J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by Boston University on 01/05/18

Check for updates

Journal of the Physical Society of Japan
Vol. 58, No. 2, February, 1989, pp. 679–683

Exact Diagonalization Study of the Spin 1/2 *XXZ* Model on the 4×4 Square Lattice

Macoto KIKUCHI and Yutaka OKABE†

Department of Physics, Osaka University, Toyonaka 560
†Department of Physics, Tohoku University, Sendai 980

(Received October 12, 1988)

We study the thermodynamic properties of the spin 1/2 quantum *XXZ* model with the *XY*-like anisotropy on the 4×4 square lattice by diagonalizing the Hamiltonian numerically. The temperature dependence of the energy, the specific heat and the uniform susceptibility are reported. The staggered and the in-plane magnetizations at the ground state are also calculated.

[quantum spin system, anisotropy, square lattice, exact diagonalization, thermodynamic property, ground state]

§1. Introduction

In a recent paper[1)] we studied the thermodynamic and ground-state properties of the spin 1/2 quantum *XXZ* model on the square lattice of up to 16×16 sites by means of a Monte Carlo (MC) simulation. The aim of the present paper is to give some numerically exact results for the same model on a smaller lattice.

The Hamiltonian of the model is given by

$$\mathscr{H}=-J\sum_{\langle ij\rangle}(S_i^x S_j^x+S_i^y S_j^y+\Delta S_i^z S_j^z).$$

Here we take $J>0$, and $\Delta=0$, 1, and -1 respectively correspond to the *XY*, the ferromagnetic (F) Heisenberg and the antiferromagnetic (AF) Heisenberg model with an appropriate unitary transformation. We treat the F and AF models with *XY*-like anisotropy as well.

Up to now, the extensive numerical studies for the AF Heisenberg[2,3)] and *XY*[4)] models using the MC methods are reported. By the MC methods, the systems as large as 256 spins can be treated, but the statistical accuracy becomes worse at low temperatures. The exact diagonalization method serves as a complementary one; we can treat only small systems, but the data obtained are numerically exact in the whole temperature range. Then it is worth studying the present model by the latter method. At present, the largest system size for which we can obtain all the eigen values of the Hamiltonian consists of 16 spins because of the restrictions of the memory and the CPU time of computers. As for the ground-state properties, Oitmaa and Betts treated the AF Heisenberg and *XY* models up to 18 sites.[5)] In the following sections we study thermodynamic and ground-state properties of the model on the 4×4 square lattice by means of the exact diagonalization method.

§2. Method of Calculation

Since the number of basis vectors for 4×4 lattice, 2^{16}, is very large, we cannot diagonalize the Hamiltonian, eq. (1), directly. Symmetry properties, therefore, are used for breaking the Hamiltonian matrix into smaller submatrices of treatable size. We do not employ all the symmetry properties of the system but use only the following ones; (i) the total number conservation of the up spins, (ii) the translational symmetry along the x axis, and (iii) the symmetry about inversion line parallel to the x axis. Spatial symmetries (ii) and (iii) are shown in Fig. 1 as T and I, respectively. The number of the different submatrices to be diagonalized thus obtained are 42 apart from the trivial cases that all the spins are alined up or down. The numbers of the basis vectors for the submatrices are listed in Table I. The submatrices of which the eigenvalues of T are $\pm i$

J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by Boston University on 01/05/18

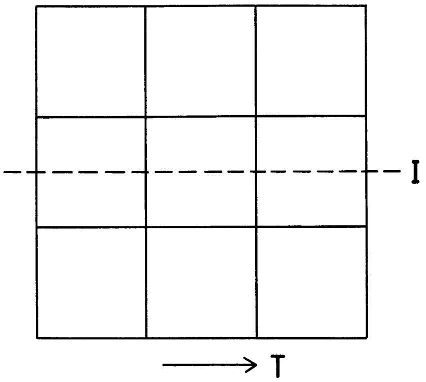

Fig. 1. Spatial symmetry operations employed for diagonalizing the Hamiltonian. The arrow and the dashed line indicate the direction of the translation operation T and the symmetry plane for the inversion operation I, respectively.

