Ground-state properties of the one-dimensional transverse Ising model in a longitudinal magnetic field

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The critical properties of the one-dimensional transverse Ising model in the presence of a longitudinal magnetic field were studied by the quantum fidelity method. We used exact diagonalization to obtain the ground-state energies and corresponding eigenvectors for lattice sizes up to 24 spins. The maximum of the fidelity susceptibility is used to locate the various phase boundaries present in the system. The type of dominant spin ordering for each phase was identified by examining the corresponding ground-state eigenvector. For a given antiferromagnetic nearest-neighbor interaction $J_2$, we calculated the fidelity susceptibility as a function of the transverse field ($B_x$) and the strength of the longitudinal field ($B_z$). The phase diagram in the ($B_x$, $B_z$)-plane shows three phases. These findings are in contrast with the published literature that claims that the system has only two phases. For $B_z < 1$, we observed an antiferromagnetic phase for small values of $B_z$ and a paramagnetic phase for large values of $B_z$. For $B_z > 1$ and low $B_z$, we found a disordered phase that undergoes a phase transition to a paramagnetic phase for large values of $B_z$.

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I. INTRODUCTION

The neighborhood of a phase transition is known to pose serious difficulties in quantum magnetic systems. For instance, such difficulties appear as one tries to obtain the location of the phase boundaries of those systems.

Several methods have been used in the literature. One was to simulate a quantum spin chain by using ultracold atoms in an optical lattice [1–4]. Another important method is the density matrix renormalization group (DMRG), which has been applied successfully to a large number of quantum many-body problems [5–8]. Other approaches include quantum Monte Carlo [9], exact diagonalization [10, 11], perturbation theory [12], and matrix product states [13]. Yet another line of investigation is the fidelity method, which relies upon the eigenvectors of finite sized models [14–17].

In the present work, we are concerned with the ground-state phase diagram of a quantum spin-$1/2$ chain, namely the transverse Ising model in a longitudinal magnetic field. Both the optical lattice and DMRG methods have been used to study the ground-state properties of that problem [1, 18]. Their phase diagrams show an antiferromagnetic phase at low fields and a paramagnetic phase for high fields. There are just these two phases presented in their results. However, we found that fidelity method reproduces the ground-state phase diagram found in the literature, as well as uncovering an additional phase boundary line between the paramagnetic and a disordered phase.

This paper is organized as follows. In Sec. II we present the model, while in Sec. III we discuss the fidelity susceptibility method. In Sec. IV we present our results, which are finally summarized in Sec. V.

II. THE MODEL

The one-dimensional transverse Ising model in the presence of a longitudinal field is written as

$$\mathcal{H} = J_2 \sum_i \sigma_i^x \sigma_{i+1}^x - B_x \sum_i \sigma_i^z - B_z \sum_i \sigma_i^z.$$  (1)

The chain consists of $L$ spin-half interacting spins, written in terms of Pauli operators, where $\sigma_i^\alpha (\alpha = x, y, z)$ is the $\alpha$-component located at site $i$. We considered a chain with periodic boundary conditions. The nearest-neighbor Ising coupling is antiferromagnetic, $J_2 > 0$, while the applied longitudinal filed $B_z > 0$ tends to align the spins ferromagnetically. Finally, quantum fluctuations are induced by a transverse magnetic field $B_x$. In what follows, we take $J_2 = 1$ as the energy unit.

In the case $B_z = 0$, the Hamiltonian is simply the Ising model in a longitudinal magnetic field. In that case the model shows a phase transition at $B_z = 2.0$. The ground state of the system in the low-field regime ($B_z < 2.0$) is antiferromagnetic, whereas for high fields ($B_z > 2.0$) it is paramagnetic.
On the other hand, for $B_z = 0$, the Hamiltonian Eq. (I) is reduced to the quantum transverse Ising model. Its ground-state properties were exactly obtained by Pfetuy in 1970 [19]. In that work it was found that quantum fluctuations induced by the transverse field drove the system through a second-order phase transition at $B_z = 1.0$. At low-fields the phase is antiferromagnetic, whereas for high fields it is disordered.

