Journal of the Physical Society of Japan
Vol. 55, No. 12, December, 1986, pp. 4448-4455

Magnetization Process of the Spin-1/2 Antiferromagnetic Ising-Like Heisenberg Model on the Triangular Lattice

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(Received July 14, 1986)

The magnetization process at $T=0$ of the spin-1/2 Heisenberg antiferromagnet on the triangular lattice with Ising-like exchange anisotropy is studied. A comparison is made to a corresponding classical system. A plateau of magnetization has been found for an interval of the external field, on which classical spin configurations dominate. Other than on the plateau, quantum effects invalidate the classical picture. A possibility of experimental confirmation of this classical-quantum crossover is also pointed out.

§1. Introduction

Cooperation of competition in interactions (or frustration) and quantum fluctuation is one of the most interesting recent problems. In this paper we study this problem in the context of magnetization process of the antiferromagnetic Ising-like Heisenberg model on the triangular lattice, which shows distinctly different behavior from its classical counterpart. The effect of frustration causes various interesting properties of spin configurations in the ground state. For example, the effect leads to vanishing long range order in some Ising systems[1-3] and also to various structures in continuous spin systems.[4] Quantum effect on the ground state spin configuration is also very interesting. In general, in the case that the order parameter $\mathcal{N}$ in the corresponding classical system and the Hamiltonian H do not commute

$$[H, \mathcal{N}]\neq 0,$$

the quantum mechanical fluctuation forbids $\mathcal{N}$ to appear with its full magnitude, which is usually termed as reduction of effective spin length. Nevertheless the essential features of the classical state remain unchanged in non-frustrated quantum spin systems as suggested by the existence of a finite sublattice long range order.[5] If the corresponding classical system is frustrated, however, a quantum spin system could have a drastically different ground state, which may be viewed as a vanishing effective spin length. For example of this case, the resonating valence bond (RVB) state has been proposed by Anderson[6] for the ground-state spin-1/2 antiferromagnet on the triangular lattice. In the RVB state no conventional long range order exists. Instead this state is characterized by a picture that singlet pairs of spins "flow around" all over the system. This picture on the ground state of the antiferromagnet on the triangular lattice is at least partially supported by numerical calculations on finite size systems.[7] Fazekas and Anderson[8] further assert that the RVB state gives an appropriate description of the ground state even in a system with Ising-like exchange anisotropy. As seen in this example, frustration enhances quantum fluctuations.

Another factor to control ground state spin configuration is an external magnetic field. If one applies an external field to an antiferromagnetic quantum spin system, the spin moments tend to align parallel to the field, and a spin flop phase often appears. With strong enough fields, all spins are forced to align parallel to the fields. This fact is true even if the underlying quantum system is frustrated. As was mentioned above, since frustration works to enhance quantum fluctuations, it should be of great interest to investigate a system with these two factors (frustration and external field). We have thus undertaken an investigation of the spin-1/2 antiferromagnetic Ising-like Heisenberg model in a field on the triangular lattice. A reason for our choice of the Ising-like system, rather than the isotropic Heisenberg model, is that this system displays a more pronounced quantum-classical crossover as a field is varied, as seen in the following sections, than the isotropic model does. Another motivation rests on the more probable amenability of the Ising-like system to experimental investigation than the perfectly isotropic system.

Before discussing quantum effects, it is useful to review what the classical theory of the antiferromagnetic Ising-like Heisenberg system on the triangular lattice predicts.[9] An important feature of the classical system is a three-sublattice long-range order in the ground state for any value of a magnetic field h applied along the z-axis. Field-dependent properties are as follows. As h approaches zero the magnetization approaches a constant value, which implies a spontaneous ferrimagnetic long-range order. The magnetization curve is so-called "metamagnetic" in contrast to the XY and isotropic Heisenberg cases: In an interval $h_{c1}<h<h_{c2}$, the magnetization takes 1/3 of the saturation value (the 1/3-plateau) which corresponds to the spin configuration that two of the sublattices have up-spins and the remaining down. Another remarkable characteristic of the classical state is the non-vanishing transverse magnetization for $h_{c2}<h<h_{c3}$ resulting from an oblique spin configuration. The purpose of the present paper is to clarify what part of these classical properties are shared by the spin-1/2 system. Our method of investigation is an explicit numerical diagonalization of Hamiltonians of finite size systems (number of spins $N\leq 21$). The magnetization at $T=0$ and other quantities of interest are determined numerically for finite systems, and the expected properties of the infinite-size system are extracted by extrapolation.

To summarize our results: No ferrimagnetism is expected as $h\to +0$. The 1/3-plateau for $h_{c1}<h<h_{c2}$ exists also in the quantum system which implies that a metamagnetic curve is obtained. The classical spin configuration dominates on the 1/3-plateau. The three-sublattice structure is valid only on the 1/3-plateau. The long-range order in the XY plane is unlikely to exist for $h_{c2}<h<h_{c3}$.

§2. Numerical Analysis of Finite-Size Systems

The Hamiltonian of the present spin-1/2 system is

$$H=2J\sum_{\langle ij\rangle}(S_i^xS_j^x+S_i^yS_j^y+AS_i^zS_j^z)-h\sum S_j^z \qquad (J>0), \quad (1)$$

where A represents exchange anisotropy and the summation extends over nearest neighbors of the triangular lattice. Our main interest is in the case $A>1$. All numerical data below are presented in units of J (i.e. we assume $J=1$). In order to calculate the magnetization $M_z(h)$ in the ground state, we first find out the lowest eigenvalue $E(M_z)$ of the Hamiltonian (1) for a given value M_z of the z-component of total magnetization (which commutes with the Hamiltonian and therefore is a classical number). The ground-state magnetization $M_z(h)$ as a function of h is determined such that $E(M_z)-hM_z$ is minimum at $M_z=M_z(h)$. The numerical diagonalization of the spin Hamiltonian was carried out using a program written by one of the authors (H.N.) and Taguchi.[7] Both periodic and free boundary conditions were employed. For the periodic case, we chose the lattice sizes

$N=12$ (Fig. 1(a), Marland-Betts type[10]),

$N=3\times 6$ (Fig. 1(b)),

$N=21$ (Fig. 1(c), Marland-Betts type).

The anisotropy parameter A assumes 0.8, 1, 1.2, 2.5 and 5. The free boundary lattice of size

$N=4\times 5$ (Fig. 1(d)),

was also investigated for the same values of A.

The resulting magnetization steps are shown in Figs. 2 to 5. From these figures the infinite-size system with $A>1$ is expected to have a metamagnetic magnetization curve as roughly sketched in Fig. 6. The quantitative features of this magnetization process are as follows. First, it is unlikely that M_z remains finite as

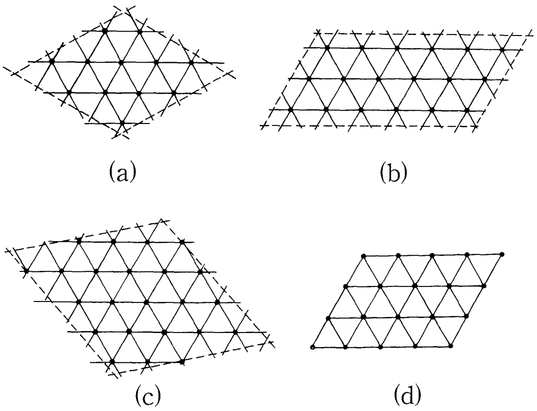


Fig. 1. Lattice shapes we have studied. Periodic boundary conditions are imposed on the lattices (a) $N=12$, (b) $N=3\times 6$, (c) $N=21$ and a free boundary is employed for the lattice (d) $N=4\times 5$.

