Lanczos exact diagonalization study of field-induced phase transitions for Ising and Heisenberg antiferromagnets

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Using an exact diagonalization treatment of Ising and Heisenberg model Hamiltonians, we study field-induced phase transitions for two-dimensional antiferromagnets. It is found that a first-order phase transition occurs for both the Ising and Heisenberg antiferromagnets. For the Ising antiferromagnet a mixture of antiferromagnetic and ferromagnetic phases exists only at a critical value of Zeeman energy, while for the Heisenberg antiferromagnet the mixed phase appears over a wide range of Zeeman energy. It is shown that the mixed phase for the Heisenberg antiferromagnet occurs owing to the presence of a spin-flop process as an intermediate step. [S0163-1829(99)13633-6]

I. INTRODUCTION

As early as 1932, Néel[1] proposed the antiferromagnetic order in order to explain the low-temperature behavior of the magnetic susceptibility of certain metals. Over the years physical properties of low-dimensional quantum antiferromagnets at low temperature have been actively pursued. The exact solution via the Bethe ansatz[2] is not extendible to multidimensional systems beyond one-dimensional integral systems. Lately one of the interesting areas of numerical studies has been to determine the character of the field-induced phase transition (i.e., the antiferromagnetic to ferromagnetic transition) involving the systems of antiferromagnetically correlated electrons under externally applied magnetic field. By applying the dynamical mean field theory (DMFT) to the Hubbard model, Held *et al.*[3] studied the microscopic origin of metamagnetism in antiferromagnets with an easy axis under external magnetic field. Their study showed that at half filling a metamagnetic phase transition arises via a first-order phase transition at low temperature and that a second-order phase transition occurs near the Néel temperature. On the other hand, Bagehorn and Hetzel[4] observed a second-order phase transition at zero temperature from the projector quantum Monte Carlo (PQMC) calculation of the Hubbard model with an easy axis. Earlier using a Landau theory of free energy, Moriya and Usami[5] revealed a second-order phase transition at low temperature involving the mixed phase of antiferromagnetic and ferromagnetic states. However, Bagehorn and Hetzel questioned whether the mixed phase would survive at a small region of magnetic field if exact electron correlations were implemented. In the present study, by performing the exact diagonalization calculations of the two-dimensional systems of antiferromagnetically correlated electrons under applied magnetic field, we examine the nature of field-induced phase transition (metamagnetism) at zero temperature for both Ising and Heisenberg antiferromagnets.

II. LANCZOS EXACT DIAGONALIZATION CALCULATIONS OF FIELD-INDUCED PHASE TRANSITIONS

For the study of field-induced phase transition for the two-dimensional Ising antiferromagnet, we consider the following model Hamiltonian with the inclusion of Zeeman coupling term:

$$H=-t\sum_{\langle ij\rangle,\sigma}(\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma}+\text{c.c.})+J_z\sum_{\langle ij\rangle}S^z_iS^z_j-h\sum_{i\sigma}\sigma c^{\dagger}_{i\sigma}c_{i\sigma}. \tag{1}$$

$\tilde{c}_{i\sigma}$ ($\tilde{c}^{\dagger}_{i\sigma}$) is the electron annihilation (creation) operator at site i with no double occupancy and S^z_i is the z component of electron spin operator at site i. t is the hopping strength, J_z is the Ising correlation strength, and h is the Zeeman energy $\mu_B B$. Here μ_B is the Bohr magneton and B is the strength of external magnetic field. $\sigma=+1$ (-1) for up spin (down spin). In the case of half filling, the above model Hamiltonian reduces to the Ising Hamiltonian.

For the study of field-induced phase transition for the two-dimensional Heisenberg antiferromagnet, we consider the t-J model Hamiltonian with the inclusion of Zeeman coupling term

$$H=-t\sum_{\langle ij\rangle,\sigma}(\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma}+\text{c.c.})+J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{1}{4}n_in_j\right)-h\sum_{i\sigma}\sigma c^{\dagger}_{i\sigma}c_{i\sigma}. \tag{2}$$

$\mathbf{S}_i$ is the electron spin operator and n_i is the electron number operator at site i. In the case of half filling, the t-J model Hamiltonian effectively reduces to the Heisenberg Hamiltonian.

The above Hamiltonians will be diagonalized by the Lanczos exact diagonalization method.[6] For the exact diagonalization treatment of antiferromagnetic correlations uniform and staggered magnetizations are defined by[7]

$$\langle(m^l_q)^2\rangle=\left\langle\left(\frac{1}{N}\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}S^l_i\right)^2\right\rangle, \tag{3}$$

where $l=x,y,z$. Here $(m^l_q)^2$ represents the square of the uniform and staggered magnetizations in the lth direction corresponding to $q=(0,0)$ and $q=Q\equiv(\pi,\pi)$, respectively. N is the total number of lattice sites. Uniform and staggered mag-

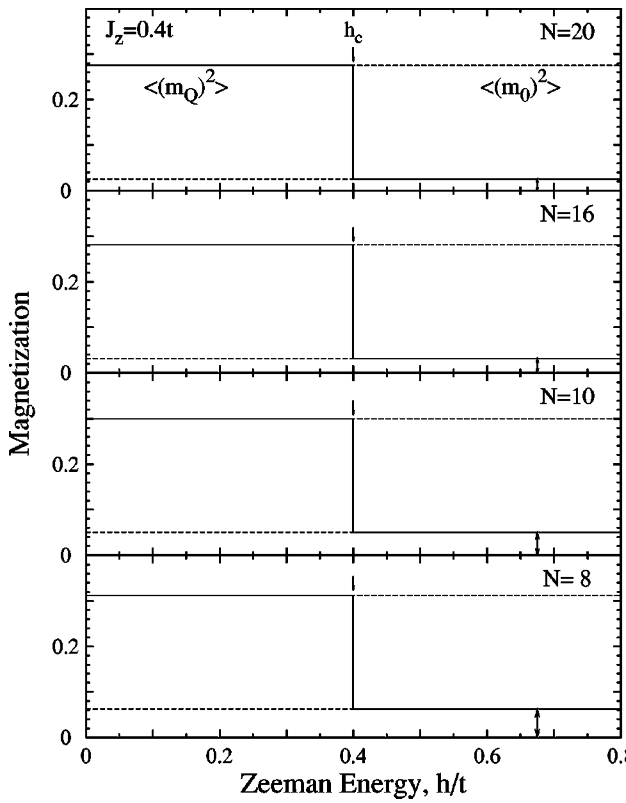

FIG. 1. Staggered and uniform magnetizations for the two-dimensional Ising antiferromagnet versus Zeeman energy. The solid line represents the staggered magnetization (m_Q) and the dashed line denotes the uniform magnetization (m_0). The Ising correlation strength is chosen to be $J_z=0.4t$. N is the number of lattice sites. h_c indicates a critical value of Zeeman energy at which discontinuities of magnetizations occur. Double-headed arrows indicate that the nonvanishing value of staggered magnetization beyond h_c is due to finite-size effect.

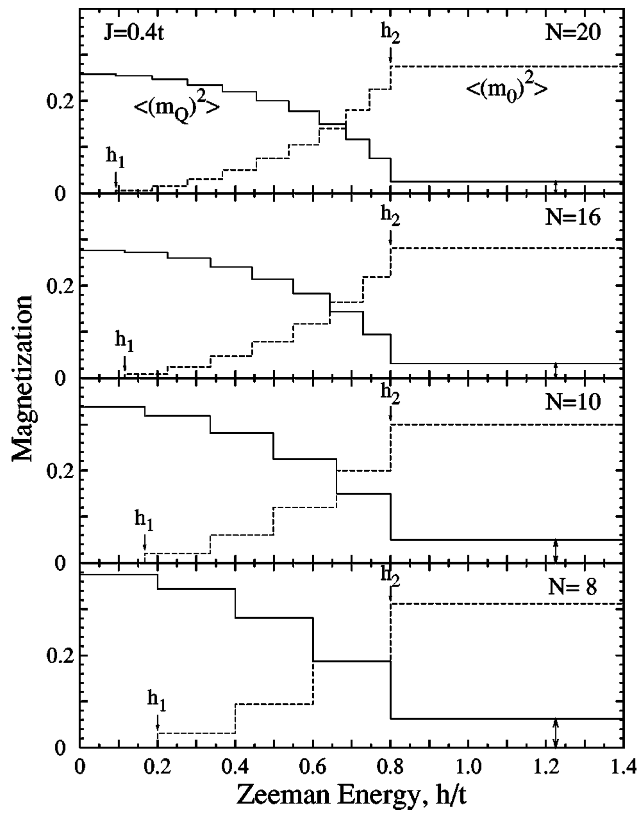

FIG. 2. Staggered and uniform magnetizations for the two-dimensional Heisenberg antiferromagnet versus Zeeman energy. The solid line represents the staggered magnetization (m_Q) and the dashed line denotes the uniform magnetization (m_0). The Heisenberg correlation strength is chosen to be $J=0.4t$. N is the number of lattice sites. h_1 indicates a value of Zeeman energy at which the uniform magnetization begins to appear (or the staggered magnetization begins to decrease). h_2 indicates a value of Zeeman energy at which the uniform magnetization saturates. Double-headed arrows indicate that the nonvanishing value of staggered magnetization beyond h_2 is due to finite-size effect.

