Quantum phase transitions in a frustrated orthogonal-dimer $S = 1$ spin system

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Abstract

We investigate quantum phase transitions in a quasi-one dimensional orthogonal-dimer $S = 1$ spin chain by means of the exact diagonalization. By taking into account the effect of the interchain coupling, we discuss how the distinct spin-gap phases found in the orthogonal-dimer chain are adiabatically connected to those in the two-dimensional Shastry-Sutherland model for the compounds SrCu$_2$(BO$_3$)$_2$ and Nd$_2$BaZnO$_5$.

Key words: orthogonal-dimer structure; exact diagonalization; frustration

Frustrated quantum spin systems have attracted current interest. A typical example is the cuprate SrCu$_2$(BO$_3$)$_2$,[1] where the Cu$^{2+}$ ions sit on the orthogonal-dimer structure, [2,3] shown in Fig. 1. In this material, novel magnetic properties were observed such as magnetization plateaus, excited states without dispersion,[1,4] which stimulate further theoretical investigations of the Shastry-Sutherland model.[3,5,6] More recently, a new orthogonal-dimer compound Nd$_2$BaZnO$_5$ was synthesized,[7] where the local moment $J = 9/2$ shows an antiferromagnetic order below $T_N = 2.4K$. Therefore, it is desirable to clarify how a higher spin generalization ($S > 1/2$), together with the competing exchange couplings, affects the ground state properties of such frustrated spin systems.

In our previous paper,[8] we have dealt with the orthogonal-dimer spin chain ($J'' = 0$) with an arbitrary spin $S$ and have shown that first-order quantum phase transitions occur ($2S$) times. In particular, in the $S = 1$ system, the Haldane spin-gap phase exists between the dimer and the plaquette phases. It is naively expected that the intermediate phase is not stable against the interchain coupling since such a quasi-one dimensional $S = 1$ spin chain is usually driven to the antiferromagnetic phase.[9–11] In this paper, we deal with the $S = 1$ orthogonal-dimer system by means of the exact diagonalization to discuss how the interchain coupling affects the spin gap phases realized in the chain.

We consider here the model Hamiltonian with the orthogonal-dimer structure as,

$$H = \sum_{(ij)} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where $\mathbf{S}_j$ indicates the $S = 1$ spin operator at the $j$th site, and $J_{ij} = J, J'$ and $J''$ represent the intra-dimer, the inter-dimer and the interchain couplings, which are...
all assumed to be antiferromagnetic. To clarify how
the spin-gap phases in the chain system are adiabati-
cally connected to those in the 2D Shastry-Sutherland model, we perform the exact diagonalization of the
orthogonal-dimer $S = 1$ spin system ($N = 4 \times 4$) with
periodic boundary condition. The results are shown in
Fig. 2. When $J'' = 0$, the system is reduced to the $S = 1$ orthogonal-dimer spin chain, where first-order
quantum phase transitions occur among three spin-gap phases. [8] Although the introduction of the interchain
coupling $J''$ enhances antiferromagnetic correlations,
the dimer phase is still stable in the small $J'$ and $J''$
region since the assembly of dimers shown by the bold
line in Fig. 1 is the exact eigenstate of the Hamiltonian.
It is remarkable that the frustration-induced Haldane
phase in the chain persists even in the 2D Shastry-
Sutherland model ($J' = J''$). The nature of the Hal-
dane phase is clearly described by the Valence Bond Solid, [12] where the spin-gap state is represented by the
assembly of the singlet bonds between the decom-
posed $S = 1/2$ spins. In the frustration-induced Haldane
phase, one of the decomposed $S = 1/2$ spins at each site is connected to the nearest neighbor spin to
form the singlet-dimer on the strong-coupling bond,
as shown in the inset of Fig. 2. Another decomposed
spin is connected to other three spins to form the pla-
quetter singlet. Therefore, this phase is composed of a
periodic arrangement of the dimer and the plaquette
singlets discussed in the $S = 1/2$ Shastry-Sutherland
model, [5] and is stable against the interchain coupling.
In the plaquette phase, the spin gap continuously
decreases with increasing the interchain coupling $J''$, and
the system may be driven to the antiferromagnetically
ordered phase. Though it is difficult to determine this
boundary, we think that the plaquette phase may not
persist on the Shastry-Sutherland line ($J' = J''$) since
the system with $S = 1$ spins favors the classical Neel
ordered state, in contrast to the plaquette phase in the
$S = 1/2$ Shastry-Sutherland model. [5,13,14] We show
this phase boundary in Fig. 2 as a guide to eyes. Al-
though our calculation is restricted to a small system,
we believe that the frustration-induced spin-gap phases
discussed here give the correct phase diagram of the
$S = 1$ Shastry-Sutherland model. [2]

Acknowledgements

This work was partly supported by a Grant-in-Aid
from the Ministry of Education, Science, Sports and
Culture of Japan. A part of computations was done
at the Supercomputer Center at the Institute for Solid
State Physics, University of Tokyo and Yukawa Insti-
tute Computer Facility.

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Fig. 2. The phase diagram of the orthogonal-dimer spin $S = 1$
system. The solid lines indicate the phase boundary where
the first-order transition occurs. The dashed line indicates the
phase boundary between the plaquette and the antiferromag-
netically ordered phases, where the second-order transition oc-
curs.