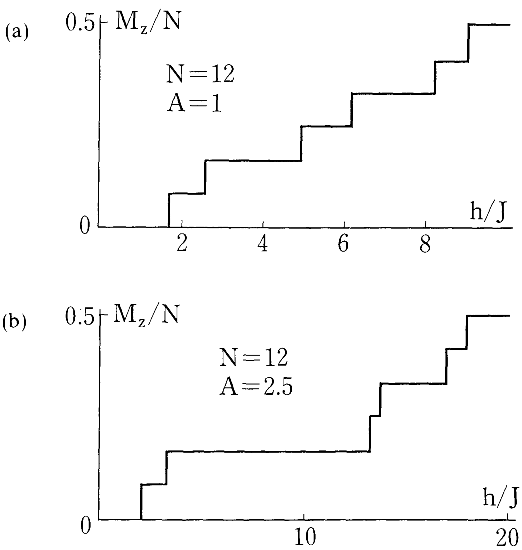


Fig. 2. Magnetization per site M_z/N as a function of the external field h on the $N=12$ lattice (Fig. 1(a)). The field h is measured in units of J. The anisotropy A assumes (a) $A=1$ and (b) $A=2.5$.

$h\to+0$ in contrast to the classical case.[9] Second, in the range $0<h<h_{c1}$ the M_z-curve is approximately straight or slightly concave downward. The 1/3-plateau is clearly present in an interval $h_{c1}<h<h_{c2}$. The first critical field h_{c1} does not strongly depend on A and is roughly at $h_{c1}=3$. The second critical field is located at about $h_{c2}=5A$. The classical values[9] are $h_{c1}^{(cl)}=3$ and $h_{c2}^{(cl)}=3(2A-1+\sqrt{4A^2+4A-7})/2$ (in units of J) for the

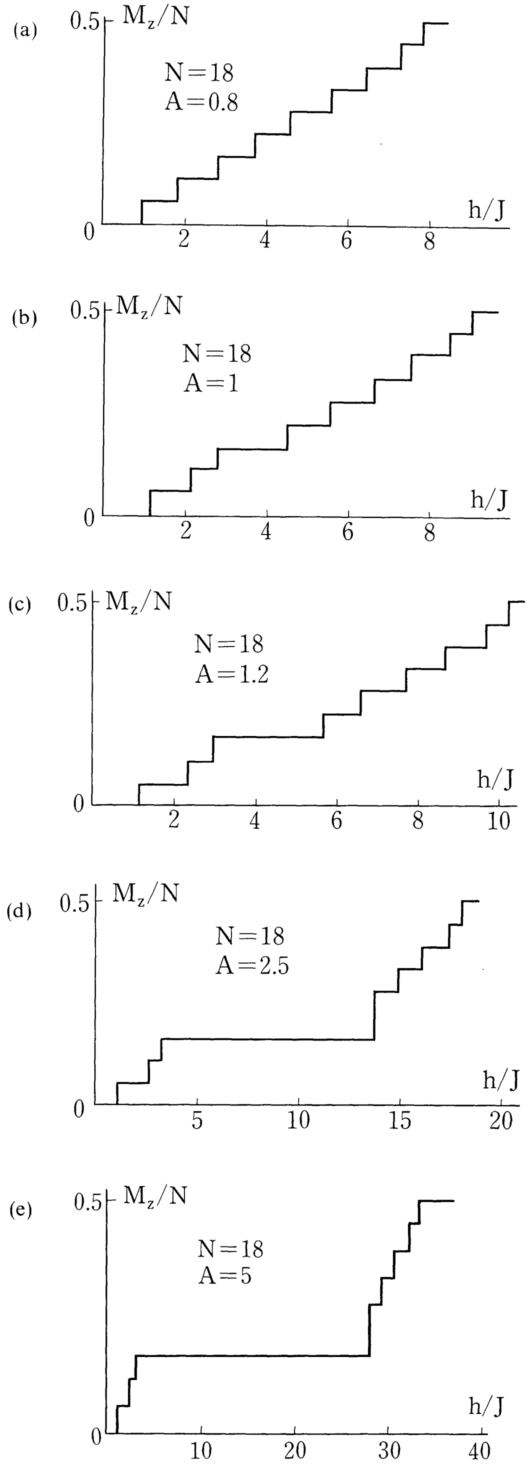


Fig. 3. Magnetization as a function of the field. The lattice size is $N=3\times 6$ (Fig. 1(b)) and the anisotropy is (a) $A=0.8$, (b) $A=1$, (c) $A=1.2$, (d) $A=2.5$, and (e) $A=5$.

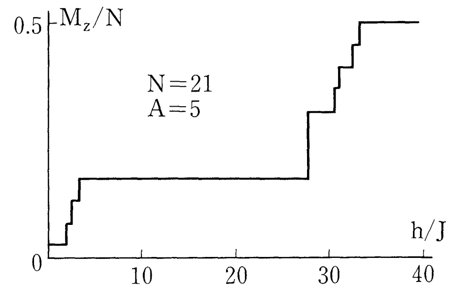
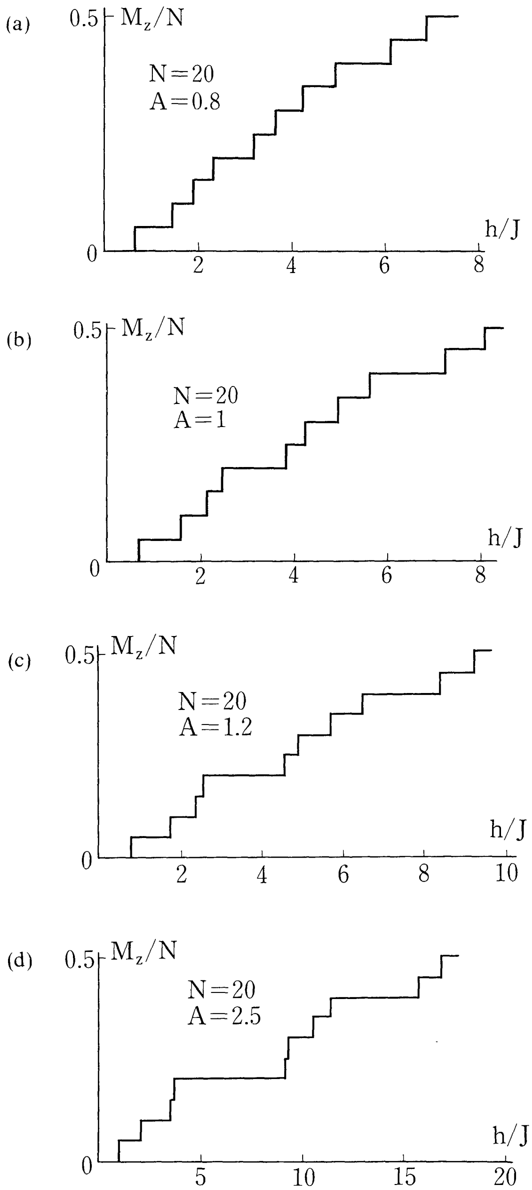


Fig. 4. Magnetization as a function of the field on the $N=21$ lattice (Fig. 1(c)) with $A=5$.



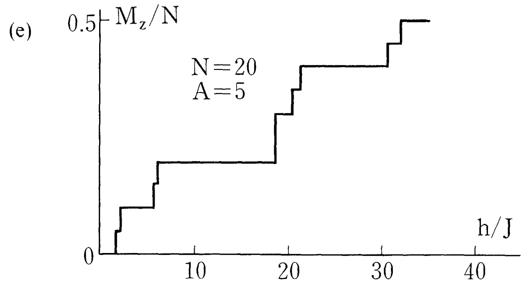


Fig. 5. Magnetization as a function of the field on the free boundary lattice of $N=4\times5$ (Fig. 1(d)). The anisotropy is (a) $A=0.8$, (b) $A=1$, (c) $A=1.2$, (d) $A=2.5$, (e) $A=5$.

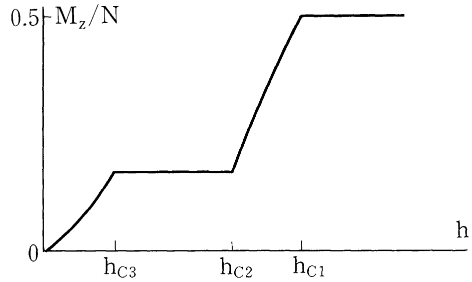


Fig. 6. Rough sketch of the magnetization as a function of the field of the infinite-size system as expected from the finite-size data in Figs. 2 to 5.

Hamiltonian

$$H=J\sum_{\langle ij\rangle}(S_i^xS_j^x+S_i^yS_j^y+AS_i^zS_j^z)-h\sum S_i^z, \quad (2)$$

with $\{S_i\}$ a classical unit vector. The coincidence of h_{c1} between classical and quantum calculations justifies the correspondence of the ratio h/J in (2) to that in the quantum Hamiltonian (1). The numerical values of the second critical field $h_{c2}^{(cl)}$ roughly agrees with $h_{c2}=5A$ of the quantum system in the range $2<A<5$. The third (saturation) field h_{c3} can be estimated by the method of Katsura and Suzuki[11] as $6A+3$. A 2/3-plateau is observed in the $N=4\times5$ and 12 systems (Figs. 2 and 5), which will be discussed in the next section.

The 1/3-plateau is present both in the classical and quantum systems. In the classical model the 1/3-plateau corresponds to the spin configuration shown in Fig. 7 (and similar two configurations obtained from Fig. 7 by exchanging three sublattices). To see if such classical states prevail in the quantum case, we have calculated a quantity defined by

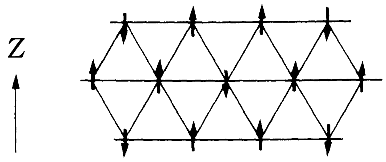


Fig. 7. The classical spin state realized in the 1/3-plateau. Spins on one of the three sublattices are down, and those on the other two sublattices are up.

$$Q=\sum_j c_j^4.$$

Here c_j is the coefficient of the j th state of the ground-state wave function

$$\psi=\sum_j c_j\phi_j \qquad (\sum_j c_j^2=1).$$

If ψ contains all c_j's in the same order of magnitude, then $c_j\sim O(1/\sqrt{L})$ (L denotes the number of states: $\Sigma_j 1=L$), which leads to $Q\sim O(1/L)$. On the other hand, if only a few states dominate, $c_j\sim O(1)$ for these dominant states and other c_j's will be negligible. In this situation $Q\sim O(1)$. Figure 8 shows the behavior of Q for $N=12$ (Marland-Betts type) and $N=3\times 6$ with $A=2.5$. As the basis we have chosen the S_i^z-diagonal states (one of which is the classical state in Fig. 7). Clearly the 1/3-plateau has a distinctly large value of Q. Other than in the 1/3-plateau Q is small and shows definite decrease as the system size increases from $N=12$ to 18. This result is compatible with the assumption that in the 1/3-plateau the classical collinear state (Fig. 7) occupies most part of the quantum wave function. A more direct method to see if the classical states dominate in the 1/3-plateau is to take projection of ψ to ϕ_1 (the state in Fig. 7), ϕ_2 and ϕ_3. Here ϕ_2 and ϕ_3 are obtained from ϕ_1 by replacing cyclically the three sublattices. If we define

$$p=\sum_{j=1}^{3} |\langle\phi_j|\psi\rangle|^2,$$

our calculations show $p=0.82$ for $N=12$ (Marland-Betts type) and $p=0.77$ for $N=3\times 6$ ($A=2.5$ for both N). These values of projection are large enough to support the classical picture and the decrease on going from $N=12$ to 18 is small enough to expect a non-negligible value in the thermodynamic limit. Therefore we may expect that on the 1/3-plateau the classical collinear states dominate. Other than in the 1/3-plateau Fig. 8 suggests that no collinear state which diagonalizes $\{S_j^z\}$ plays a distinctly important role.

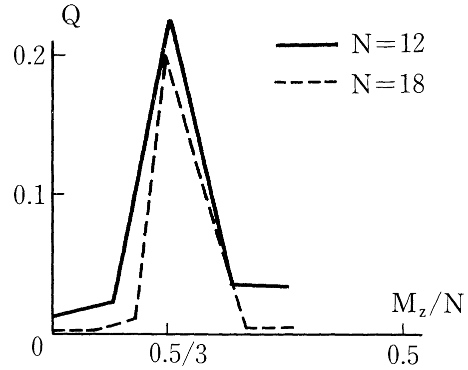


Fig. 8. Concentration ratio of the ground state wave function to particular states to diagonalize $\{S_i^z\}$. The peak at the 1/3-plateau is compatible with the assumption of domination of the classical state of Fig. 7.

Another support for this classical-quantum crossover is provided by the sublattice long-range order parameter

$$\mathcal{S}_z^2=4\langle(\sum_{j\in A} S_j^z)^2+(\sum_{j\in B} S_j^z)^2+(\sum_{j\in C} S_j^z)^2\rangle/N^2,$$

where the first sum is over one of the sublattices A, the second over B and the third over the remaining C. If the classical prediction is correct, the existence of a sublattice long-range order leads to $\mathcal{S}_z^2\sim O(1)$ in the limit $N\to\infty$. We present our result for $\mathcal{S}_z^2$ in Fig. 9 for $N=12$ and 18 ($A=2.5$). The sublattice order parameter has a large value at the 1/3-

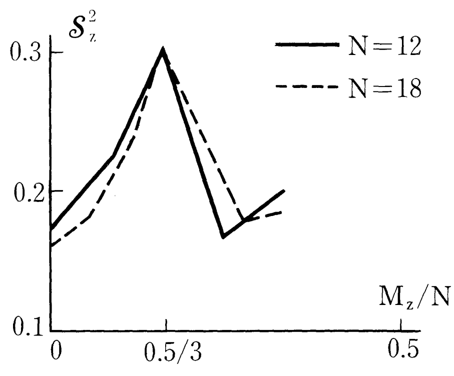


Fig. 9. Sublattice long-range order as a function of magnetization. The 1/3-plateau has a large value of the order parameter.

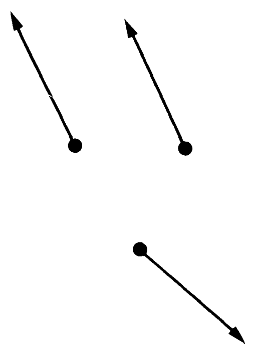


Fig. 10. The classical state realized in the range $h_{c2}<h<h_{c3}$.[9] This state has a non-vanishing transverse magnetization.

plateau and no decrease as N increases is observed at the plateau. Our conclusion is that the classical picture is valid on the 1/3-plateau and quantum effects are important other than in the plateau.

As mentioned in the Introduction the classical theory predicts a non-vanishing transverse magnetization for $h_{c2}<h<h_{c3}$ (Three sublattices have spin configurations as described in Fig. 10). To check if this prediction remains valid in the quantum system, we have calculated the total transverse magnetization M_{xy}^2 and the sublattice transverse magnetization $\mathcal{S}_{xy}^2$ defined by

$$M_{xy}^2=\langle(\sum_j S_j^x)^2+(\sum_j S_j^y)^2\rangle/N^2,$$

$$\mathcal{S}_{xy}^2=4\langle\sum_{L=A,B,C}\{(\sum_{j\in L} S_j^x)^2+(\sum_{j\in L} S_j^y)^2\}\rangle/N^2.$$

As seen in Fig. 11, both quantities show definite decrease as the system size is increased except at $M_z=0$. (The increase of the total transverse magnetization in the space of $M_z=0$ as N is increased is not compatible with any classical or quantum expectation and is left as a future problem). Our main interest is at $h_{c2}<h<h_{c3}$ where the data in Fig. 11 deny the transverse long-range order in the thermodynamic limit. In the classical system the sublattice structure is always complete and the relation

$$\mathcal{S}^2\equiv\mathcal{S}_z^2+\mathcal{S}_{xy}^2=\frac{1}{3},$$

is satisfied. On the other hand in the quantum system, $\mathcal{S}^2$ itself vanishes at $0<h<h_{c1}$ and $h_{c2}<h<h_{c3}$. This result indicates that the

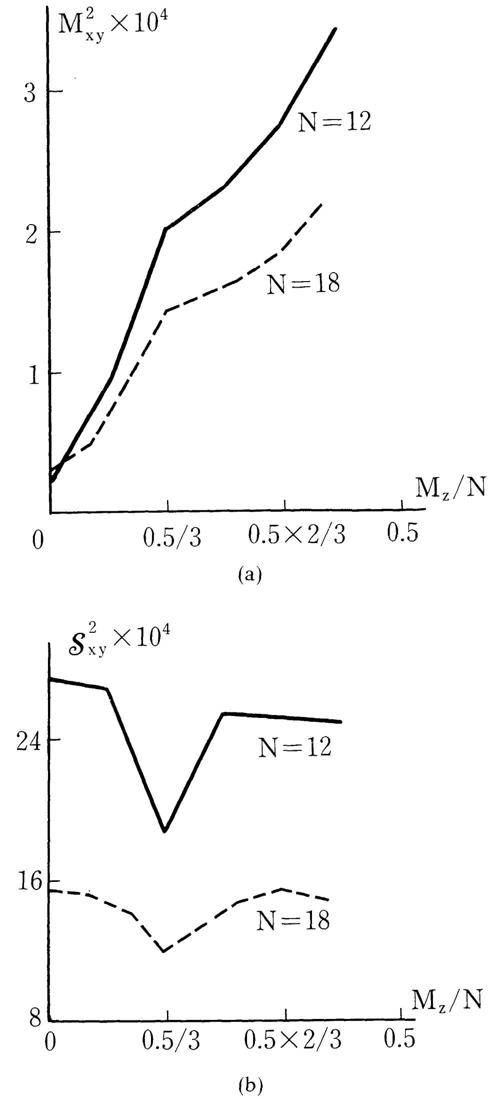


Fig. 11. Transverse magnetization of the quantum system as a function of the longitudinal magnetization. (a) Total transverse magnetization and (b) sublattice transverse magnetization. The clear decrease of both total and sublattice orders suggests the absence of the transverse magnetization in the thermodynamic limit.

system is in quite quantum mechanical state and it verifies that the three sublattice structure (Fig. 10) of the classical theory is broken down in spin-1/2 systems.

§3. Discussion

In the preceding section we have shown that quantum fluctuations do not modify the classical picture on the 1/3-plateau. It is possible to intuitively understand the existence of this classical plateau in the quantum system. The ground state of the Ising model ($A=\infty$) is infinitely degenerate (the Wannier states[12]) and is separated from the first excited state by a finite gap (Fig. 12(a)). On introduction of quantum transverse interactions ($A<\infty$), both the Wannier and excited states split into energy bands. The spin configuration in the 1/3-plateau shown in Fig. 7 is one of the levels in the lower band which is shown by a bold line in Fig. 12(b). If we apply an external field, almost all levels in the bands are bent downward, and for $h_{c1}<h<h_{c2}$ the spin configuration as in Fig. 7 stays to be the ground state (Fig. 12(b)). For a larger field $h>h_{c2}$ the lowest level of the upper band comes below the lowest level of the lower band. Hence the 1/3-plateau is closely related to the existence of an energy gap in the Ising limit.

It is also interesting to discuss the case with $A=1$. In the absence of an external field the isotropic case ($A=1$) is the boundary between the XY-like ($A<1$) and Ising-like ($A>1$) systems. When a field is applied in the z-direction, Figs. 3(a), 3(b) and 5(a), 5(b) suggest that the 1/3-plateau remains in the isotropic case ($A=1$) while it disappears in the slightly XY-like case ($A=0.8$). This result is not inconsistent with symmetry arguments since a system with $h>0$ is anisotropic even when $A=1$. The magnetic field effectively enhances the interaction in the z-direction, leading to the Ising-like behavior of the isotropic system. One should not forget, however, that our system may not be large enough and the existence of a plateau at the isotropic case $A=1$ should be further checked in larger systems.

A 2/3-plateau is observed in some systems (Figs. 2(b) and 5(b) to (e)). The classical theory[9] does not predict a 2/3-plateau; in fact the quantity Q defined in §3 and the sublattice long range order are both unlikely to have appreciable values in the thermodynamic limit (Figs. 8 and 9). Thus the 2/3-plateau, even if it remains in the $N=\infty$ system, is not of classical nature. Of course the absence of this plateau in many lattices (Figs. 3 and 4) may suggest that this plateau comes from a finite-size effect. A careful analysis of larger system is required in future studies.

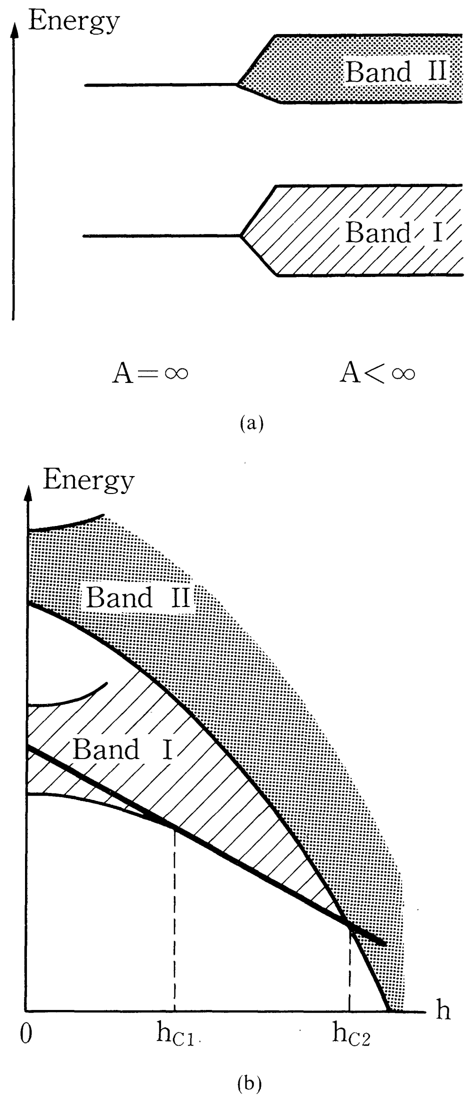


Fig. 12. (a) The ground and first excited states are degenerate in the Ising case ($A=\infty$). By the transverse term of the Hamiltonian (a) both energy levels split into bands. (b) When an external field is applied, the levels in the bands change their energy by the Zeeman term. The appearance of the 1/3-plateau is a consequence of the fact that the classical configuration of Fig. 7 (represented by the bold line in the present figure) stays to be the lowest level in an interval $h_{c1}<h<h_{c2}$.

It should be interesting to check our predictions experimentally. The point is to verify the classical character of the 1/3-plateau. In neutron scattering experiments, for instance, a sharp Bragg peak corresponding to the classical states will be observed only for an interval $h_{c1} < h < h_{c2}$.

Acknowledgement

We thank Yoshihiro Taguchi for his assistance in numerical calculations at the initial stage of this work. This work is partially supported by the Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture.

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