

## Perturbational Method for the Numerical Evaluation of the Ground-State Energy of the Heisenberg Model

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A perturbational method is developed and applied to the numerical calculation for the energy of the ground state  $E_g$  of antiferromagnetic Heisenberg model of finite size systems. In this method the system is divided into two subsystems and each one is treated exactly, while the interactions between the subsystems are taken into account by the second order perturbation. This process saves the memory space of computer, and moreover the relative error is very small and decreases as the size of system is increased. Actual calculations for the triangular lattice are performed up to the number of spins  $N=36$  and  $E_g$  for the infinite lattice is estimated as  $-(1.04 \pm 0.01)N|J|$ , where  $|J|$  is the exchange integral.

[ perturbational method, diagonalization of Hamiltonian, computer, Heisenberg  
 model, triangular lattice ]

### §1. Introduction

In order to obtain the energy of the ground state  $E_g$  in an infinite quantum spin system (e.g. antiferromagnetic Heisenberg model), we often use the method to compute exactly the energy of the ground state  $E_g(N)$  for a finite system which consists of  $N$  spins ( $N=2, 3, 4, \dots$ ), and then extrapolate the results to the limit  $N \rightarrow \infty$ . The linear chain lattice is the most suitable for such an extrapolation. (See Fig. 1. Bonner and Fisher<sup>1)</sup> obtained the results up to  $N=12$  under the periodic boundary condition.) On the other hand, for two- or three-dimensional lattices,  $N$  increases rapidly as the linear size of the system grows, so that the computations quickly reach the limit set by the memory space of the computer. As our experience shows,<sup>2)</sup> if we could obtain the numerical values of  $E_g(N)$  up to  $N \sim 30$ , we would be able to estimate the ground state energy for the infinite size system even if we could not carry out the computations for  $N > 30$ , because we could probably extrapolate the data for  $N < 30$  with considerable accuracy to the infinite-size system.

In a previous paper,<sup>3)</sup> we presented a new

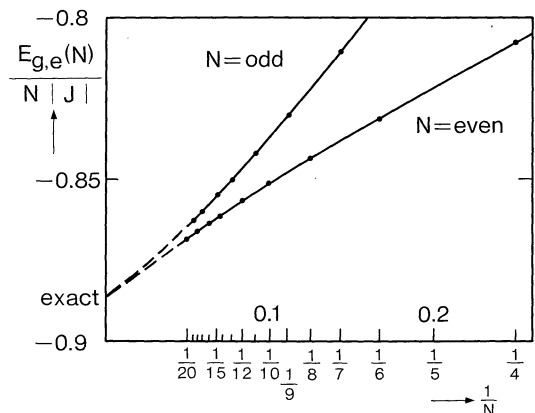


Fig. 1.  $E_{g,e}(N)/N$  versus  $1/N$  calculated under the free boundary condition for linear chain lattices consisting of  $N$  spins, where  $E_{g,e}(N)$  is the exact energy of the ground state for finite  $N$ . The exact value for  $N \rightarrow \infty$   $E_g/N = -0.8863|J|$  is marked exact. Bonner and Fisher<sup>1)</sup> obtained the results up to  $N=12$  under the periodic boundary condition.

method in which we divided the total system into several subsystems and each was treated exactly by the Trotter formula<sup>4)</sup> for finite Trotter number  $n$ , and extrapolated the results to infinite  $n$ .

In the present paper we give another method.<sup>5)</sup> We divide the system consisting of

$N$  spins into two (or more if necessary) subsystems A and B, each of which consists of  $N_A$  and  $N_B=N-N_A$  spins, respectively. Their properties are computed exactly, and the interactions between them are treated by the perturbational methods.

The Hamiltonian of the total system  $\mathcal{H}_{\text{tot}}$  can be written as

$$\mathcal{H}_{\text{tot}} \equiv 2|J| \sum_{\langle ij \rangle} S(i) \cdot S(j) = \mathcal{H}_A + \mathcal{H}_B + \mathcal{H}', \tag{1.1}$$

where  $S(i)$  is the spin operator at the  $i$ -th site, whose magnitude is  $\frac{1}{2}$ , and  $\mathcal{H}_A$  and  $\mathcal{H}_B$  represent the Hamiltonian of the subsystems and  $\mathcal{H}'$  is that of the interactions between A and B subsystems. Hereafter we use the unit of  $|J|=1$ . Since  $[\mathcal{H}_A, \mathcal{H}_B]=0$ , we may compute the energy of the ground state  $E_g(N_A)$  and  $E_g(N_B)$  of two subsystems separately. Therefore our requirement of computer storage can be reduced from  $k \times (2^N \times 2^N)$  bytes to  $k \times (2^{N_A} \times 2^{N_A} + 2^{N_B} \times 2^{N_B})$  bytes, where  $k$  is a numerical factor of the order 10. The product  $2^M \times 2^M$  ( $M=N_A$  or  $N_B$ ) appears since we have to solve completely the eigenvalue equations of the Hamiltonian in each subspace.

**§2. Linear Chain Lattices**

At first we explain our method which is applied to the case of a linear chain lattice consisting of  $N$  spins. In this section  $N$  is confined to multiples of 4, and other cases will be treated in the next section. The system is divided into the A and B subsystems each consisting of  $N/2$  spins as is shown in Fig. 2. We use the free boundary condition in this paper. (Periodic boundary condition is unsuitable, because we will consider an application of the

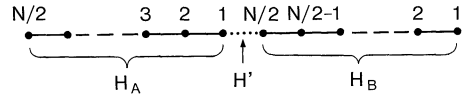


Fig. 2. A linear chain lattice. The numerals express the ordinal number of sites counted from the right end.

method to the triangular lattice in §4, in which case the toroidal frustration<sup>6)</sup> under the periodic boundary condition complicates the problem.)

In a numerical diagonalization of the Heisenberg Hamiltonian, it is useful to carry out calculations in the space of a definite  $M \equiv \sum S^z(i)$ , because the Hamiltonian of subsystem commutes with the  $z$  component of the total spin in subsystem. Using the computer we get the eigenvalues  $\epsilon_{M,i}$  and  $\epsilon_{M,j}$ , and the eigenfunctions  $\phi_{M,i}$  and  $\psi_{M,j}$  for each subsystem A and B, respectively, as follows,

$$\mathcal{H}_A \phi_{M,i} = \epsilon_{M,i}^A \phi_{M,i}, \tag{2.1a}$$

$$\mathcal{H}_B \psi_{M,j} = \epsilon_{M,j}^B \psi_{M,j}, \tag{2.1b}$$

where the suffix  $i$  or  $j$  represents the energy level. We denote the energy of the ground state by  $\epsilon_{0,0}^A = \epsilon_{0,0}^B$ . Note that the ground state is included in the space of  $M=0$ .<sup>7)</sup>

The Hamiltonian of the perturbation is written by

$$\mathcal{H}' = 2|J|(S_A(1) \cdot S_B(N/2)), \tag{2.2}$$

which is indicated by dotted line in Fig. 2. The unperturbed wave functions and energies for the combined A and B subsystems without  $\mathcal{H}'$  are  $\phi_{M,i} \psi_{M',j}$  and  $\epsilon_{M,i}^A + \epsilon_{M',j}^B$  respectively. The energy of the ground state  $E_g(N)$  for the total system is given by the second order perturbational method as follows,

$$E_g(N) = E_0 + \Delta E, \tag{2.3a}$$

where

$$E_0 = \epsilon_{0,0}^A + \epsilon_{0,0}^B, \tag{2.3b}$$

$$\Delta E = \sum_M \sum_{M'} \sum_i \sum_j \frac{|\langle \phi_{M,i} \psi_{M',j} | 2|J|[S_A(1) \cdot S_B(N/2)] | \phi_{0,0} \psi_{0,0} \rangle|^2}{\epsilon_{0,0}^A + \epsilon_{0,0}^B - \epsilon_{M,i}^A - \epsilon_{M',j}^B}. \tag{2.3c}$$

Actual calculations were carried out using the computer program already reported<sup>8,9)</sup> and also the theorem proved in Appendix. The obtained results are given in Table I. As is clearly seen in Table I, our results  $E_g(N)/N$  are very accurate compared with the exact values  $E_{g,e}(N)/N$ , i.e. the relative error for  $N=4$  is less than 1.4%, and it decreases as  $N$  is increased (see Fig. 3), because the expectation value of the unperturbed Hamiltonian  $\mathcal{H}_A + \mathcal{H}_B$  grows so that the perturbation  $\mathcal{H}'$  is

relatively less important as  $N$  is increased.

**§3. The Case for  $N_A=N_B=$ Odd Number**

When the numbers of spins,  $N_A$  and  $N_B$ , in the subsystems are odd, eq. (2.3) cannot be used directly, because all unperturbed energy levels including the ground states in the subsystems are degenerate, i.e. Kramers doublets.

Let us consider the linear chain lattice in which  $N_A=N_B=$ odd number. We denote the degenerate ground states of the A(B) subsystem by  $\phi_{\frac{1}{2},0}$  and  $\phi_{-\frac{1}{2},0}$  ( $\psi_{\frac{1}{2},0}$  and  $\psi_{-\frac{1}{2},0}$ ). We have the quartet unperturbed ground states for the total system without the interactions between subsystems as follows,

$$\phi_{\frac{1}{2},0}\psi_{\frac{1}{2},0}, \quad \phi_{\frac{1}{2},0}\psi_{-\frac{1}{2},0}, \quad \phi_{-\frac{1}{2},0}\psi_{\frac{1}{2},0}, \quad \phi_{-\frac{1}{2},0}\psi_{-\frac{1}{2},0}. \tag{3.1}$$

It is easy to diagonalize the perturbation  $\mathcal{H}' = 2|J|(S_A(1) \cdot S_B(N/2))$  in the above quartet space. This perturbation splits the quartet into the upper triplet (3.2) and the lower singlet (3.3), shown in Fig. 4. They are

$$\phi_{\frac{1}{2},0}\psi_{\frac{1}{2},0}, \quad \phi_{-\frac{1}{2},0}\psi_{-\frac{1}{2},0}, \quad (\phi_{\frac{1}{2},0}\psi_{-\frac{1}{2},0} + \phi_{-\frac{1}{2},0}\psi_{\frac{1}{2},0})/\sqrt{2}, \tag{3.2}$$

and

$$(\phi_{\frac{1}{2},0}\psi_{-\frac{1}{2},0} - \phi_{-\frac{1}{2},0}\psi_{\frac{1}{2},0})/\sqrt{2} \equiv \Psi_0. \tag{3.3}$$

Then we calculate the energy shift of  $\Psi_0$  by the second-order perturbation. If we denote the perturbation  $2|J|(S_A^z(1)S_B^z(N/2))$  by  $\mathcal{H}'_{zz}$  and  $|J|\{S_A^+(1)S_B^-(N/2) + S_A^-(1)S_B^+(N/2)\}$  by  $\mathcal{H}'_{xy}$ , the bras which connect with  $\mathcal{H}'_{zz}|\Psi_0\rangle$  are  $\langle\phi_{\frac{1}{2},i}\psi_{-\frac{1}{2},j}|$  and  $\langle\phi_{-\frac{1}{2},i}\psi_{\frac{1}{2},j}|$  and similarly those which connect with  $\mathcal{H}'_{xy}|\Psi_0\rangle$  are  $\langle\phi_{\frac{3}{2},i}\psi_{-\frac{3}{2},j}|$ ,  $\langle\phi_{\frac{1}{2},i}\psi_{-\frac{1}{2},j}|$ ,  $\langle\phi_{-\frac{1}{2},i}\psi_{\frac{1}{2},j}|$  and  $\langle\phi_{-\frac{3}{2},i}\psi_{\frac{3}{2},j}|$ . There are no such relations as described in the Appendix in the present case, so that the calculations concerning  $\mathcal{H}'_{zz}$  and  $\mathcal{H}'_{xy}$  must be performed independently. These contributions are denoted by  $\Delta E^{zz}$  and  $\Delta E^{xy}$ , respectively, in Table II. The errors of the present results in Table II are larger than those in Table I. This can be understood as follows: Generally  $E_g(N_A)$  in the case of  $N_A=$ odd number is larger than those in the case of  $N_A=$ even

number as shown in Fig. 1. When the numbers of both subsystem are  $N/2$ , which is an odd number, the unperturbed energy  $2E_g(N/2)$  is considerably larger than  $E_{g,c}(N)$  though the former is lowered to  $E_0$  by  $E_{sp}$  as a result of the splitting of Kramers degeneracy, see Fig. 4.

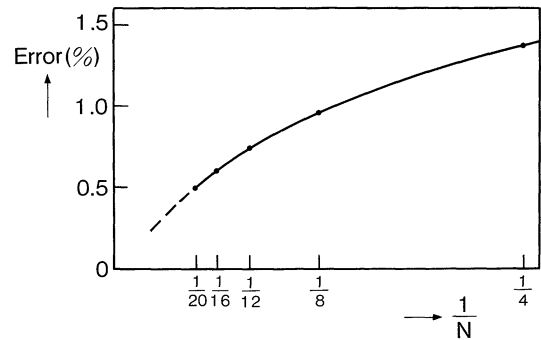


Fig. 3. The error for the energy  $E_g(N)$  of the ground state obtained by the present method relative to the exact one  $E_{g,c}(N)$  for linear chain lattices.

Table I. Numerical values of the energy for linear chain lattices consisting of  $N$  spins.  $E_0$ ,  $\Delta E$ ,  $E_g(N)$  are defined in (2.3).  $E_{g,c}(N)$  is the exact value. Error means  $\{E_g(N) - E_{g,c}(N)\}/|E_{g,c}(N)|$ .

$N$	$E_0$	$\Delta E$	$E_g(N)/N$	$E_{g,c}(N)/N$	Error (%)
4	$-1.5000 \times 2$	-0.1875	-0.7969	-0.8080	1.37
8	$-3.2321 \times 2$	-0.2212	-0.8357	-0.8437	0.95
12	$-4.9872 \times 2$	-0.2343	-0.8507	-0.8570	0.74
16	$-6.7499 \times 2$	-0.2409	-0.8588	-0.8640	0.60
20	$-8.5161 \times 2$	-0.2448	-0.8639	-0.8682	0.50

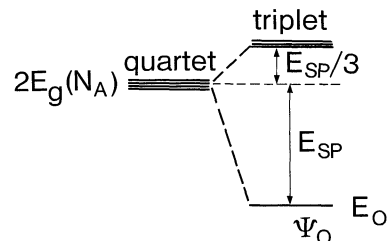


Fig. 4. Unperturbed quartet ground levels are split into the triplet eq. (3.2) and the singlet  $\Psi_0$  eq. (3.3). The energy level of the singlet is given by  $E_0 = 2E_g(N_A) + E_{sp}$ .

Table II. The numerical results in the case of linear chain lattices with  $N_A=N_B$ =odd number.  $E_0=2E_g(N_A)+E_{sp}$  (see Fig. 4). The present result is  $E_g(N)=E_0+\Delta E^{zz}+\Delta E^{xy}$ .

$N$	$N_A=N_B$	$2E_g(N_A)$	$E_{sp}$	$E_0$	$\Delta E^{zz}$	$\Delta E^{xy}$	$E_g(N)/N$	$E_{g,c}(N)/N$	Error (%)
10	5	-7.7116	-0.3927	-8.1043	-0.0309	-0.0724	-0.8208	-0.8516	3.62
14	7	-11.3450	-0.2649	-11.6099	-0.0427	-0.0887	-0.8387	-0.8610	2.59
18	9	-14.9452	-0.1936	-15.1387	-0.0510	-0.1026	-0.8496	-0.8663	1.93

Furthermore, the energy gained by the perturbation  $\Delta E^{zz}+\Delta E^{xy}$  in the case of  $N/2$ =odd number is about half of  $\Delta E$  in the case of  $N/2$ =even number.

The similar treatment can be carried out when  $N_A$  is an even number and  $N_B$  an odd number.

#### §4. Triangular Lattices

In this section we apply our method to the triangular lattice. As the first example, the systems we calculated are shown in Fig. 5 where the subsystems are drawn by solid lines while the interactions treated by the perturbational method are drawn by dotted lines. By use of our method we obtained the results which are given in Table III. It is interesting to see that the absolute values of errors diminish as the length is increased in (a), (b<sub>1</sub>), (c<sub>1</sub>) and

(d<sub>1</sub>), while they grow in (a), (b<sub>2</sub>), (c<sub>2</sub>) and (d<sub>2</sub>). Thus, in the latter case the perturbational method does not work excellently. An unexpected feature is that the errors have the opposite sign to those in linear chains (compare with Tables I and II). This might be caused by the following reason: The triangular lattice antiferromagnet has frustration which increases the energy. The energy obtained by the second order perturbational method is the simple sum of the perturbed energy of each bond which does not take account of frustration, so that the perturbational energy would lower  $E_g(N)$  so much.

Next, we estimate the energy of the ground state  $E_g$  of the antiferromagnetic Heisenberg model on the triangular lattice. In our previous paper<sup>2)</sup> we considered lattices of the railroad trestle shape. First the width of the

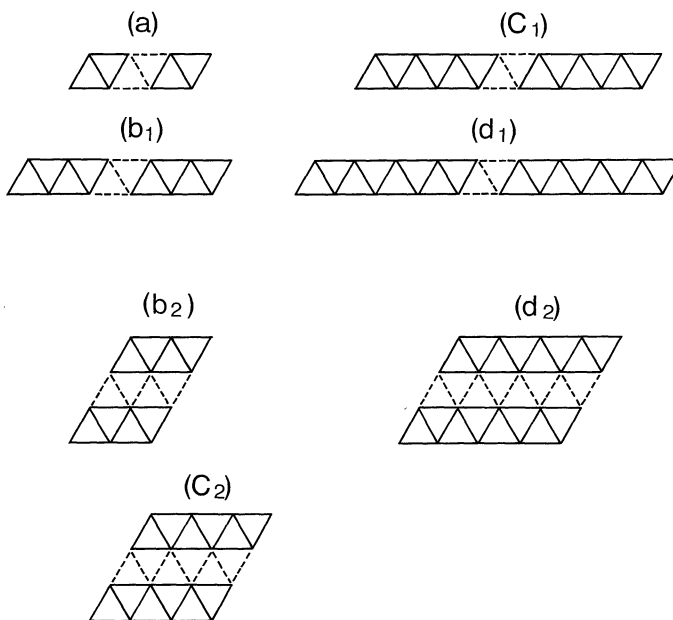


Fig. 5. Several examples of finite triangular lattices. Subsystems are drawn by solid lines while interactions by dotted lines. The number of spins  $N$  are (a) 8; (b<sub>1</sub>), (b<sub>2</sub>) 12; (c<sub>1</sub>), (c<sub>2</sub>) 16; (d<sub>1</sub>), (d<sub>2</sub>) 20.

Table III. Numerical values for the triangular lattices shown in Fig. 5.

Fig. 5	$N$	$E_0$	$\Delta E$	$E_g(N)/N$	$E_{g,c}(N)/N$	Error (%)
(a)	8	$-3.5000 \times 2$	$-0.4826$	$-0.9353$	$-0.9204$	$-1.62$
(b <sub>1</sub> )	12	$-5.4174 \times 2$	$-0.5390$	$-0.9478$	$-0.9374$	$-1.11$
(c <sub>1</sub> )	16	$-7.3631 \times 2$	$-0.5246$	$-0.9532$	$-0.9461$	$-0.75$
(d <sub>1</sub> )	20	$-9.3070 \times 2$	$-0.5006$	$-0.9557$	$-0.9513$	$-0.47$
(b <sub>2</sub> )	12	$-5.4174 \times 2$	$-0.8415$	$-0.9730$	$-0.9454$	$-2.92$
(c <sub>2</sub> )	16	$-7.3631 \times 2$	$-1.1671$	$-0.9933$	$-0.9637$	$-3.07$
(d <sub>2</sub> )	20	$-9.3070 \times 2$	$-1.4879$	$-1.0051$	$-0.9737$	$-3.22$

railroad trestle is fixed, and the length is increased to estimate the infinite-length energy. Then the width is increased to estimate the energy of the infinite width-length lattice. Our prediction for  $E_g$  was  $-1.05N$ . It would give a better estimation if we could avoid the double extrapolation. In fact Marland and Betts<sup>6</sup> estimated  $E_g$  for the triangular lattice by a single extrapolation using the diamond shape lattice with specific size. Unfortunately their estimation was not accurate,<sup>2,10</sup> probably owing to the toroidal frustration caused by the periodic boundary condition and even-odd alternation.

In the present paper we use the regular triangular shape. We calculate  $E_g(N)$  for the regular triangular lattices consisting of  $N=3, 6, 10, 15, 21, 28$  and  $36$  spins under the free boundary condition.

The results are shown in Table IV, where  $E_g(N)/N$  was obtained by the direct diagonalization of  $\mathcal{H}_{\text{tot}}$  for  $N$  up to 21. It should be noticed that their ground states are degenerate irrespective of the fact that  $N$  is even or odd number. For  $N=28$ , we divided the triangle into three subsystems  $12+8+8$  shown in Fig. 6(a). For  $N=36$ , we divided the triangle into 3 subsystems each of which contains 12 spins, but we had two different kinds of shape of subsystems as shown in Figs. 6(b) and 6(c). Using the perturbational method we

Table IV. Exact  $E_{g,c}(N)/N$  for the regular triangular shape lattice consisting of  $N$  spins.

$N$	$E_{g,c}(N)/N$	Degeneracy
3	$-0.5000$	2
6	$-1.5000$	2
10	$-0.8363$	2
15	$-0.8786$	6
21	$-0.9162$	4

got  $E_g(N)/N$  for these lattices shown in Table V. It must be stressed that the relative difference of  $E_g(N)/N$  for two different divisions (a) and (b) in the case of  $N=36$  is only 0.07%. This observation serves as a confirmation of reliability of the numerical results in Table V.

Finally we plot  $E_g(N)/N$  versus  $1/N$  in Fig. 7. If we use the data of (i)  $N=28, N=36$ (a), (ii)  $N=28, N=36$ (b), (iii)  $N=15, N=21$ , neglecting those of  $N=15, 10, 6, 3$ , and extrapolate each case by a straight line, our predictions for  $E_g/N$  are (i)  $-1.04$ , (ii)  $-1.04$ , (iii)  $-1.01$ . In view of the fact that  $E_g/N$  estimated by the use of spin systems with odd numbers is larger than that by even numbers as shown in Fig. 1, the present results would be consistent and reliable.

In conclusion, our prediction for  $E_g/N$  of the infinite triangular lattice is  $-(1.04 \pm 0.01)$ .

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**Appendix: Proof of**  $|\langle \alpha | S^z(\mathbf{1}) | g \rangle|$   
 $= |\langle \alpha^+ | S^+(\mathbf{1}) | g \rangle| / \sqrt{2}$   
 $= |\langle \alpha^- | S^-(\mathbf{1}) | g \rangle| / \sqrt{2}$

It is useful to exploit symmetry relations in calculating the expectation value in eq. (2.3c). As the Hamiltonian of the subsystem  $\mathcal{H}_A$  ( $\mathcal{H}_B$ ) commutes with  $S_{\text{tot}}^2$  and  $S_{\text{tot}}^z$ , ( $S_{\text{tot}} \equiv \sum_i S(i)$ , where the summation is taken over all sites in the A (B) subsystem), all eigenfunctions of  $\mathcal{H}_A$  ( $\mathcal{H}_B$ ) have definite  $S(S+1)$  and  $M$ , which are eigenvalues of  $S_{\text{tot}}^2$  and  $S_{\text{tot}}^z$ , respectively. In §2 and 3, we did not need to explicitly denote  $S$ -dependence of the eigenfunction, but here it is necessary to express  $S$ . We write the eigenket by  $|S, M\rangle$  or  $|S, M, i\rangle$  if necessary, where  $i$  is the same  $i$  as in  $\phi_{M,i}$  which

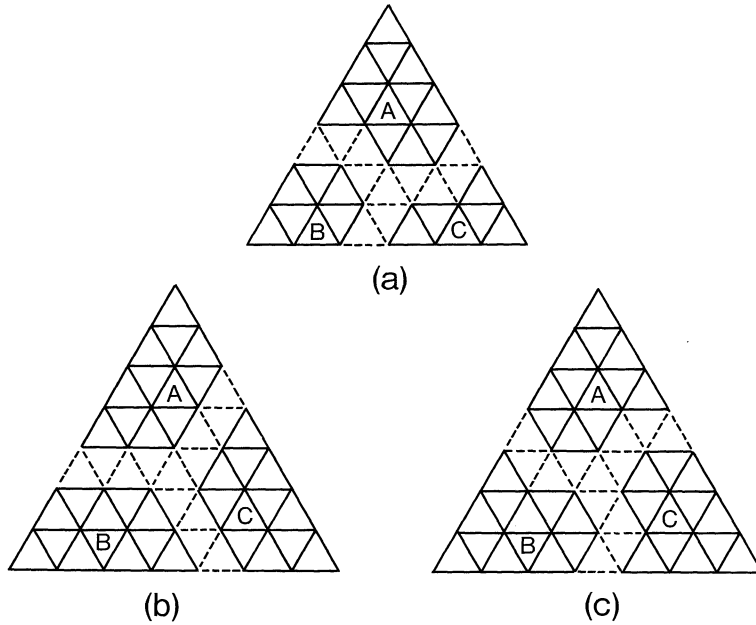


Fig. 6. Regular triangular shape lattices consisting of (a)  $N=28$  spins are divided into three subsystems  $N_A=12$ ,  $N_B=8$  and  $N_C=8$ , (b), (c)  $N=36$  spins,  $N_A=N_B=N_C=12$ , but the shapes of subsystems are different.

Table V.  $E_g(N)/N$  for the regular triangular shape lattices shown in Fig. 6.

$N$	$E_A$	$E_B$	$E_C$	$\Delta E$	$E_g(N)/N$
28	-11.0324	-7.4036	-6.6946	-2.4210	-0.9840
38(b)	-10.8892	-10.8892	-10.8892	-3.2071	-0.9965
36(c)	-11.0324	-11.0324	-11.0324	-2.8025	-0.9972

appeared in §2. The ground ket is  $|0,0\rangle$  or  $|0, 0, 0\rangle$  when  $N/2$  is an even number which is the case we consider here. In the following we often denote the ground ket by  $|g\rangle$  for simplicity.

By use of the commutation relations of spin operators and the identities:  $S_{tot}^+ |g\rangle = S_{tot}^- |g\rangle = 0$ , we have

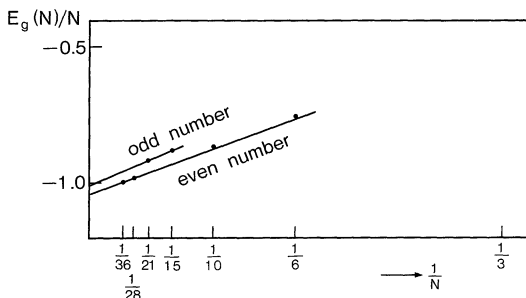


Fig. 7.  $E_g(N)/N$  versus  $1/N$  for finite regular triangular lattices.

$$S_{tot}^+ S^z(1) |g\rangle = -S^+(1) |g\rangle, \tag{A·1}$$

$$(S_{tot}^+)^2 |g\rangle = 0, \tag{A·2}$$

$$(S_{tot}^- S_{tot}^+) S^z(1) |g\rangle = 2S^z(1) |g\rangle. \tag{A·3}$$

It is obvious that  $S^z(1) |g\rangle$  is in the space of  $M=0$ . From (A·2),  $S$  of  $S^z(1) |g\rangle$  is  $S \leq 1$ . However,  $S$  must be 1, because if  $S$  were 0,  $S^z(1) |g\rangle$  must be 0 from the left side of (A·3). By normalization we have