III. THE FIDELITY APPROACH

Consider an Hamiltonian that depends on an arbitrary parameter $\lambda$, which drives the system through a phase transition when $\lambda = \lambda_c$. We define the quantum fidelity of a ground-state as the magnitude of the overlap between two neighboring ground-states; namely,

$$F(\lambda, \delta) = |\langle \psi(\lambda) | \psi(\lambda + \delta) \rangle|,$$

where $|\psi\rangle$ is the normalized non-degenerate ground-state eigenvector of the system evaluated near a given value of $\lambda$ by an arbitrary small shift $\delta$.

Quantum fidelity also depends on the system size. As the system approaches a quantum transition the fidelity behavior changes dramatically. It drops from a level close to unity on either side of the transition point to a minimum value at the transition point. This is caused by the distinct nature of the ground-state on each side of that transition point.

Due to its simplicity and ability to locate phase transitions, quantum fidelity has been used in quantum information theory [14] and for the identification of topological phases in condensed matter physics [15–16].

Instead of working with quantum fidelity as defined above, it is preferable to work with the fidelity susceptibility, which is obtained by expanding the fidelity as a Taylor’s series for very small $\delta$, about $\lambda$. Assuming that the ground state is normalized, the fidelity susceptibility can be written as

$$\chi(\lambda) = 2(1 - F(\lambda, \delta))/\delta^2 + O(\delta^2).$$

The ground-state energy and eigenvector for a given $\lambda$ are found using both Lanczos and conjugate gradient methods. The latter has been used in Hamiltonian models in statistical physics and transfer-matrix techniques [21, 22]. For a given accuracy, both methods give the same results for the ground-state eigenvectors and energies.

Since the Hamiltonian (I) depends on two independent parameters, $B_x$ and $B_z$, we must investigate each of their associated susceptibilities. To differentiate between them, we use the notation $\chi_{z}(\lambda)$, where $\lambda$ is chosen as one of the fields, and $\gamma$ is the other field, which is kept fixed during the calculations. The boundary lines are then found by using Eq. (II) with $\delta = 0.001$ in a range of accuracy between $10^{-12}$ and $10^{-14}$ for the ground-state energy, depending on the chain size. For each $\lambda$, the location of the phase boundary is determined by the maximum of the fidelity susceptibility.

Our procedure started out by finding the ground-state energies and corresponding eigenvectors, where we used a complete set of orthogonal basis vectors. The basis vectors were then used to express the Hamiltonian in matrix form. The eigenvalues and eigenvectors were calculated numerically using exact diagonalization.

The standard basis consists of a tensor product of $L$ eigenstates of the $z$-component of the Pauli operator $\sigma_i^z$ located at site $i$, namely $|n> = \prod_i^L |s_i>$. This basis is then used to find both the eigenvalues and eigenvectors of the Hamiltonian, and to identifying the ground-state configuration on each phase, where $s = 0, 1$. Here $|1> >$ denotes the eigenvector of $\sigma_i^z$ for an up-spin, and $|0> >$ the corresponding eigenvector for a down-spin at site $i$. The index $n$ labels the basis states and has the values $n = 0, 1, ..., N - 1$, with $N = 2^L$ denoting the size of the Hilbert space.

By writing the basis index $n$ in binary notation, each of the $L$ binary digits will represent the $z$-component of the spin at a given site $i$ of a lattice with $L$ spins. As an example, for a chain with $L = 10$ spins, the state $|792> >$ is written in binary notation as $|1100110100> >$, where the state represents a periodic configuration with 2 up-spins followed by 3 down-spins. An arbitrary eigenstate of the Hamiltonian can therefore be written as:

$$|\phi_\alpha > = \sum_{n=0}^{N-1} a_\alpha(n)|n> >,$$

where the energy levels are labeled by $\alpha = 0, 1, ..., N - 1$. In particular, $\alpha = 0$ is assigned to the ground-state.

Because of the symmetry of the Hamiltonian (I), the coefficients $a_\alpha(n)$ are real. The full wave vector can be visualized by plotting the amplitudes $a_\alpha(n)$ for any lattice size $L$, as a function of the state index $n$ in a single graph [24, 25].

IV. RESULTS

In our numerical calculations we used even lattice sizes from $L = 8$ to 24. This choice of lattice sizes preserves the symmetry of the ground state when the system is in the antiferromagnetic phase. In addition, it avoids undesirable frustration effects due to the finite size of the system and the imposed periodic boundary conditions.

To obtain the phase diagram of the model, we first calculated the fidelity susceptibility as a function of the transverse field $B_x$ for a fixed longitudinal field $B_z$. We represented this susceptibility as $\chi_{B_z}(B_x)$ in Fig. (I). We show the behavior of $\chi_{B_z}(B_x)$ for three lattice sizes $L = 12, 16$ and 24, for the particular value of the longitudinal field $B_z = 0.5$. In all calculations involving the susceptibility, we have used $\delta = 0.001$. The maximum of the susceptibility for each lattice size is taken as the quantum transition
FIG. 1: (color online) Fidelity susceptibility as a function of the transverse field $B_x$ for a fixed longitudinal field $B_z = 0.5$, and lattice sizes $L = 12, 16, 24$. The maximum of the susceptibility specifies the location of the transition point. We set $J_2 = 1$ as the unity of energy for this and the subsequent figures.

FIG. 2: (color online) Phase diagram in the ($B_x$, $B_z$)-plane for chains sizes $L = 12$ (circles), 16 (squares) and 24 (diamonds), obtained from the maximum of $\chi_{B_z}$. The model shows two phase regions, antiferromagnetic and paramagnetic. The transition points $(B_x, B_z) = (0, 2)$ and $(B_x, B_z) = (1, 0)$ are exact results. The dashed line is the critical line from DMRG results (Ref. [18]).

FIG. 3: (color online) Fidelity susceptibility vs longitudinal field $B_z$ for a chain of size $L = 24$, and fixed transverse fields $B_x = 1.5$ and 0.5 (inset). The maximum of the susceptibility locates the transition point.

FIG. 4: (color online) Phase diagram in the ($B_x$, $B_z$)-plane for chains with $L = 12$ (circles), 16 (squares), and 24 (diamonds), obtained from the maxima of $\chi_{B_x}$. The model shows three phase regions, antiferromagnetic, paramagnetic, and disordered. The transition points at $(B_x, B_z) = (0, 2)$ and $(B_x, B_z) = (1, 0)$ are known exact results. The dashed line is the critical line from DMRG (Ref. [18]).

point from antiferromagnetic to paramagnetic phases for this particular value of longitudinal field.

By carrying out such calculations for different values of longitudinal fields in the interval $(0, 2)$, we obtained the phase diagram shown in Fig. 2. The results for $L = 12$ (open circles), 16 (squares) and 24 (diamonds) are shown together with the critical boundary (dashed line) from [18] calculated using DMRG. As one can see, by increasing the lattice sizes from $L = 12$ to 24 the critical line from the fidelity method gradually approaches the DMRG results. The critical line for $L = 24$ is almost indistinguishable from that of DMRG. This is the full phase diagram of the model, as reported in the literature [1, 18].
However, an analysis of the phase transitions for small longitudinal or transverse fields shows an inconsistency in the phase diagram of Fig. 2. For instance, for small transverse fields we expect an antiferromagnetic-paramagnetic phase transition boundary near $B_z = 1$. On the other hand, in the limit of small longitudinal fields, and based on the exact results for the transverse Ising model, we expect an antiferromagnetic-disordered transition near $B_x = 1$.

Another way to see this is that for low $B_x$ and high $B_z$, the spins should be pointing in the $z$-direction and opposite case, namely low $B_z$ and high $B_x$, the spins should be pointing in the $x$-direction. Thus these two configurations cannot be part of the same phase. Therefore a phase boundary between the disordered-paramagnetic phase must be present in the phase diagram, Fig. 2.

We will show below that by evaluating a second fidelity susceptibility for a fixed transverse field $(\chi_{B_x})$ this missing phase boundary can be located. As in the case of Fig. 2 we first calculated the susceptibility $\chi_{B_x}$ as a function of $B_z$ for fixed values of $B_x$. Figure 3 shows the results for $B_x = 1.5$ and 0.5 (inset). The value $B_z = 0.5$ lies within the antiferromagnetic phase, while $B_z = 1.5$ is in the disordered phase.

A point worth noticing is the relatively high ratio between the two fidelity susceptibility maxima. The susceptibility maximum of the antiferromagnetic phase is about 35 times larger than that of the disordered phase. The small value in the disordered phase indicates a weak transition between the disordered and paramagnetic phases. Perhaps that is why it has been overlooked using other methods 1 18.

The phase diagram obtained using the maxima of $\chi_{B_x}$ for magnetic fields in the interval $(0 \leq B_z, B_z \leq 2)$ for lattice sizes $L = 12, 16, 24$ is depicted in Fig. 4. For comparison, we have also included the DMRG results (dashed line). The transition boundary between the antiferromagnetic and paramagnetic phases gets closer to the DMRG results as the chain size increases (although the convergence is slower for the susceptibility $\chi_{B_x}$). Our fidelity results for the phase boundaries of different lattice sizes converge quite rapidly. The boundary between the disordered and paramagnetic phases for $L = 16$ and $L = 24$ are already indistinguishable in the scale of the figure. Thus, the two fidelity susceptibilities $\chi_{B_x}$ and $\chi_{B_z}$ complement each other in the determination of the phase boundaries. By combining the results of the present work and those of DMRG, we arrived at the full phase diagram for the model, depicted in Fig. 5.

The spin configuration of each phase can be found by plotting the ground-state eigenvector amplitudes as a function of the ground-state index $n$. As a working example we shall use $L = 12$. For the point $(B_x, B_z) = (0.5, 0.2)$ inside the antiferromagnetic phase, we obtained the plot depicted in Fig. 6. The two largest amplitudes are at $n=1365$ and $n=2730$, corresponding to a ground-state in the binary representation $|01010101011\rangle$ and $|101010101010\rangle$, respectively. The much smaller amplitudes are transverse field effects.

Moving to the disordered phase, we consider now the point $(B_x, B_z) = (2.0, 0.1)$, where the ground-state amplitudes are shown in Fig. 4. Although the antiferromagnetic component is still present (due to the Ising interactions) as the larger component of the amplitudes, many other components with comparable amplitudes are also present.

Finally, we considered $(B_x, B_z) = (1.5, 2.0)$, inside the
paramagnetic phase. We obtained the graph shown in Fig. 3. The largest amplitude at \( n = 4096 \) corresponds to the ferromagnetic configuration with all spins pointing in the direction of the field. The second largest amplitudes also correspond to a ferromagnetic configuration with all spins but one aligned with the field. The third largest amplitudes still correspond to a ferromagnetic configuration with all spins but two aligned with the field. Similar ferromagnetic configurations are found for the smaller amplitudes.

V. SUMMARY AND CONCLUSIONS

The ground-state properties of the transverse Ising model in the presence of a longitudinal field was analyzed using the quantum fidelity method. The phase diagram in the \( (B_x, B_z) \)-plane shows three phases in contrast with previously reported results from the literature, which show only two phases. The phases are antiferromagnetic, paramagnetic, and disordered. We have also analyzed the spin configuration of the ground-state of each corresponding phase. The spins configuration on each phase clearly show distinct characteristics.

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