)$ by numerically solving eq. (2), and then extrapolated these results for $N=8$, 10 and 12 to $N \to \infty$ by assuming that their $N$-dependences are quadratic functions of $N^{-2}$. Examples are shown in Fig. 4(a) and Table I. Thus, we

\begin{figure}[h]
(a) \hspace{1cm} (b)
\begin{center}
\includegraphics[width=0.8 \textwidth]{fig2.png}
\end{center}
\caption{(Color) The ground-state phase diagram on the $\Delta-D$ plane determined in the present work; in (b), part of (a) is enlarged. Note that the H and LD states belong to the same phase. See the text for more details.}
\end{figure}
have obtained the Haldane-ID and ID-LD boundaries, which are shown, respectively, by the red and blue solid lines in Fig. 3.

![Graph showing the Haldane-ID and ID-LD transitions](image)

**Fig. 4.** (a) Examples of the Haldane-ID and ID-LD transitions with $D = 1.82$ and $N = 12$, where $\Delta E_{\text{ID}}^{\text{ID}}(N) \equiv E_0(N, 0, -1; \text{tbc}) - E_0(N, 0, +1; \text{tbc})$. From this, we obtain $\Delta c_{(\text{H-ID})}(12) = 2.23793$ and $\Delta c_{(\text{H-ID})}(12) = 2.16639$ by the interpolation. We note that $E_0(N, 0; \text{pbc})$ is higher than $E_0(N, 0, +1; \text{tbc})$ in this regime. (b) An example of the XY1-LD transition with $D = 1.82$ and $N = 12$, where $\Delta c_{(\text{ID})}^{\text{ID}}(N) \equiv E_0(N, 2; \text{pbc}) - E_0(N, -1; \text{tbc})$. From this, we obtain $\Delta c_{(\text{XY1-ID})}(12) = 2.14265$ by the interpolation. We note that $E_0(N, 0, -1; \text{tbc})$ is higher than $E_0(N, 0, +1; \text{tbc})$ in this regime.

**Table 1.** Examples of critical values of $\Delta$ in the case of $D = 1.82$ obtained by the LS method.

| N   | $\Delta c_{(\text{H-ID})}^{\text{ID}}(N)$ | $\Delta c_{(\text{H-ID})}^{\text{ID}}(N)$ | $\Delta c_{(\text{XY1-ID})}^{\text{ID}}(N)$ |
|-----|------------------------------------------|------------------------------------------|------------------------------------------|
| 6   | 2.17687                                  | 2.14971                                  | 2.08931                                  |
| 8   | 2.22262                                  | 2.16106                                  | 2.12246                                  |
| 10  | 2.23529                                  | 2.16527                                  | 2.13607                                  |
| 12  | 2.23793                                  | 2.16639                                  | 2.14265                                  |
| $\infty$ | 2.241 ± 0.001                             | 2.167 ± 0.001                             | 2.156 ± 0.001                             |

We have found that the maximum value of $D$ for which eq. (2) has two solutions exists for each value of $N$ and that, although this maximum value increases as $N$ increases, it approaches a finite value in the limit of $N \to \infty$. For example, eq. (2) has two solutions only when $D \lesssim 2.05$, $D \lesssim 2.14$ and $D \lesssim 2.17$, respectively, for $N = 8$, 10 and 12. We have also found that, when eq. (2) has no solution, the relation $E_0(N, M, +1; \text{tbc}) < E_0(N, M, -1; \text{tbc})$ always holds. These show that, for sufficiently large values of $D$, the ID state does not appear in the ground-state phase diagram and the crossover between the Haldane and LD states may take place, which means that the Haldane and LD states belong to the same phase. In fact, the extrapolated lines of the phase boundary line between the Haldane and ID states and that between the ID and LD states, which are shown, respectively, by the red and blue dotted lines in Fig. 3, merge at the point $(\Delta, D) \sim (2.64, 2.19)$.