Table I. Number of the basis states of the submatrices to be diagonalized. T and I are the eigenvalues of the translation and the inversion operations, respectively. The values for the total S_z are given in the first row. The matrices for $T=\pm i$ are Hermitian, while the others are real symmetric.

T	I	$\pm\Sigma S_z=7$	6	5	4	3	2	1	0
1	1	2	18	70	240	546	1022	1430	1638
1	-1	2	14	70	224	546	994	1430	1600
-1	1	2	18	70	236	546	1022	1430	1632
-1	-1	2	14	70	224	546	994	1430	1600
$\pm i$	1	2	14	70	224	546	994	1430	1600
$\pm i$	-1	2	14	70	224	546	994	1430	1600

are Hermitian and are conjugate to each other, while others are real symmetric. We diagonalize these submatrices numerically and obtain all the eigenvalues of the Hamiltonian. It takes about 600 seconds for diagonalization by NEC SX-2N of the Computer Center of Osaka University for each value of Δ. Unfortunately, we cannot get all the eigenvectors and calculate the several correlation functions because of the restriction of the memory and the CPU time. As a result thermodynamic properties we can study are the energy, the specific heat and the uniform (ferromagnetic) susceptibility of z direction. Only for the ground state, we obtain the eigenvector and study the staggered and the in-plane magnetizations.

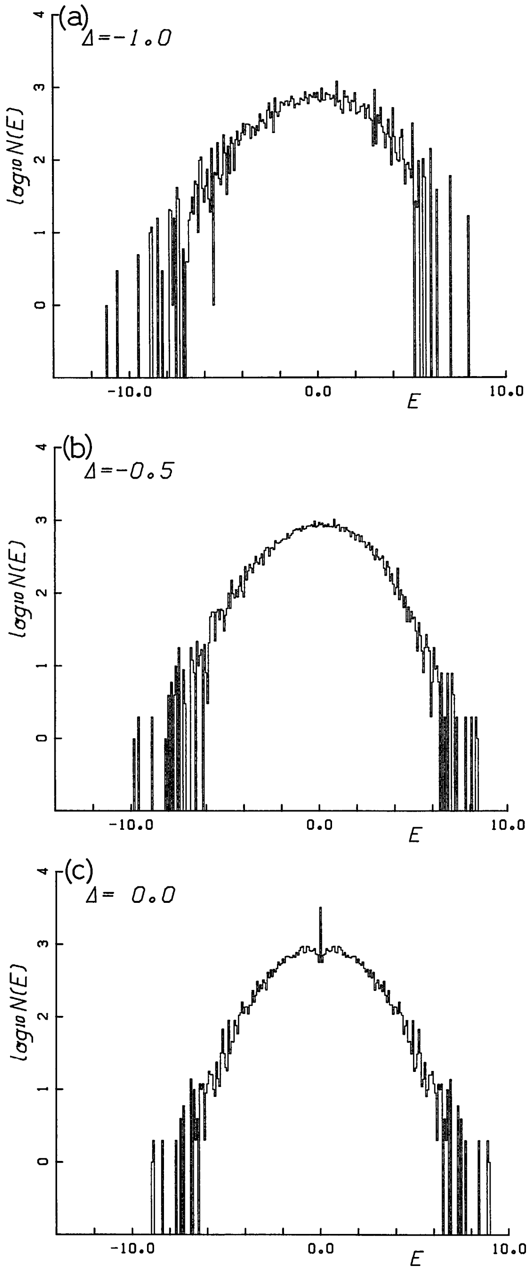

Fig. 2. Logarithm of the density of states for (a) $\Delta=-1$, (b) $\Delta=-0.5$ and (c) $\Delta=0$.

