Lanczos exact diagonalization study of field-induced phase transition 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 transition for two-dimensional antiferromagnets. For the system of Ising antiferromagnet the predicted field-induced phase transition is of first order, while for the system of Heisenberg antiferromagnet it is the second-order transition. We find from the exact diagonalization calculations that the second-order phase transition (metamagnetism) occurs through a spin-flop process as an intermediate step.

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I. INTRODUCTION

Much earlier (in 1932) the antiferromagnetic order was proposed by Néel in order to explain the low temperature behavior of the magnetic susceptibility of certain metals. Currently physical properties of low-dimensional quantum antiferromagnets at low temperature are actively pursued. The exact solution via Bethe Ansatz is limited to one-dimensional integral systems, but not extendible to multidimensional systems. Recently, one among the interesting subjects is a numerical study of field-induced phase transition, namely, the antiferromagnetic to ferromagnetic transition in the two-dimensional 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. studied the microscopic origin of metamagnetism along an easy axis in antiferromagnets under external magnetic field. Their study showed that at half filling a metamagnetic phase transition arises via the first-order phase transition at low temperature and that the second-order phase transition occurs near the Néel temperature. On the other hand, Bagehorn and Hetzel observed the 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 revealed the second-order phase transition at low temperature involving the mixed phase of ferro- and antiferromagnetic 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 0 K for both Ising and Heisenberg antiferromagnets.

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

With the inclusion of Zeeman coupling term, the two-dimensional t-J model Hamiltonian is written,

\[ H = -t \sum_{\langle ij \rangle, \sigma} \left( (1 - n_{i,-\sigma})c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j,-\sigma}) + c.c. \right) + J \sum_{\langle ij \rangle} (S_i \cdot S_j - \frac{1}{4} n_in_j) - h \sum_{i\sigma} \sigma c_{i\sigma}^\dagger c_{i\sigma}, \]

(1)

where \( c_{i\sigma} \) \( (c_{i\sigma}^\dagger) \) is the electron annihilation (creation) operator, \( S_i \) is the electron spin operator at site \( i \), and \( h \) is the Zeeman energy. \( \mu_B \) 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 t-J model Hamiltonian effectively reduces to the Heisenberg model Hamiltonian.

The above Hamiltonian in Eq. (1) will be diagonalized by the Lanczos exact diagonalization method. For the exact diagonalization treatment of antiferromagnetic correlations uniform and staggered magnetizations are defined by

\[ \langle (m_\ell^\ell)^2 \rangle = \left\langle \left( \frac{1}{N} \sum_i e^{i q \cdot r_i} S_i^\ell \right)^2 \right\rangle, \]

(2)

where \( \ell = x, y, z \). Here \( (m_\ell^\ell)^2 \) represents the square of the uniform and the staggered magnetizations in the \( \ell \)th direction corresponding to \( q = (0,0) \) and \( q = Q \equiv (\pi, \pi) \) respectively. \( N \) is the total number of lattice sites. We calculate the variation of the uniform and the staggered magnetizations with vertically applied magnetic field to a \( 4 \times 4 \) square lattice of antiferromagnetically correlated electrons by satisfying periodic boundary conditions. For the parameters we choose \( t = 1 \) and \( J = 0.4 \). Lanczos iteration is terminated when the ground state energy is converged within the error bound of \( 10^{-10} \).
For the Ising systems, \( H = J \sum_{\langle ij \rangle} S_i^z S_j^z \), we find that the metamagnetic phase transition is of first order, as is shown in Fig. 1. In our previous work,\(^9\) we calculated the staggered and the uniform magnetizations for the Ising system by using Hubbard model Hamiltonian in mean-field approximation. The first-order phase transition was also predicted. In both approaches we note that there exists no mixed phase (of both \( m_Q \neq 0 \) and \( m_0 \neq 0 \)). In other words, discontinuity from staggered to uniform magnetization is observed at a critical magnetic field, say, \( h = 0.4t \) in Fig. 1 (the staggered magnetization beyond the critical field and the uniform magnetization below the same point did not completely vanish owing to finite-size effect). Thus in the Ising systems metamagnetism occurs as a first-order phase transition. This is in agreement with the DMFT study of Held et al.\(^3\) On the other hand, Bagehorn and Hetzel showed from their PQMC calculation that metamagnetism occurs via a second-order phase transition.

\[ <(m_Q)^2> \quad t=1, J_z=0.4 \]

\[ <(m_0)^2> \quad t=1, J=0.4 \]

**FIG. 1.** Staggered and uniform magnetizations for the two-dimensional Ising system as a function of Zeeman energy. (a) staggered magnetization \( m_Q \) and (b) uniform magnetization \( m_0 \).