The fact that the Haldane and LD states belong to the same phase is very reasonable for the following reasons: (A) as discussed above, $P = +1$ for both states; (B) in the case in which open boundary conditions are imposed, it is clear that there exists no edge state in the LD state (see Fig. 1(b)), and also Pollmann et al.\(^{15,16}\) showed very recently that two $S = 1/2$ spins left at each edge in the Haldane state are in the $(S_{\text{tot}}, S_{\text{tot}}) = (1, 0)$ state, which leads to the no-edge state, at least if $\Delta > 1$ and $D > 0$ are satisfied; (C) Pollmann et al.\(^{15}\) constructed a one-parameter matrix product state which interpolates the Haldane and LD states without any quantum phase transition. Although the Haldane and LD states are apparently different from each other from the valence-bond pictures in Figs. 1(a) and (c), they belong to the same phase. Here, we give two examples for such a situation. One is an antiferromagnetic $S = 1$ chain with the bond alternation and the on-site anisotropy,\(^{17,18}\) in which the LD state and the dimer state belong to the same phase. The other is an antiferromagnetic $S = 1$ two-leg ladder,\(^{19}\) where the Haldane state and the rung-dimer state belong to the same phase called the four-site plaquette singlet phase.

In a similar way, for a fixed $D$, the critical values $\Delta c_{(\text{XY1-H})}^{(\text{XY1-H})}$ and $\Delta c_{(\text{XY1-LD})}^{(\text{XY1-LD})}$ of the XY1-Haldane and XY1-LD transitions, respectively, can be obtained from

$$E_0(N, 0, +1; \text{tbc}) = E_0(N, 2; \text{pbc}) < E_0(N, 0, -1; \text{tbc}).$$

(3)

An example is shown in Fig. 4(b) and Table I. For the critical value $\Delta c_{(\text{XY1-ID})}$ of the XY1-ID transition, we have to solve

$$E_0(N, 0, -1; \text{tbc}) = E_0(N, 2; \text{pbc}) < E_0(N, 0, +1; \text{tbc})$$

(4)

instead of eq. (3). Thus, we have obtained the phase boundary lines between the XY1 state and one of the Haldane, ID and LD states, which are depicted, respectively, by the brown, black and cyanic lines in Fig. 3.

Finally, the phase transition between the Haldane and Néel states is of the 2D Ising type, since the $Z_2$ symmetry is broken in the Néel state. In this case the phenomenological renormalization group (PRG) method\(^{20}\) is useful for determining the phase boundary line. We have numerically solved the PRG equation,

$$(N - 2) \{ E_1(N - 2, 0; \text{pbc}) - E_0(N - 2, 0; \text{pbc}) \} = N \{ E_1(N, 0; \text{pbc}) - E_0(N, 0; \text{pbc}) \},$$

(5)

to obtain the solution $\Delta c_{(\text{H,N})}^{(\text{H,N})}(N)$ for a given value of $D$. Then, we have extrapolated, to estimate the critical value $\Delta c_{(\text{H,N})}^{(\text{H,N})}$, these results for $N = 8, 10$ and 12 to $N \to \infty$ by assuming that their $N$-dependences are quadratic functions of $(N - 1)^{-2}$, and have determined the phase boundary line as shown by the green line in Fig. 3. It is expected that $D c_{(\text{H,N})}^{(\text{H,N})}$ approaches $D c_{(\text{H,N})}^{(\text{H,N})} = \Delta$ in the $\Delta \to \infty$ limit. This is because in the case of the Ising limit, governed by the Hamiltonian $H_{\text{Ising}} = \Delta \sum_{j} S_{j}^{z} S_{j+1}^{z} + D \sum_{j}(S_{j}^{x})^{2}$, when $D > \Delta$ the ground state of the present system is the $S_{j}^{z} = 0$ state, and when $D < \Delta$ it is the Néel state with $S_{j}^{z} = 2(1)^{j}$ and that with $S_{j}^{z} = 2(-1)^{j+1}$ state which are degenerate with each other. In the $\Delta \to \infty$ limit the transition line between the Néel state and the Haldane state becomes of the first order, as is expected from the above Ising limit Hamiltonian $H_{\text{Ising}}$. Therefore, on the Haldane-Néel transition line, there should exist a
special point at which the transition changes from the second order to the first order as \( \Delta \) increases. The details of this point are left for a future study.

