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In this work we investigate the quantum phase transitions at zero temperature of the one-dimensional transverse Ising model with an extra term containing four-spin interactions. The competition between the energy couplings of the model leads to an interesting zero-temperature phase diagram. We use a modified Lanczos method to determine the ground state and the first excited state energies of the system, with sizes of up to 20 spins. We apply finite size scaling to the energy gap to obtain the boundary region where ferromagnetic to paramagnetic transition takes place. We also find the critical exponent associated with the correlation length. We find a degenerate $\langle 3,1\rangle$ phase region. The first-order transition boundary between this phase and the paramagnetic phase is determined by analyzing the behavior of the transverse spin susceptibility as the system moves from one region to the other.

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I. INTRODUCTION

In recent years, there has been a considerable interest in models exhibiting quantum phase transitions.[1–3] These transitions occur at the absolute zero of temperature as a given parameter of the Hamiltonian is changed across a critical value. At the transition, the ground state of the system undergoes a substantial change. There are a few real systems where quantum transitions play a major role, such as magnetic-field-tuned superconductor-insulator transition in TiN films,[4] superconductor-insulator transition in granular materials,[5] heavy fermion materials,[6] gas of ultracold atoms in a periodic potential,[7] optically trapped Bose-Einstein condensates,[8] two-dimensional electron gas in semiconductors,[9] spin ladder materials,[10] and Josephson-junction arrays,[11] among others.

Since the transition happens at $T=0$, one can search for its signature in one-dimensional (1D) models, which are more amenable to analysis. Such is the case with the transverse Ising model in 1D, originally meant to be a pseudospin model to describe the effects of proton tunneling in hydrogen-bonded materials.[12] It has been known since Pfeuty[13] that the ground state of that model undergoes a ferromagnetic to paramagnetic phase transition as the transverse field interaction energy crosses a threshold value. That kind of transition driven by a transverse field has indeed been observed in the insulator $LiHoF_4$.[14]

The Ising model with four-spin interactions was proposed, independently, by Wu[15] and by Kadanoff and Wegner[16] in 1971. Those authors showed that the Baxter eight-vertex model was equivalent to two regular Ising models of two-spin coupling interacting with each other through a four-spin coupling term. Soon thereafter, Blinc and Zeks[17,18] suggested that the addition of a four-spin interaction term to the transverse Ising model could lead to a first-order transition, such as the ferroelectric transition of potassium dihydrogen phosphate (KDP). Ever since, the influence of higher-order exchange interactions in the critical properties of Ising models has been studied theoretically with several different methods, among them, mean-field calculations,[19–21] renormalization group methods,[22,23] and Monte Carlo simulations.[24,25] Some results from series expansions[22,26] have also been reported in the literature. Models with four-spin interactions can show unusual properties which are not present in regular spin systems with two-spin interactions only. For instance, they may account for nonuniversal critical phenomena[15,16,27] and deviations from Bloch $T^{3/2}$ law at low temperatures.[28,29]

Models of multispin interactions have also been used to explain the thermodynamical properties of hydrogen-bonded ferroelectrics $PbHPO_4$ and $PbDPO_4$,[30] squaric acid crystal $(H_2C_2O_4)$,[19,31] binary alloys,[24] ferroelectric thin films,[32] and some copolymers.[33] They have been used to understand the experimental results of spin gaps,[20,34] Raman peaks,[35] and optical conductivity[36] seen in the copper oxyde ladder $La_xCa_{14-x}Cu_{24}O_{41}$.[37] In addition, four-spin interactions seem to play a role in the physics of the two-dimensional antiferromagnet La_2CuO_4,[38] the precursor of high-T_c superconductors.

In the present paper, we investigate the phase transitions at the ground state of the $s=1/2$ transverse Ising model with the addition of a term of four-spin interactions, in one dimension. We are interested in the phases which result from the interplay between the competing two-spin Ising coupling and the four-spin coupling in the presence of a transverse field. We use a modified Lanczos method[39] to exactly determine the ground state and the first excited state energies as well as the corresponding eigenvectors. We then use finite-size scaling analysis to determine the ferromagnetic-paramagnetic transition line and the critical exponent associated with the correlation length. In addition, by analyzing the transverse magnetization we also find the line of first-order transition separating the paramagnetic state from a novel phase, the antiphase $\langle 3,1\rangle$ where a long-range order is formed by the repetition of a unit cell with three like spins followed by a single opposite spin. We also take advantage of the knowledge of the ground-state eigenvectors that we obtain to visualize the phases of the model. This paper is arranged as follows: In Sec. II we introduce the model and outline the methods used; in Sec. III, we present and discuss our results.

II. THE MODEL

The system here studied is described by the Hamiltonian

$$H = -\sum_{i=0}^{N-1} [2J_1 S_i^z S_{i+1}^z + 8J_4 S_i^z S_{i+1}^z S_{i+2}^z S_{i+3}^z + B_x S_i^x], \quad (1)$$

where S_i^α denotes the α component of a spin-1/2 operator, $\alpha=x,y,z$, located at site i in a chain with N spins, with periodic boundary conditions. The quantity J_1 is the Ising coupling between neighboring spins, whereas J_4 is the Ising-like four-spin interaction and B_x is the strength of the transverse magnetic field along the x direction. For $J_4=0$ the model reduces to the usual Ising model in a transverse field (TIM). We shall be concerned with a Ising ferromagnetic coupling, $J_1>0$, competing with the four-spin term $J_4<0$, which disfavors ferromagnetism, but might favor other phases. The transverse field B_x drives the system toward the paramagnetic phase. All of these provide the ingredients for an interesting phase diagram, even at zero temperature.

In this work we present a systematic study of the quantum behavior of the model described by Eq. (1) at $T=0$. We are particularly interested in the identification of the different phases induced by changes in both the four-spin coupling and the magnetic field. To identify the critical couplings and fields separating the various quantal phases we shall use different approaches depending on the nature of the phase transition.

To determine the second-order transition line, we employ a finite-size method which was used recently to study the quantum phase transition in the transverse Ising model with nearest and next-to-nearest neighbor interactions.[40] That approach assumes that at the critical region, the energy gap between the ground state and first excited state varies linearly with the reciprocal of the size of the system, namely,

$$G_N \equiv (E_1^N - E_0^N) \propto N^{-1}. \quad (2)$$

Here $G_N=G_N(J,B)$ is a function of the two parameters, $J \equiv J_4/J_1$ and $B\equiv B_x/J_1$. Therefore, for two different system sizes,

$$N(E_1^N - E_0^N) = N'(E_1^{N'} - E_0^{N'}). \quad (3)$$

The critical fields B_c are found by calculating the point where the scaled energy gap $\Delta_N \equiv N(E_1^N - E_0^N)$ coincides for two different system sizes, for a given value of J.

The critical exponent ν associated with the correlation length is calculated from the relationship[40]

$$\nu = \frac{\ln(N/N')}{\ln(\Gamma_N/\Gamma_{N'})}, \quad (4)$$

where

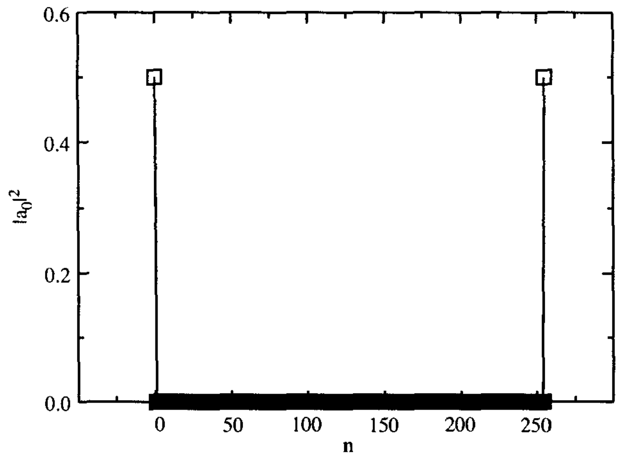

FIG. 1. Ground state of the model in the ferromagnetic phase $(J,B)=(-0.3,0.0)$, for a system size $N=8$. The horizontal axis shows the labels of the basis states, while the vertical axis depicts the squared amplitudes for each of the basis states in the ground state. The nonzero amplitudes correspond to the basis states with all the spins down ($n=0$) and all spins up ($n=255$).

$$\Gamma_N = \left. \frac{\partial \Delta_N(J,B)}{\partial B} \right|_{B=B_c} \quad (5)$$

is the slope of the scaled energy gap for a given J, evaluated at the critical field B_c.

We carry out numerical calculations on chains containing up to $N=20$ spins, with periodic boundary conditions. The first two lowest energies of the system and eigenstates are determined using a modified Lanczos method. The convergency precision used in our calculation depends on the system size, as follows: between 10^{-9} and 10^{-12} for the ground state energy, and from 10^{-5} to 10^{-9} for the first excited state energy. We use a state basis in which the vectors are eigenstates of $S^z = \sum_{i=0}^{N-1} S_i^z$. A basis state is represented by $|n\rangle$, with state labels $n=0,\ldots,M-1$, where $M=2^N$ is the total number of states. The state $|n\rangle$ is given by a sequence of N digits, containing only zeros or ones, which is the binary representation of the label n. The zeros represent down spins and the ones up spins. In this way, there is a simple connection between the basis state labels n and how the spins are distributed along the chain in that state. A general state is written as a linear combination of the basis states, as follows,

$$|\psi_\alpha\rangle = \sum_{n=0}^{M-1} a_\alpha(n)|n\rangle, \quad (6)$$

where $\alpha=0$ for the ground state and $\alpha=1$ for the first excited state, etc. By using this notation we were able to draw a picture of the entire wave function in a single diagram.

Consider a graph in which the horizontal axis represents the labels of the basis states while the vertical axis shows the squared amplitudes $|a_\alpha(n)|^2$ corresponding to the weights of each basis state $|n\rangle$ in $|\psi_\alpha\rangle$, as in Eq. (6). We plot in Fig. 1 the squared amplitudes for the ground-state ($\alpha=0$) ferromagnetic phase when $(J,B)=(-0.3,0.0)$ for a system of $N=8$

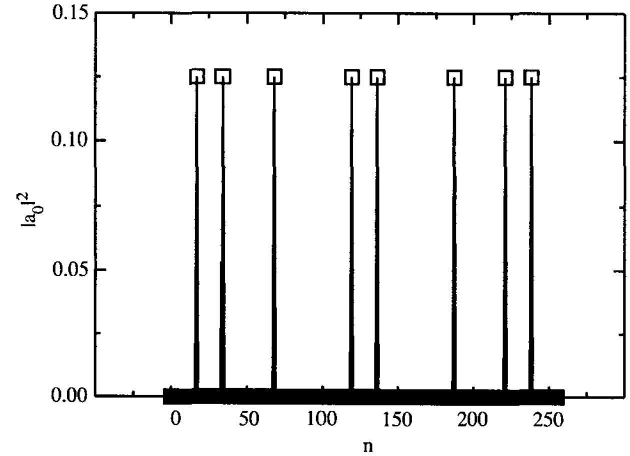

FIG. 2. Ground state for the $\langle 3,1\rangle$ antiphase for $(J,B)=(-0.8,0.0)$ and $N=8$. The axes represent the same quantities as in Fig. 1. The nonzero amplitudes correspond to the basis states with three neighboring spins up (down) followed by one spin down (up). For example, the first peak from the left is at label $n=17$ and corresponds to the basis state $|00010001\rangle$, whose argument is simply the number 17 in binary representation.

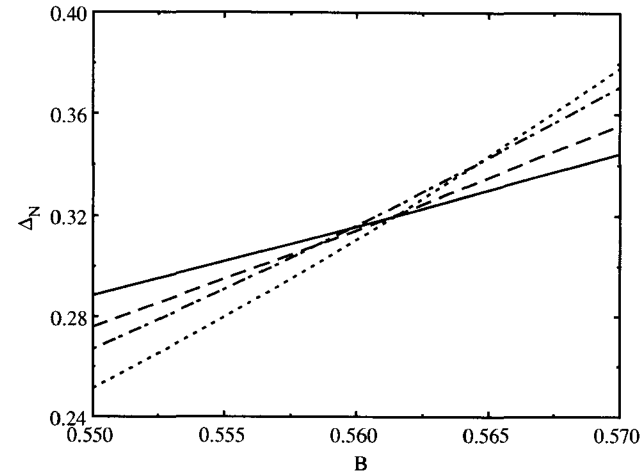

FIG. 3. Scaled energy gap Δ_N as a function of the transverse magnetic field B, for various lattice sizes. The intersection between two lines gives an estimate for the critical field B_c. Here, $J=-0.3$ and $N=8,12,16,20$. The lines are drawn according to the system size: solid line, $N=8$; dashed line, $N=12$; dotted-dashed line, $N=16$; and dotted line, $N=20$.

spins. The two peaks correspond to the state where the spins are either all down $|n=0\rangle=|00000000\rangle$ or up $|n=255\rangle=|11111111\rangle$. The zeros (ones) in the binary representation of n indicate down (up) spins.

In Fig. 2 we show the squared amplitudes of the basis states of the ground state of a novel phase, $\langle 3,1\rangle$, corresponding to the configuration where there are three consecutive spins in the up (down) direction followed by a single spin in the down (up) direction, also for $N=8$. The basis vectors now contributing to the ground state are

$$|17\rangle = |00010001\rangle,$$

$$|34\rangle = |00100010\rangle,$$

$$|64\rangle = |01000100\rangle,$$

$$|134\rangle = |10001000\rangle,$$

each with net magnetization in the down direction, and

$$|119\rangle = |01110111\rangle,$$

$$|187\rangle = |10111011\rangle,$$

$$|221\rangle = |11011101\rangle,$$

$$|238\rangle = |11101110\rangle,$$

with net magnetization in the opposite (up) direction.

The critical line that separates the antiphase $\langle 3,1\rangle$ from the paramagnetic phase is a line of first order. To locate this line we rely on the behavior of the ground-state transverse magnetization with the applied magnetic field. The ground-state magnetization is defined as

$$M^x(J,B) \equiv \langle \psi_0|S_T^x|\psi_0\rangle, \tag{7}$$

where

$$S_T^x = \sum_{i=0}^{N-1} S_i^x, \tag{8}$$

and $|\psi_0\rangle$ is the ground-state eigenvector. We determine the critical field B_c by the location of the maximum of the ground-state transverse susceptibility $\chi=\partial M^x/\partial B$ for a given value of the coupling ratio J.

III. RESULTS AND CONCLUSIONS

To locate the critical line that separates the ferromagnetic phase from the paramagnetic phase, we plot the scaled energy gap as a function of the applied magnetic field B, for several values of the four-spin coupling parameter, J. This is shown in Fig. 3 for $J=-0.3$ and lattice of sizes $N=8,12,16$, and 20. Results for lattice sizes in between these are not shown, mainly not to clog the picture. The crossing of two lines indicates the critical field B_c. To find the value of the critical field B_c in the thermodynamic limit $(N\to\infty)$ we estimate the value of the field at the crossing point between Δ_8 and Δ_N for $N=9,10,\dots,20$. The critical field in the thermodynamic limit is then estimated by extrapolating these values for large N, as shown in Fig. 4. The process is then repeated for other values of the coupling ratio J, so that we obtain the ferromagnetic-paramagnetic line in the phase diagram. For the first-order transition boundary that occurs for $-J>0.5$, the location of the transition line is obtained by examining the behavior of transverse susceptibility, χ. A typical result is shown in Fig. 5 for $J=-0.8$. The transverse susceptibility of finite-sized chains shows a peak at the critical value of B. As the system size grows, the peak becomes higher and narrower, thus indicating a discontinuity at the thermodynamic

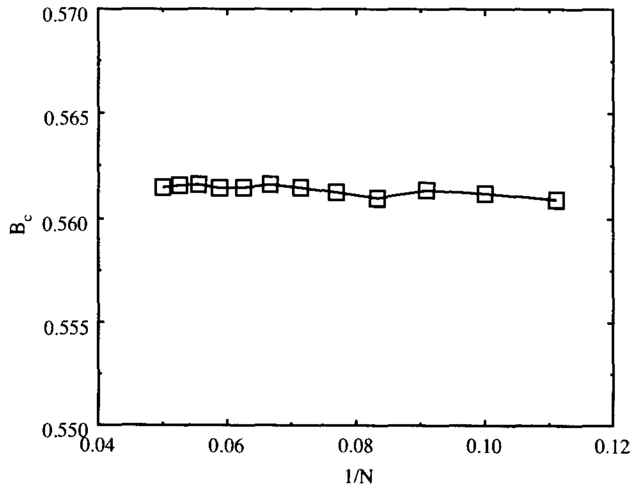

FIG. 4. Dependence of the critical field, B_c, with the reciprocal of the system size for $J=-0.3$. The critical field is found from the crossings of the scaled energy gap Δ_8 with each Δ_9, $\Delta_{10},\ldots$, and Δ_{20}, and then by extrapolating the values to the thermodynamic limit, $1/N \to 0$.

limit. We then estimate the critical fields B_c for several values of the four-spin coupling $-J>0.5$. By examining the ground-state wave vector, we find that the first-order transition line separates the paramagnetic phase from the antiphase $\langle 3,1\rangle$, in which threelike spins followed by one opposite spin is a basic structure that repeats itself leading to long-range order. The combined results for both transition lines are shown in Fig. 6. For $-J<0.5$ we have a second-order transition line separating a ferromagnetic phase at low fields from a paramagnetic phase at high fields. On the other hand,

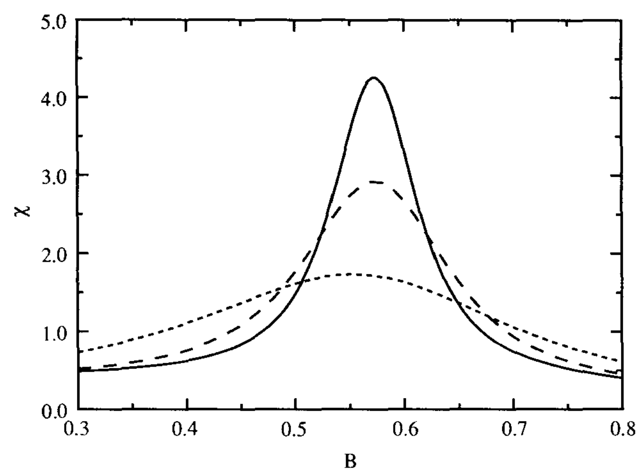

FIG. 5. Ground-state transverse susceptibility χ, as a function of the applied field B, for $J=-0.8$. The value of B at the maximum of the curves are the critical fields B_c that separate the antiphase $\langle 3,1\rangle$ from the paramagnetic phase. Note that as the system size N increases, so does the height of χ. The thermodynamic limit of the critical field is obtained by extrapolating the results to the thermodynamic limit.

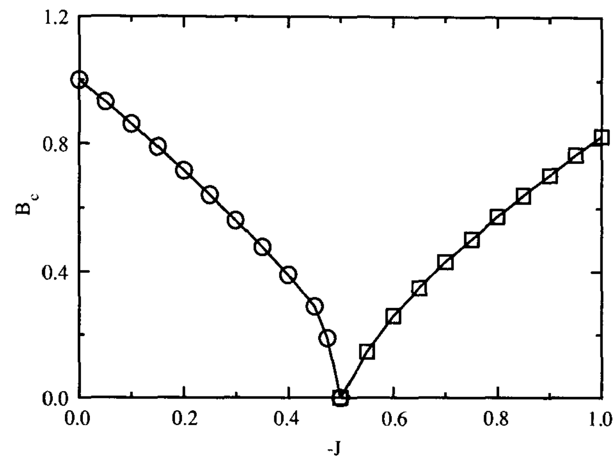

FIG. 6. Phase diagram for the ground state of the transverse Ising model with additional term with four-spin interactions. The open circles are the critical fields obtained from finite-size scaling for the second-order phase transition between the ferromagnetic and paramagnetic phases. The squares separate the antiphase $\langle 3,1\rangle$ from the paramagnetic phase, through a first-order transition. The critical fields are calculated from the location of the peak of the transverse magnetic susceptibility magnetization at the boundary for the fixed coupling constant ratio, J.

for $-J>0.5$ the transition line is of first-order and separates the antiphase $\langle 3,1\rangle$ at low fields from the paramagnetic phase at higher fields. A typical ground-state picture of the antiphase is shown in Fig. 2. Finally, the critical exponent ν associated with the correlation length is shown in Fig. 7. The evaluation of the exponent is done using Eq. (4) for magnetic fields along the critical boundary separating the ferromagnetic phase from the paramagnetic phase. The plots in Fig. 7 indicates the trend of the values of the exponent towards the

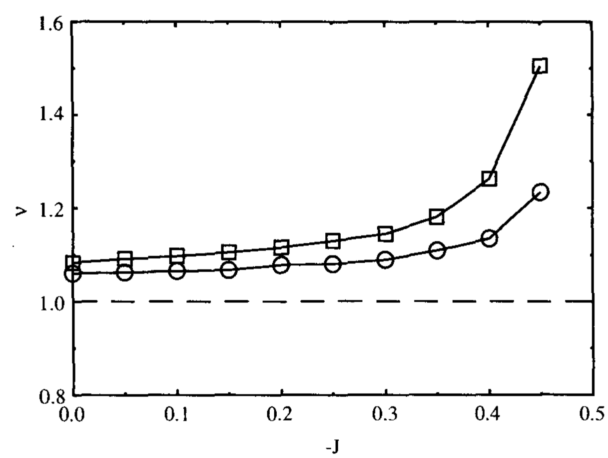

FIG. 7. Correlation length critical exponent ν along the second-order phase transition line. Squares are the results for $(N,N')=(8,10)$, and circles for $(N,N')=(12,14)$. The dotted line denotes the value $\nu=1$, corresponding to the system in the thermodynamic limit. Large deviations from the exact result are found for coupling ratios in the neighborhood of $J=-0.5$.

exact value $\nu=1$, as the size of the system increases.

To conclude, we studied the quantum properties of the transverse Ising model with an added term with four-spin interactions. The quantum phases at $T=0$ induced by the four-spin interaction and the magnetic field are identified, and the transition boundaries separating these phases are numerically calculated by using finite-size scaling as well as the calculation of the ground-state transverse magnetization. We observed a phase, denoted here as the antiphase $\langle 3,1\rangle$, for $-J>0.5$ and low magnetic fields, where the ground state consists of a linear combination of three consecutive up (down) spins followed by one down (up) spin.

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