netizations as a function of the applied magnetic field are computed for small clusters of various sizes ($\sqrt{8}\times\sqrt{8}$, $\sqrt{10}\times\sqrt{10}$, 4×4, and $\sqrt{20}\times\sqrt{20}$) with periodic boundary conditions. Lanczos iteration is terminated when the ground state energy is converged within the error bound of 10^{-10}.

For the case of Ising antiferromagnet, predicted magnetizations are shown in Fig. 1 for small clusters of various sizes and $J_z=0.4t$. The staggered magnetization is represented by a solid line and the uniform magnetization is denoted by a dashed line. The nonvanishing values of staggered magnetization at high Zeeman energies is due to finite-size effect, as is indicated by double-headed arrows in the figure. Discontinuity from the staggered to uniform magnetizations occurs at a critical Zeeman energy $h_c=J_z=0.4t$. Although not shown here, the same behavior of staggered and uniform magnetizations is observed for other values of J_z. A mixture of antiferromagnetic and ferromagnetic phases exists at a critical field corresponding to h_c. Thus the field-induced phase transition for the Ising antiferromagnet is found to be of first order. In our previous work,[8] we calculated the staggered and uniform magnetizations for the Ising system by using Hubbard model Hamiltonian in mean-field approximation. The first-order phase transition was also predicted.

For the case of the Heisenberg antiferromagnet, predicted magnetizations are shown in Fig. 2 for small clusters of various sizes and $J=0.4t$. The stepwise curves are formed owing to the finite-size effect. This is because the difference in number between up ($N_\uparrow$) and down ($N_\downarrow$) spins discretely varies with the change of magnetic field, e.g., $N_\uparrow-N_\downarrow=0,2,\ldots,10$ for a half-filled $\sqrt{10}\times\sqrt{10}$ lattice. As the number of lattice sites and thus the number of electron spins increase, the stepwise curves are expected to turn smooth. Indeed the computed results showed such a trend as is shown in Fig. 2. The uniform magnetization appears at a low Zeeman energy of h_1 and reaches a maximum (or saturates) at a Zeeman energy of h_2. The staggered magnetization beyond h_2 does not completely vanish owing to the finite-size effect, as is indicated by double-headed arrows in the figure. It is found that as the size of cluster increases, h_1 tends to reach 0 while h_2 remains unchanged with the value of $h_2=2J=0.8t$. This observation is displayed in Fig. 2. Although not shown here, the same behavior for $h_1=0$ and $h_2=2J$ is observed for other values of J. Thus a mixed phase of antiferromagnetic and ferromagnetic states is found to occur in the range of $h_1=0<h<h_2=2J$ for the two-dimensional Heisenberg antiferromagnet. The coexistence of the two phases is not seen to change substantially as the lattice size

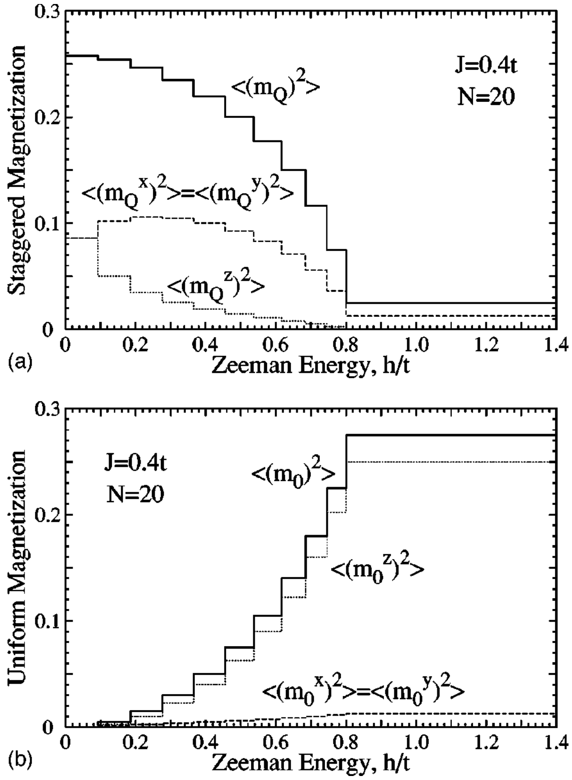

FIG. 3. Decomposition of (a) staggered and (b) uniform magnetizations for the two-dimensional Heisenberg antiferromagnet of lattice size $\sqrt{20}\times\sqrt{20}$ into directions parallel (x and y components) and perpendicular (z component) to the plane.

increases, thus indicating that there exists no significant finite-size effect on the mixed phase. The field-induced phase transition is of first order because the system is at coexistence of the two phases, the antiferromagnetic and ferromagnetic phases. Although not to be directly compared owing to differences in the space dimension of antiferromagnet, such a tendency of uniform magnetization was experimentally observed for the three-dimensional crystal of $Y(Co_{1-x}Al_x)_2$ at low temperature by Goto *et al.*[9] The DMFT of the infinite-dimensional Hubbard model by Held *et al.*[3] yielded a first-order transition. Bagehorn and Hetzel[4] argued in favor of a second-order transition from the PQMC calculations of the Hubbard model with an easy axis. However, their results were obtained for the case of weak coupling ($U=2t$) and are not directly comparable to our strong-coupling results.

In order to find the cause of the mixed phase for the Heisenberg antiferromagnet, we show both the staggered and uniform magnetizations in the direction parallel to and perpendicular to the xy plane, respectively, in Fig. 3. As the external magnetic field increases, the x and y components of the staggered magnetization are predicted to increase particularly in the region of low field, $h\lesssim 0.3t$ in Fig. 3(a), whereas the z component decreases in the same region. The antiferromagnetic order projected onto the xy plane (perpendicular to the external magnetic field) tends to persist, while its z component m_Q^z monotonically decreases and vanishes at $h=0.8t$. This can be further explained as follows. In the absence of magnetic field, spins align into a strong antiferromagnetic state due to the Heisenberg interaction as is shown in Fig. 4(a). As the magnetic field in the z direction increases, spin-flop process occurs as an intermediate state by exhibiting the components of antiferromagnetic spin alignment on the xy plane, as depicted in Fig. 4(b). For the Heisenberg antiferromagnet, the spin flop, that is, the x and y components of the staggered magnetization peak at a particular value of the applied magnetic field, say, $h\simeq 0.3t$ as is shown in Fig. 3(a). As the external magnetic field further increases, the Zeeman effect begins to dominate the Heisenberg interaction with disappearance of the spin-flop process by allowing ferromagnetic configurations, as is shown in Fig. 4(c). On the other hand, for the Ising system the spin-flop process is not involved and the mixed phase does not occur except at the critical Zeeman energy, as is shown in Fig. 1. Thus we claim that the spin-flop process due to antiferromagnetic interactions involving x and y components of spins are responsible for the mixed phase of the Heisenberg system.

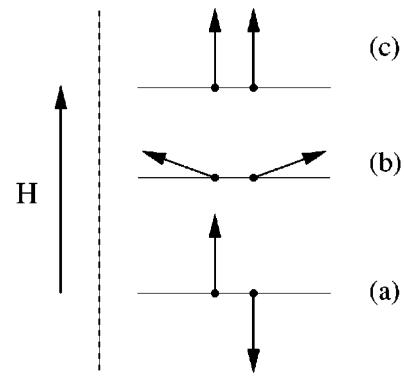

FIG. 4. Spin-flop process and metamagnetism under applied magnetic field. The magnetic field is applied in the z direction. The horizontal solid line represents the two-dimensional xy plane. (a) antiferromagnetic spin order, (b) spin flop, and (c) ferromagnetic spin order.

III. CONCLUSION

By applying the exact diagonalization method to the Ising and Heisenberg antiferromagnets in external magnetic fields, we have examined the field-induced phase transition from an antiferromagnetic to a ferromagnetic state. For both the Ising and Heisenberg antiferromagnets the first-order phase transition is predicted to occur. For the Ising antiferromagnet a mixture of antiferromagnetic and ferromagnetic phases exists only at a critical value of Zeeman energy, while for the Heisenberg antiferromagnet the mixed phase appears over a wide range of Zeeman energy. It was shown that the mixed phase for the Heisenberg antiferromagnet occurs through the spin-flop process as an intermediate step.

ACKNOWLEDGMENTS

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