§3. Results

3.1 Level scheme and density of states

In Figs. 2(a)–2(c) we show the density of states (DOS) for $\Delta=-1$, -0.5 and 0. The histogram shows the logarithm of the number of levels within intervals $\Delta E=0.16$ against the energy. DOSs for $\Delta=0.5$ and 1 can be ob-

J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by Boston University on 01/05/18

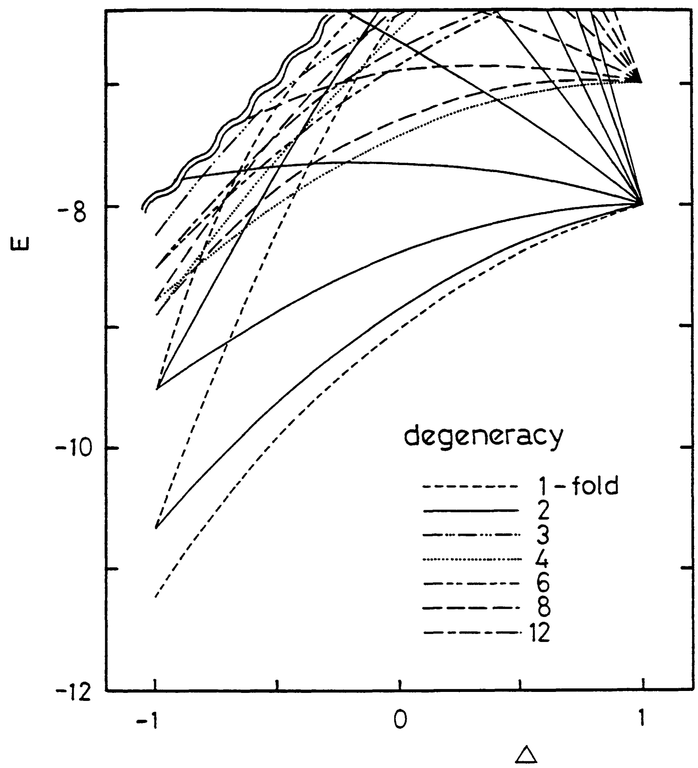

Fig. 3. Energy levels near the ground state. The calculated eigenvalues are connected smoothly by the lines; the line types indicate the degeneracy of the level as shown in the figure. To avoid complexity, the levels higher than the wavy line are not shown.

tained from those for -0.5 and -1 by changing the sign of the energy, respectively. The DOS for the XY model has special features; it is symmetric about $E=0$, and a large number of the states degenerate just at $E=0$.

Level scheme near the ground state is of special interest because low temperature properties are relating to them. Figure 3 shows several levels near the ground state as functions of Δ. The line types indicate the degeneracy of the levels. There is no crossing of the levels for the ground state, that is, the symmetry of the ground state does not change within the present parameter range; the ground state is found to be invariant under all the symmetry operations. There is a finite gap between the ground state and the first excited state, which decreases as Δ increases and disappeares at $\Delta=1$. It is expected that the gap vanishes in the thermodynamic limit.

3.2 *Energy and specific heat*

The energy E and the specific heat C are calculated from the n-th eigenvalue of the Hamiltonian E_n as;

$$E=\frac{1}{Z}\sum_n E_n \exp(-E_n/T),$$

and

$$C=\frac{1}{T^2}\left(\frac{1}{Z}\sum_n E_n^2 \exp(-E_n/T)-E^2\right),$$

where Z is the partition function. In Fig. 4 we show the temperature dependence of the energy E per spin in units of J. At sufficiently low temperature, the value of E varies monotonically with Δ, while the curves cross at finite temperature. Figure 5 shows the specific heat per spin. The small peaks at $T\approx 0.1$ reflect the finite gap. The peak near $T=0.5$ for the XY model may correspond to the critical temperature, if the model exhibits

J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by Boston University on 01/05/18

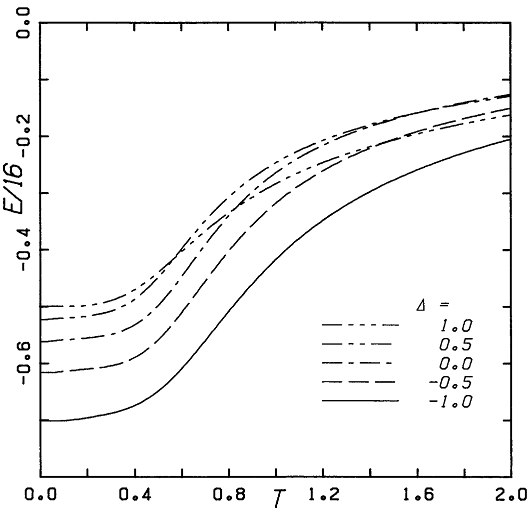

Fig. 4. Temperature dependence of the energy per spin.

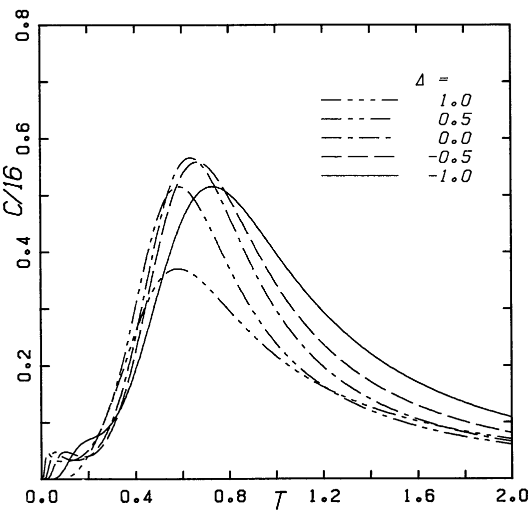

Fig. 5. Temperature dependence of the specific heat per spin.

the Kosterlitz-Thouless-type phase transition.

3.3 *Uniform susceptibility*

The uniform susceptibility χ is obtained from the magnetization M_{zn} of the n-th eigenstate as

$$\chi=\frac{1}{TZ}\sum_{n}(M_{zn})^2\exp(-E_n/T).$$

In Fig. 6, we plot the susceptibility per spin. In the case of the AF Heisenberg model, χ has a flat peak around $T\approx 1.0$, which behavior has

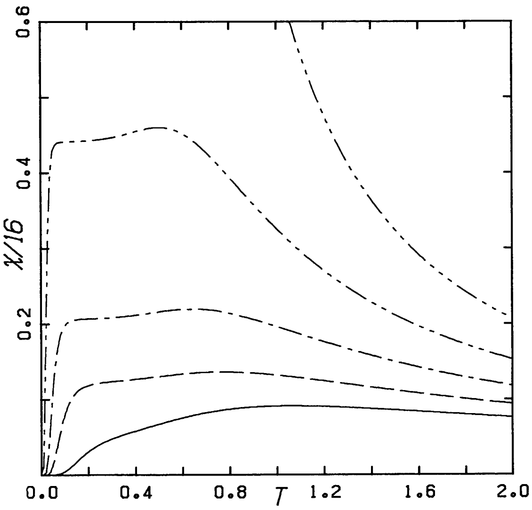

Fig. 6. Temperature dependence of the uniform susceptibility per spin. The same lines are used as in Figs. 4 and 5.

already been pointed out from MC studies.[1,2] That flat peak shifts to lower temperature with increasing Δ, and becomes higher at the same time. The uniform susceptibility approaches zero as $T\to 0$ except for the F Heisenberg model, which is a direct consequence of the finite gap. It is clear from the structure of low energy levels that χ for the F Heisenberg model diverges as $1/T$ (Curie law) at low temperature. The present system size is too small to observe non-classical critical behavior.

3.4 *Ground state properties*

For the ground state we obtain eigenvector of the Hamiltonian, and calculate the square of the staggered magnetization $\langle N_z^2\rangle$ and the square of the in-plane magnetization $\langle M_x^2\rangle$. For the XY and the AF Heisenberg model, Oitmaa and Betts calculated these values.[4] We list the data of $\langle M_x^2\rangle$ and $\langle N_z^2\rangle$ in Table II together with the ground-state energy. The values vary smoothly with Δ, which shows the

Table II. The energy per spin and the squares of the staggered and the in-plane magnetization per spin for the ground state.

	$\Delta=-1$	-0.5	0	0.5
$E/16$	-0.70178	-0.61678	-0.56249	-0.52415
$\langle N_z^2\rangle/16$	0.09218	0.03812	0.02572	0.02021
$\langle M_x^2\rangle/16$	0.09218	0.12238	0.13282	0.13846

J. Phys. Soc. Jpn.
Downloaded from journals.jps.jp by Boston University on 01/05/18

continuity of the ground state in the present parameter region.

§4. Summary

By diagonalizing the Hamiltonian, we have studied the ground state and thermodynamic properties of spin 1/2 *XXZ* model on the 4×4 square lattice. The density of states and the level scheme near the ground state have been discussed in terms of the anisotropy parameter Δ. The energy, the specific heat and the uniform susceptibility have been calculated at finite temperature. We have also studied the staggered magnetization and in-plane magnetization at the ground state. The present results will serve as reference data for the numerical studies by MC or the other methods. Some data are already used for discussing the size dependence in ref. 1.

Recently, Barnes *et al.* discussed a ground-state phase transition at $\Delta=-1$ based on their Monte Carlo study.[6] The possibility of the disappearance of the order parameter at $\Delta=-1$ argued by some authors[2,7] is closely related to that phase transition. A detailed study of the structure of low energy levels as in Fig. 3 for $\Delta<-1$ combined with the present results will be helpful for the discussion, which will appear in near future.

Acknowledgements

We would like to thank Professors H. Shiba and S. Miyashita for fruitful discussions. Thanks are also due to T. Barnes for informing us of his work prior to publication and valuable discussions. The present study is supported by Grant-in-Aid for Encouragement of Young Scientists and also by Grant-in-Aid for Scientific Research from The Ministry of Education, Science and Culture.

References

1) Y. Okabe and M. Kikuchi: J. Phys. Soc. Jpn. **57** (1988) 4351.
2) S. Miyashita: J. Phys. Soc. Jpn. **57** (1988) 1934.
3) J. D. Reger and A. P. Young: Phys. Rev B**37** (1988) 5978.
4) E. Loh, Jr., D. J. Scalapino and P.M. Grant: Phys. Rev. B**31** (1985) 4712; B**33** (1986) 5104; H. De Raedt, B. De Readt and A. Lagendijk: Z. Phys. B**57** (1984) 209; H. De Raedt and A. Lagendijk: Phys. Rev. B**33** (1986) 5102; T. Onogi, S. Miyashita and M. Suzuki: *Quantum Monte Carlo Methods in Equilibrium and Non-Equilibrium Systems*, ed. M. Suzuki (Springer, Berlin, 1987) p. 75; I. Morgenstern and D. Wurts: *ibid.* p. 163; S. Homma, H. Matsuda and N. Ogita: preprint.
5) J. Oitmaa and D. D. Betts: Can. J. Phys. **56** (1976) 897.
6) T. Barnes, D. Kotchan and E. S. Swanson: preprint.
7) S. Fujiki and D. D. Betts: Can. J. Phys. **64** (1986) 876.

Note added in proof—After submitted the present paper, we noticed that there are some previous works. Kelland calculated all the eigenvalues for the *XY* case for N up to 16 (J. Phys. Soc. Jpn. **52** (1983) Suppl. 11). Coombs and Oitmaa computed the ground-state energy as a function of Δ for systems up to 16 spins (J. Magn. & Magn. Mater. **15–18** (1980) 345). We wish to thank Professor J. Oitmaa for kindly informing us on the above papers.