$$S^z(1) |g\rangle = \frac{1}{2} |1, 0, i\rangle \equiv \frac{1}{2} |\alpha_i\rangle, \tag{A·4}$$

where  $|\alpha_i\rangle$  is indicated in Fig. A·1. Multiplying both sides in (A·4) by  $S_{tot}^+$  and using the formula

$$S_{tot}^\pm |S, M\rangle = \sqrt{(S \mp M)(S \pm M + 1)} |S, M \pm 1\rangle, \tag{A·5}$$

we get

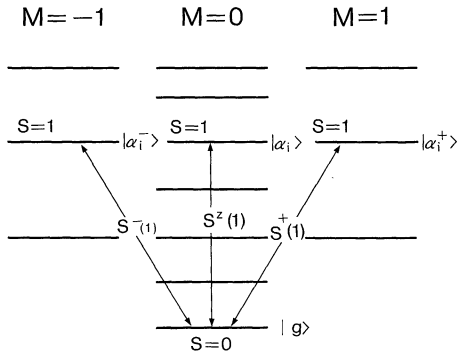


Fig. A·1. Energy level diagram for  $M=0, \pm 1$ , which shows the eigenket  $|\alpha_i\rangle$  connected by  $S^z(1)$  and  $|\alpha_i^\pm\rangle$  by  $S^\pm(1)$  with  $|g\rangle$ .

$$S_{\text{tot}}^+ S^z(1) |g\rangle = \frac{1}{\sqrt{2}} |1, 1, i\rangle \equiv \frac{1}{\sqrt{2}} |\alpha_i^+\rangle, \quad (\text{A} \cdot 6)$$

where  $|\alpha_i^+\rangle$  is the degenerate eigenket with  $|\alpha_i\rangle$  (see Fig. A·1). On the other hand the left side in (A·6) is  $-S^+(1)|g\rangle$  from (A·1), so that we have

$$S^+(1) |g\rangle = -\frac{1}{\sqrt{2}} |\alpha_i^+\rangle. \quad (\text{A} \cdot 7)$$

Therefore we obtain an important relation;

$$|\langle \alpha_i | S^z(1) |g\rangle| = |\langle \alpha_i^+ | S^+(1) |g\rangle| / \sqrt{2}. \quad (\text{A} \cdot 8)$$

Similarly we have

$$|\langle \alpha_i | S^z(1) |g\rangle| = |\langle \alpha_i^- | S^-(1) |g\rangle| / \sqrt{2}, \quad (\text{A} \cdot 9)$$

where  $|\alpha_i^-\rangle$  is  $|1, -1, i\rangle$ . Thus we obtain

$$\begin{aligned} |\langle \phi_{0,i} \psi_{0,j} | S_A^z(1) S_B^z(N_B/2) | \phi_{0,0} \psi_{0,0} \rangle| &= |\langle \phi_{1,i} \psi_{-1,j} | \frac{1}{2} S_A^+(1) S_B^-(N_B/2) | \phi_{0,0} \psi_{0,0} \rangle| \\ &= |\langle \phi_{-1,i} \psi_{1,j} | \frac{1}{2} S_A^-(1) S_B^+(N_B/2) | \phi_{0,0} \psi_{0,0} \rangle|. \end{aligned} \quad (\text{A} \cdot 10)$$

In this way we may replace the numerator in (2.3c) by

$$3 |\langle \phi_{0,i} \psi_{0,j} | 2 | J | S^z(1) S^z(N/2) | \phi_{0,0} \psi_{0,0} \rangle|^2. \quad (\text{A} \cdot 11)$$

This is a very useful relation, because we may confine ourselves to the subspace of  $M=0$  and only consider the  $z$  component of the perturbational Hamiltonian. However, this relation cannot be used when  $N_A$  is an odd number.

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*Note added in proof*—One of the authors (H. N.) and H. Nakanishi (J. Phys. Soc. Jpn, submitted) recently obtained  $E_g/N|J| = -1.09 \pm 0.02$  by directly diagonalizing finite-size systems up to  $N=27$ .