# Ground-State Phase Diagram of an Anisotropic $S=2$ Antiferromagnetic Chain with Quartic, Uniaxial, On-Site Anisotropy

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## Purpose and Model:

Employing mainly numerical methods, we determine the ground-state phase diagram of an $S=2$ $XXZ$ antiferromagnetic chain with one-site anisotropies, which is described by the Hamiltonian,

$$\mathcal{H} = \sum_{i=1}^{N} \{ S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \} + D \sum_{i=1}^{N} (S_i^z)^2 + D' \sum_{i=1}^{N} (S_i^z)^4 \, ,$$

where $\vec{S}_i = (S_i^x, S_i^y, S_i^z)$ is the $S=2$ operator at the $i$th site; $\Delta$ is the $XXZ$ anisotropy parameter of the nn interactions; $D$ and $D'$ are, respectively, the quadratic and quartic uniaxial on-site anisotropy parameters.

## Results of Our Recent Study:

In the case where $\Delta \geq 0$, $D \geq 0$ and $\boldsymbol{D' = 0}$, we have determined the ground-state phase diagram on the $D$ versus $\Delta$ plane by **the twisted-boundary-condition level spectroscopy (TBCLS) analysis** [1,2] and **the phenomenological renormalization (PR) analysis** [3] of the numerical results of exact-diagonalization calculations.

[1] A. Kitazawa, J. Phys. A: Math. Gen. **30** (1997) L285.
[2] K. Nomura and A. Kitazawa, J. Phys. A: Math. Gen. **31** (1998) 7341.
[3] M. P. Nightingale, Physica A **83** (1976) 561.

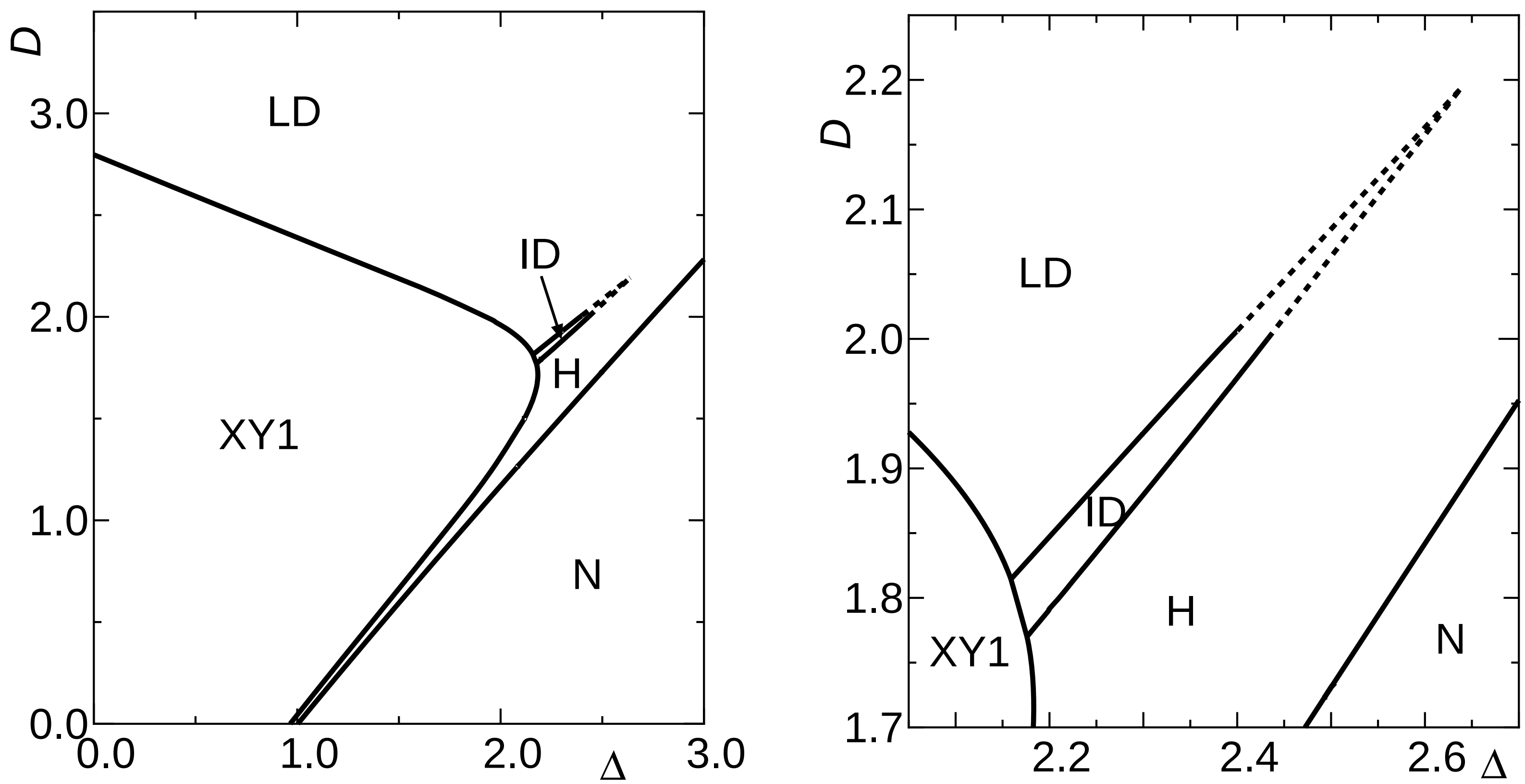
The interaction between two boundary spins $\vec{S}_N$ and $\vec{S}_1$:

$$S_N^x S_1^x + S_N^y S_1^y + \Delta S_N^z S_1^z \qquad \text{in PBC}$$

$$\Downarrow$$

$$-(S_N^x S_1^x + S_N^y S_1^y) + \Delta S_N^z S_1^z \qquad \text{in } \mathbf{TBC}$$

**Obtained Phase Diagram:** [4]





[4] T.T., K. Okamoto, H. Nakano, T. Sakai, K. Nomura and M. Kaburagi, J. Phys. Soc. Jpn **80** (2011) 043001.


The phase diagram consists of the four phases; **the Haldane/LD, ID, $XY1$, and Néel phases.**

One of the remarkable features of the phase diagram is the fact that **the intermediate-$D$ (ID) state appears as the ground state**.

**The existence of the ID states in $S \geq 2$ integer spin chains was predicted by Oshikawa in 1992** [5]. After then, considerable efforts by performing density-matrix renormalization-group (DMRG) calculations [6,7,8] were devoted to find this state in the $S = 2$ case, but fruitful results were not obtained.

[5] M. Oshikawa, J. Phys.: Cond. Matter **4** (1992) 7469.
[6] H. Aschauer and U. Schollwöck, Phys. Rev. B **58** (1998) 359.
[7] U. Schollwöck and Th. Jolicœur, Europhys. Lett. **30** (1995) 493.
[8] U. Schollwöck, O. Golinelli and Th. Jolicœur, Phys. Rev. B **54** (1996) 4038.

We would like to emphasize that **in order to find the ID state, it is essential to emply the TBCLS analysis** [9].

[9] K. Okamoto, T.T., H. Nakano, T. Sakai, K. Nomura and M. Kaburagi, J. Phys.: Conf. Series **320** (2011) 012018.

## Purpose of the Present Work:

The region for the ID state is fairly narrow in the previously obtained phase diagram. In order to clarify the nature of the ID state in more details, it is necessary to investigate that case where a wider ID region appears in the ground-state phase diagram. For this purpose, **we treat the case of $\boldsymbol{D' \neq 0}$**. Since the ID state in the $S=2$ chain corresponds essentially to the Haldane state in the $S=1$ chain, we can expect that, when $D'$ is positive and sufficiently large, the ID region in the ground-state phase diagram becomes to be wide.

# Results for Two Cases: