Numerical study of the spin-flop transition in anisotropic spin-$\frac{1}{2}$ antiferromagnets

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Magnetization processes of the spin-1/2 antiferromagnetic XXZ model in two and three spatial dimensions are studied using a quantum Monte Carlo method based on stochastic series expansions. A recently developed operator-loop algorithm enables us to show clear evidence of a first-order phase transition in the presence of an external magnetic field. Phase diagrams of closely related systems, hard core bosons with nearest-neighbor repulsions, are also discussed, focusing on the possibilities of phase-separated and supersolid phases.

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There has been much interest in the magnetic properties of anisotropic quantum antiferromagnets since Néel first predicted a first-order phase transition in the presence of an external magnetic field.[1] One of the simplest models for anisotropic antiferromagnets in an external magnetic field is described by the spin-1/2 XXZ model Hamiltonian

$$H=J\sum_{\langle\mathbf{i},\mathbf{j}\rangle}(S_{\mathbf{i}}^{x}S_{\mathbf{j}}^{x}+S_{\mathbf{i}}^{y}S_{\mathbf{j}}^{y}+\Delta S_{\mathbf{i}}^{z}S_{\mathbf{j}}^{z})-h\sum_{\mathbf{i}}S_{\mathbf{i}}^{z},\qquad(1)$$

where $S_{\mathbf{i}}^{\alpha}$ is the $\alpha(=x,y,z)$ component of the spin-1/2 operator at site $\mathbf{i}$, h is an external magnetic field applied in the z direction, and $\langle\mathbf{i},\mathbf{j}\rangle$ runs over all the nearest-neighbor pairs of spins at sites $\mathbf{i}$ and $\mathbf{j}$. $J(>0)$ is an antiferromagnetic coupling constant, and $\Delta(\geqslant 0)$ is an anisotropic constant. Mean-field calculations of the spin-1/2 XXZ model,[2] supporting Néel's prediction, found a first-order phase transition from a Néel-ordered state to a spin-flipping state with increasing magnetic field h. Contrary to these studies, it is known from the Bethe ansatz solution that the one-dimensional (1D) spin-1/2 XXZ model shows a second-order transition in the presence of an external magnetic field.[3] This discrepancy is assigned to the inadequacy of treating quantum fluctuations by mean-field theories. It is thus important to use an unbiased numerical method for understanding the correct nature of the magnetization process even for the simplest systems [such as one given by Eq. (1)] in higher spatial dimensions, since there exist no analitically exact solutions. This is preciely one of our purposes in this paper.[4]

Another importance of studing the spin-1/2 XXZ model defined by Eq. (1) comes from the fact that the model is mapped onto a system of hard core bosons with nearest-neighbor repulsions described by the Hamiltonian

$$H_B=-t\sum_{\langle\mathbf{i},\mathbf{j}\rangle}(c_{\mathbf{i}}^{\dagger}c_{\mathbf{j}}+c_{\mathbf{j}}^{\dagger}c_{\mathbf{i}})+V\sum_{\langle\mathbf{i},\mathbf{j}\rangle}n_{\mathbf{i}}n_{\mathbf{j}}-\mu\sum_{\mathbf{i}}n_{\mathbf{i}},\qquad(2)$$

with $t=J/2$, $V=J\Delta$, and $\mu=h+zJ\Delta/2$ (z is the coordination number).[5] Here $c_{\mathbf{i}}^{\dagger}$ is a creation operator of a hard core boson at site $\mathbf{i}$, and $n_{\mathbf{i}}=c_{\mathbf{i}}^{\dagger}c_{\mathbf{i}}$. The total magnetization $M_z=\Sigma_{\mathbf{i}}S_{\mathbf{i}}^{z}$ thus relates to $\Sigma_{\mathbf{i}}(n_{\mathbf{i}}-1/2)$ in the boson model. The boson Hamiltonian H_B is proposed as a model Hamiltonian to study properties of liquid ^{4}He,[6] granular superconducting arrays,[7] and flux lines in superconductors.[8] The ground-state phase diagram was studied using mean-field theories[2,9] and numerical methods,[10] and shows a Mott insulating phase, a superfluid phase, and a phase having both orders simultaneously (a *supersolid* phase). The correspondence of these states to those in the spin model is as follows: Mott insulating and Néel states, superfluid and spin-flipping states, and supersolid and "intermediate" spin states,[2] respectively.

The main purpose of this paper is to show clear evidence of the first-order phase transitions of 2D and 3D spin-1/2 XXZ models in the presence of a magnetic field, using a recently developed numerical method; we also present ground-state phase diagrams. The presence of a phase-separated phase and the absence of a supersolid phase, in a closely related system of hard core bosons with nearest-neighbor repulsions, are also discussed.

The magnetization process of the 2D and 3D spin-1/2 XXZ models, defined by Eq. (1), is studied numerically on square (number of spins $N_s=L\times L$) and cubic ($N_s=L\times L\times L$) lattices using a quantum Monte Carlo (QMC) technique based on stochastic series expansions (SSE's).[11] Very recently an important technical improvement was achieved by Sandvik.[12] He found an algorithm of cluster-type updates (operator-loop updates) within the SSE QMC scheme which reduces the autocorrelation time drastically compared to simulations using only local updates. While this method is very similar to the loop algorithm in the world-line QMC method proposed by Evertz *et al.*,[13] one major advantage of the SSE method with operator-loop updates is that there is no difficulty in simulating systems with anisotropic couplings in external magnetic fields, owing to not needing "freezing" configurations and "global" weights which make the loop algorithm in the world-line QMC method highly inefficient.[12] This reduced autocorrelation time enables us to go down to very low temperatures in very high magnetic fields; therefore, the method is suitable for our purpose. Another advantage of this study using the SSE scheme over other earlier numerical studies[4,10,14] is that the simulations are performed directly in the ground canonical ensemble, i.e., the magnetization per site $m_z=M_z/N_s$ is calculated for a given magnetic field h. In this paper temperatures T are set to be $J/k_BT=2L$, which is low enough to study ground-state properties on finite lattices,[15] and a periodic boundary condition is used. The exchange coupling J will be taken to be the energy unit. Since there exists a long-range Néel-ordered state only for $\Delta\geqslant 1.0$, from which the first-order spin-flip

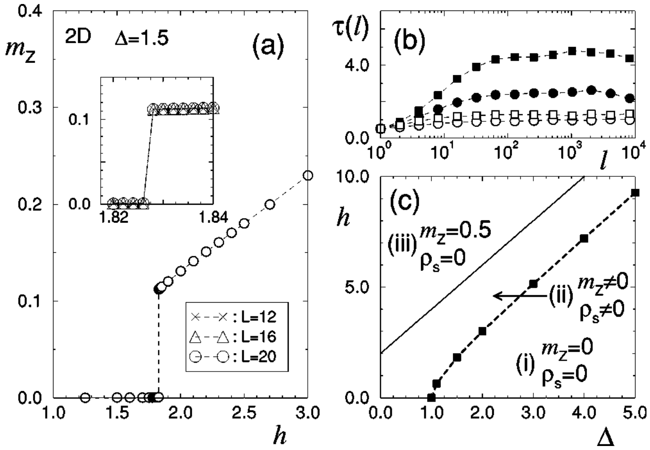

FIG. 1. (a) Magnetization curve of the 2D spin-1/2 XXZ model with $\Delta=1.5$. Inset: an enlarged scale is used. Error bars are smaller than symbols. (b) Correlation time $\tau(l)$ (for a definition, see in the text) of m_z (circles) and $S(\pi,\pi)$ (squares) as a function of bin length l. The parameters are $N_s=12^2$, $T=1/24$, $\Delta=1.5$, and $h=2.0$. Solid (open) marks are data for operator-loop updates with closed loops constructed as many as 25 (100) times per MC step. (c) The ground-state phase diagram of the 2D spin-1/2 XXZ model with anisotropic constant Δ in the presence of the magnetic field h. There exist three phases: (i) a Néel-ordered phase, (ii) a spin-flipping phase, and (iii) a fully saturated ferromagnetic phase. The solid line is $2(1+\Delta)$ (see the text). The dashed line is a guide to the eye.

transition can take place by applying a finite external field, our main focus in this paper will be on this anisotropic regime.

Let us first study the magnetization process in two dimensions. A typical example of the magnetization curves is shown in Fig. 1(a). One can see that at a certain critical magnetic field h_c the magnetization m_z changes discontinuously from 0 to a finite value m_z^c. For this example in the figure, with $\Delta=1.5$, the magnetization jumps at $h_c\sim 1.83$ to $m_z^c\sim 0.11$.[16] Working on various system sizes [see in the inset of Fig. 1(a)], we confirm that finite-size effects are small, and conclude that the jump in magnetization is not due to extrinsic factors working on finite-size lattices. The result already gives clear evidence of a first-order phase transition.

In order to illustrate that autocorrelation times of our QMC measurements are short enough, the integrated autocorrelation time $\tau_{\rm int}$ is estimated as follows: we first divide a sequence of Monte Carlo data points into bins of length l, and, for each bin length l, the average of the data in the bth bin and the variance $\sigma^2(l)$ of the bin averages are calculated. The integrated autocorrelation time $\tau_{\rm int}$ is then estimated by the asymptotic value of $\tau(l)=l\sigma^2(l)/2\sigma^2(l=1)$ at large l, above which $\tau(l)$ does not depend on l.[17] The results of $\tau_{\rm int}$ for m_z and spin structure factor $S(\mathbf{q})$ at $\mathbf{q}=(\pi,\pi)$ are shown in Fig. 1(b) for $\Delta=1.5$ and $h=2.0$. From this figure, $\tau_{\rm int}$'s are estimated to be no longer than 4–5 MC steps. Since we use a bin length of $l=1000$ or more to estimate the statistical errors, we can be sure that our error bar is accurate. It should be noted here that $\tau_{\rm int}$ can be controlled by changing how many times closed loops are constructed in the operator-loop updates. In this paper we have to construct closed loops as many as about 1000 times per MC step for larger values of Δ.

Repeating the same procedure for different values of Δ, the ground-state phase diagram of the 2D spin-1/2 XXZ model is completed. The result is given in Fig. 1(c). There exist three different phases denoted by (i) $m_z=0$, (ii) $m_z\neq 0$, and (iii) $m_z=0.5$ in the figure. The third phase (iii) corresponds to a fully saturated ferromagnetic phase, and is separated from the second phase (ii) by a critical magnetic field $h_c^{\rm max}$. This transition is trivial, and is not of interest here. The critical magnetic field $h_c^{\rm max}$ is indeed easily calculated by going to the boson model described by Eq. (2): the critical chemical potential required to have just one particle in the d-dimensional boson system is $-2dt$; therefore $h_c^{\rm max}/J$ is found to be $d(1+\Delta)$.

To show further evidence of a first-order transition between phases (i) and (ii) we calculate the spin structurefactor $S(\mathbf{q})=1/N_s\Sigma_{\mathbf{i},\mathbf{j}}e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\mathbf{S_i}\cdot\mathbf{S_j}$ at $\mathbf{q}=(\pi,\pi)$ and the spin stiffness (helicity modulus) ρ_s as a function of h for a fixed Δ. The spin stiffness ρ_s is calculated, for example, by $\rho_s=T\langle w_x^2+w_y^2(+w_z^2)\rangle/dL^{d-2}$ in two (three) dimensions