The LS method\(^{10,11} \) is based on the sine-Gordon theory or, equivalently, the \( c = 1 \) conformal field theory with the perturbation, where \( c \) is the central charge. Then, in order to check the applicability of the LS method, we have calculated the central charge \( c \) from the finite-size correction of the ground-state energy per one spin,\(^{21–23} \)

\[
\frac{E_0(N, 0; \text{pbc})}{N} \approx \lim_{N \to \infty} \frac{E_0(N, 0; \text{pbc})}{N} - \frac{\pi v_s c}{6N^2} \quad (6)
\]

where \( v_s \) is the spin wave velocity. The central charge \( c \) is defined only in the gapless region, and it becomes zero in the gapped region if the above formula is formally applied. Along the line \( D = 1.9 \), where the ground-state changes as \( XY1 \Rightarrow LD \Rightarrow ID \Rightarrow \text{Haldane} \Rightarrow \text{Néel} \) with the increase of \( \Delta \) from zero, we found that the values of “apparent \( c \)” are \( c \approx 1 \) for \( 0 < \Delta < 2.7 \) and \( c \approx 0 \) for \( \Delta > 2.7 \). This result shows that our system is effectively described by the sine-Gordon theory, which ensures the applicability of the LS method and is consistent with the smallness of gaps in the LD, ID and Haldane states along this line. Nomura and Kitazawa\(^{11} \) also found that \( c \approx 1 \) at the Haldane/\( XY1 \) and \( XY1\)-LD transition points on the \( \Delta = 1 \) line and at the \( XY1\)-Haldane transition point on the \( D = 0 \) line.

In conclusion, we have determined rather precisely the ground-state phase diagram on the \( D \)-plane of the \( S = 2 \) quantum spin chain described by the Hamiltonian (1), employing various numerical methods based on the exact-diagonalization calculation. The resulting phase diagram (see Fig. 3) consists of the \( XY1 \) phase, the Haldane/LD phase, the ID phase and the Néel phase. It is noted that in the Haldane/LD phase, the crossover between the Haldane and ID states may occur. In our opinion, the most significant result of the present work is that the ID phase appears in the phase diagram. The existence of this phase was predicted by Oshikawa\(^{9} \) about twenty years ago. After then, considerable efforts by performing DMRG calculations\(^7–9 \) were devoted to find this phase in the \( S = 2 \) case, but fruitful results were not obtained. We now think that the reason for this is clear. In the DMRG method, the distinctions between the \( XY1 \) state and the gapped states are made by extrapolating the excitation gaps of finite-\( N \) systems to \( N \to \infty \). Namely, the state is determined to be gapless or gapped depending on whether the extrapolated gap is zero or finite. Since, of course, the values of extrapolated gap have numerical errors, it is very difficult to discriminate between the gapless state and the state with a very small gap. This situation is clearly seen in Fig. 7 of the paper of Aschauer and Schollwöck.\(^7 \) In other words, the apparent boundaries between the \( XY1 \) phase and the gapped phases determined by the DMRG method shift into the gapped region, because the system with \( \xi > N \) behaves to be gapless, where \( \xi \) is the correlation length. In fact, in the case of \( \Delta = 1 \), the transition point between the \( XY1 \) phase and the LD phase is estimated as \( D_{c2} \approx 3.0 \) by the DMRG method,\(^9 \) which is considerably larger than \( D_{c2} = 2.39,^{11} \) obtained by the LS method. As can be seen from Fig. 3, the region of the ID phase is fairly narrow, and thus the whole region of the ID phase was completely masked by the “apparent \( XY1 \) region”. Although we have tried to detect the edge state with \( S^z = 1/2 \) (see Fig. 1(b)) around each end of the open chain in the ID state by the DMRG method, this has also led to fruitless results. The reason why the LS method\(^{10,11} \) is very useful is undoubtedly the fact that it can sharply distinguish three phases, the \( XY1 \), ID and Haldane/LD phases, by the crossing of the excitations under periodic and twisted boundary conditions.

We would like to express our appreciation to Professor Masaki Oshikawa for his invaluable discussions and comments as well as for his interest in this study. We are deeply grateful to Dr. Frank Pollmann for his stimulating discussions. We also thank the Supercomputer Center, Institute for Solid State Physics, University of Tokyo, the Computer Room, Yukawa Institute for Theoretical Physics, Kyoto University and the Cyberscience Center, Tohoku University for computational facilities. The present work has been supported in part by a Grant-in-Aid for Scientific Research (B) (No. 20340096), and a Grant-in-Aid for Scientific Research on Priority Areas “Novel states of matter induced by frustration” from the Ministry of Education, Culture, Sports, Science and Technology.

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