For the Heisenberg systems, we show the predicted magnetization as a function of applied field in Fig. 2. The stepwise curves are inevitably formed owing to the size effect. As the number of lattice sites increases, the stepwise curves are expected to turn smooth. The solid curves in the figure are interpolated ones only for the visual aid. The second-order field-induced transition is observed for metamagnetism at 0 K. The magnetic susceptibility, \( \chi = \frac{dm}{dh} \) changes from a negative to a positive value at a crossing point between the lines of the staggered magnetization (solid line) and of the uniform magnetization (dotted line). This indicates the occurrence of a mixed phase of the ferro- and antiferromagnetic phases during the process of metamagnetism. The predicted antiferromagnetic susceptibility vanishes beyond a ‘critical field’ corresponding to the Zeeman energy, \( h \simeq 0.8t \) (the staggered magnetization did not completely vanish owing to the size effect). The uniform magnetization is predicted to remain constant beyond the same point. Although not to be directly compared, due 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.\(^8\)

\[ <(m_Q)^2> \quad t=1, J_z=0.4 \]

\[ <(m_0)^2> \quad t=1, J=0.4 \]

**FIG. 2.** Staggered \( m_Q \) (solid line) and uniform \( m_0 \) (dotted line) magnetizations for the two-dimensional Heisenberg system as a function of Zeeman energy. Solid curves are guide lines for the eyes.

In order to find the cause of the second-order phase transition with the Heisenberg antiferromagnet, in Fig. 3 we show both the staggered and uniform magnetizations in the direction parallel to and perpendicular to the plane respectively. 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, \( h < 0.3t \) in Fig. 3(a), whereas the \( z- \)component decreases in the same region. The antiferromagnetic order projected onto the plane (perpendicular to the external magnetic field) tends to persist to a point, while its \( z- \)component \( m_Q^z \) monotonically decreases and vanishes at \( h \simeq 0.8t \). 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 x-y 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, \( h \approx 0.3t \) as is shown in Fig. 4(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 first-order phase transition was predicted with no involvement of spin-flop process before the metamagnetic transition, as is shown in Fig. 1. Thus we claim that antiferromagnetic spin interactions involving x- and y-components are responsible for the second-order phase transition accompanying a spin-flop process as an intermediate step.

![Staggered and uniform magnetizations](image)

**FIG. 3.** Staggered and uniform magnetizations for the two-dimensional Heisenberg system as a function of Zeeman energy. (a) Decomposition of staggered magnetization \( (m_Q) \) and (b) decomposition of uniform magnetization \( (m_0) \) into directions parallel \( (m_Q^x) \) and \( (m_Q^y) \) and perpendicular \( (m_Q^z) \) to the plane respectively for \( q = Q, 0 \).

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

### III. CONCLUSION

By applying the exact diagonalization method to Heisenberg antiferromagnets under external magnetic field, we examined how the second-order phase transition occurs from an antiferromagnetic to a ferromagnetic state at a critical magnetic field. The second-order phase transition occurred in the presence of the mixed phase near the critical magnetic field. According to the present exact diagonalization study, the second-order phase transition was induced through the presence of spin-flop process owing to the influence of the x- and y-components of antiferromagnetic spin interactions. In short we observed that for the case of two-dimensional Ising systems the field-induced transition from the antiferromagnetic state to the ferromagnetic state is of first order with no involvement of spin-flop process, while for the case of two-dimensional Heisenberg antiferromagnetic systems it is of second order with the involvement of the spin-flop process as an intermediate process.

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