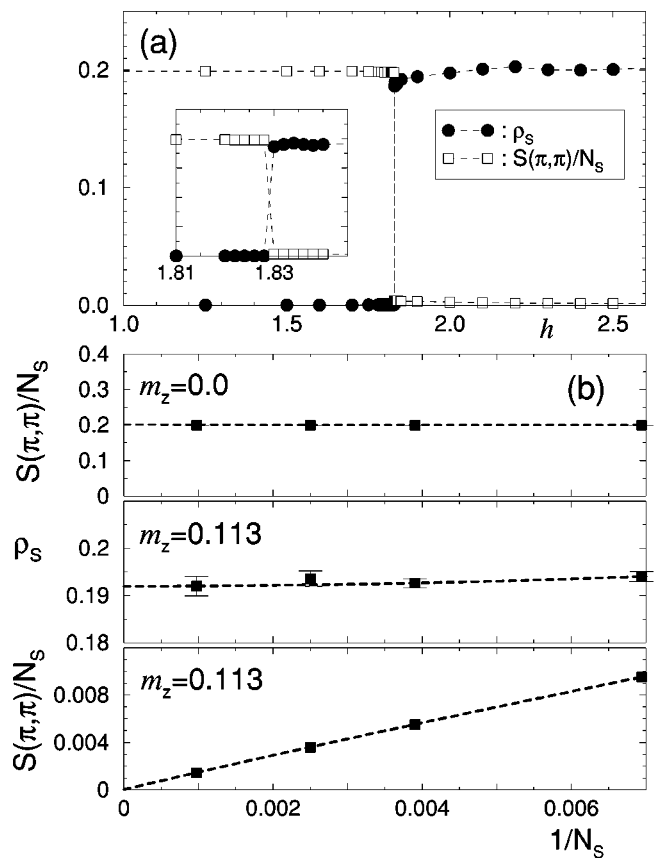

FIG. 2. (a) $S(\pi,\pi)$ and ρ_s for the 2D spin-1/2 XXZ model with $\Delta=1.5$ and $N_s=20^2$ as a function of the magnetic field h. Inset: an enlarged scale is used. (b) Finite-size scaling of $S(\pi,\pi)/N_s$ and ρ_s for different magnetizations with $\Delta=1.5$. The top figure shows $S(\pi,\pi)/N_s$ for $m_z=0$ and the middle (bottom) figure shows ρ_s ($S(\pi,\pi)/N_s$) for $m_z=0.113$. Dashed lines are liner fitting curves for QMC data, extrapolating to $1/N_s\to 0$.

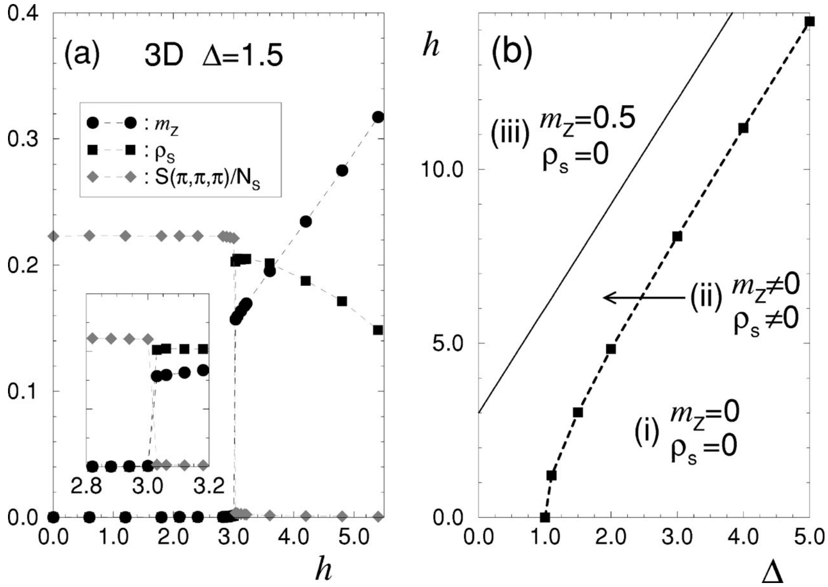

FIG. 3. (a) m_z, $S(\pi,\pi,\pi)$, and ρ_s for the 3D spin-1/2 XXZ model with $\Delta=1.5$ and $N_s=8^3$ as a function of the magnetic field h. Inset: an enlarged scale is used. (b) The ground-state phase diagram of the 3D spin-1/2 XXZ model with an anisotropic constant Δ in the presence of a magnetic field h. The diagram consists of (i) a Néel-ordered phase, (ii) a spin-flipping phase, and (iii) a fully saturated ferromagnetic phase. The solid line is $3(1+\Delta)$ (see the text). The dashed line is a guide to the eye.

where w_α is the winding number per linear spatial lattice size L in the α direction.[18] ρ_s corresponds to the superfluid density in the boson model, and is used to detect the superfluid phase in the system.[9,10,18] The results are shown in Fig. 2(a) for $\Delta=1.5$ as a function of h. When h is small, $S(\mathbf{q})$ has a peak at $\mathbf{q}=(\pi,\pi)$ (the $\mathbf{q}$ dependence is not shown) and $\rho_s=0$. With increasing h these quantities change discontinuously at h_c where the magnetization m_z jumps, and $S(\pi,\pi)$ becomes zero while ρ_s has a finite value.[19] Apparently these two phases are (i) a Néel-ordered phase (for $h<h_c$) and (ii) a spin-flipping phase (for $h>h_c$), and are separated through a first-order transition.[20]

Earlier studies found the supersolid phase in the 2D boson model characterized by simultaneously possessing finite values of $S(\pi,\pi)$ and ρ_s in a region between phases (i) and (ii) of the phase diagram.[9,10] One can indeed barely see small but finite values of $S(\pi,\pi)$ for $h>h_c$, where ρ_s is finite [see Fig. 2(a)]. In order to elucidate the possibility of the existence of the supersolid phase systematically in two dimensions, we carry out finite-size scaling analyses of $S(\pi,\pi)$ and ρ_s for fixed magnetizations. The results are presented in Fig. 2(b). One can see that $S(\pi,\pi)/N_s$ (ρ_s) stays finite in the limit of $N_s\to\infty$ for $h<h_c$ ($h>h_c$) while $S(\pi,\pi)/N_s$ approaches zero at $N_s\to\infty$ for $h>h_c$. Doing similar analyses for different values of Δ and m_z it is found that whenever $h>h_c$, $S(\pi,\pi)/N_s$ goes to zero in the thermodynamic limit. We therefore conclude that the supersolid phase does not exist in the 2D spin-1/2 XXZ model. The results are consistent with very recent studies by Batrouni and Scalettar.[14]

We now carry out similar calculations for the 3D spin-1/2 XXZ model to study the nature of the phase transition induced by the external magnet field. Strong evidence of the first-order transition is provided in Fig. 3(a). In this figure the magnetization m_z, spin structure factor $S(\pi,\pi,\pi)$, and spin stiffness ρ_s for $\Delta=1.5$ are plotted as functions of the external magnetic field h. It is clearly seen that as in the case of the 2D model, these quantities change discontinuously at a critical magnetic field h_c. Working with different values of Δ, a ground-state phase diagram is constructed and the result is shown in Fig. 3(b). As in two dimensions the phase diagram consists of three different phases: (i) a Néel-ordered phase, (ii) a spin-flipping phase, and (iii) a fully saturated ferromagnetic phase.[21] The critical magnetic field h_c in three dimensions is observed to be larger compared to that in two dimensions for a given Δ. This is simply because the increased coordination number in three dimensions makes the needed magnetic field larger to destroy the Néel state. Similar finite-size scaling analyses, done for the 2D model, do not find a supersolid phase in the 3D model.

Finally we summarize our results in Fig. 4 by showing the ground-state phase diagrams of the 2D and 3D spin-1/2 XXZ models on the parameter space of anisotropic constant Δ and

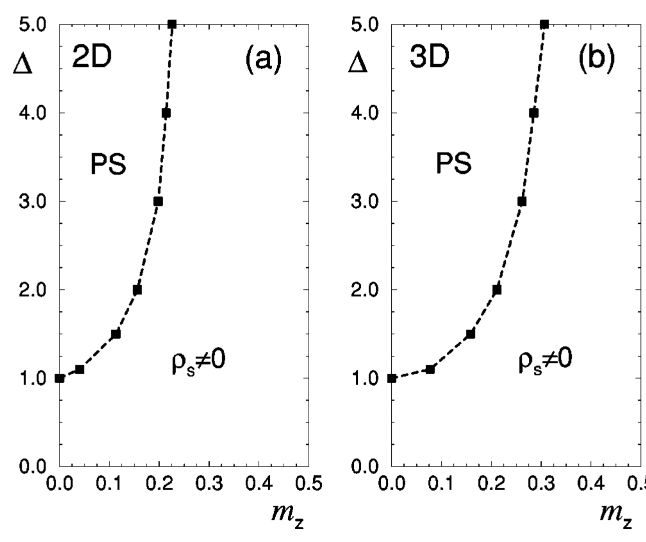

FIG. 4. The ground-state phase diagrams of the (a) 2D and (b) 3D spin-1/2 XXZ models on the parameter space of anisotropic constant Δ and magnetization m_z. PS stands for phase separation. The Néel (fully saturated ferromagnetic) state exists in the region of $\Delta\geqslant 1.0$ and $m_z=0.0$ ($m_z=0.5$). The spin-flipping phase is in the region denoted by $\rho_s\neq 0$. The dashed line is a guide to the eye. For the boson model defined by Eq. (2) m_z and Δ correspond to $0.5-n$ and $V/2t$, respectively.

magnetization m_z. The phase diagrams show (i) a Néel-ordered state at $\Delta \geqslant 1.0$ and $m_z = 0.0$, (ii) a spin-flipping state with $\rho_s \neq 0$, (iii) a fully saturated ferromagnetic state at $m_z = 0.5$, and (iv) a phase-separated state (denoted by PS in the figures). The phase-separated region exists because, as seen in Figs. 1(a) and 3(a), there is a region in magnetization m_z which we cannot reach in a thermodynamically stable way no matter how finely the magnetic field h is tuned. In other words, if one could have a state with m_z in this magnetization region, the state would be phase separated between a Néel state with $m_z = 0$ and a spin-flipping state with $m_z = m_z^c$. Some earlier studies predicted two phase coexisting regions working with a canonical ensemble (i.e., fixed m_z), and their results were interpreted as a supersolid phase.[9,10] However, our calculations conclude that these phases are thermodynamically unstable and phase separated. Our conclusions are consistent with recent studies by Batrouni and Scalettar for the 2D boson model.[14]

In conclusion, we have numerically studied the magnetization process of the spin-1/2 anisotropic XXZ model in two and three spatial dimensions using the QMC method based on the SSE, and have shown clear evidence of a first-order phase transition in the presence of an external magnetic field. Based on the calculated ground-state phase diagrams, the existence of a phase-separated region and the absence of a supersolid phase were pointed out in the related systems of hard core bosons with nearest-neighbor repulsions.

It would be of great interest to study effects of random anisotropic constant Δ on phase diagrams,[22] since one can elucidate *quantum* effects on recently proposed impurity-induced quantum-critical-point-like behavior near *first*-order phase transitions in Ising models.[23] Another interesting issue to address is the effects of long-ranged Coulomb repulsions between bosons on the phase-separated region in the phase diagram. There is a general belief that introducing Coulomb interactions replaces the phase-separated state by thermodynamically stable states such as a dropletlike state and perhaps a stripe state.[24] The model studied here provide an ideal system to examine the possibilities of those exotic states using unbiased numerical methods.

Note added in proof. Phase diagrams at finite temperatures for the 2D boson model [described by Eq. (2)] with $V = 3t$ have been reported recently by G. Schmid *et al.*[25] Our results in this paper are in good agreement with their results at low temperatures.

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[15] Except for $\Delta \sim 1.0$, for which we have to go down to lower temperatures to see a clear jump in the magnetization curve.
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[19] In phase (iii), ρ_s is zero. This is understood simply because the superfluid density is proportional to the number density n for the boson model; in phase (iii), $n = 0$.
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[21] Note that in phase (ii) $\langle w_x^2 \rangle = \langle w_y^2 \rangle = \langle w_z^2 \rangle$.
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