Finite-temperature phase transitions in the quantum fully frustrated transverse-field Ising models

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The quantum antiferromagnetic spin-1/2 Ising model on a triangular lattice and analogous fully frustrated Ising model on a square lattice with quantum fluctuation induced by the application of the transverse magnetic field are studied at finite temperatures by constructing an exact mapping onto a purely classical model with a more complex interaction. It is shown that in weak fields the temperatures of the phase transitions separating the critical phase from the ordered and disordered phases in both models are proportional to the magnitude of the field.

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I. INTRODUCTION

In recent years interest in quantum frustrated magnetic systems is constantly growing due to the permanent appearance of new materials belonging to this class (see Ref. 1 for a recent review). In many cases, an interplay between fluctuations (quantum and thermal) and a macroscopic degeneracy of the classical ground states makes understanding the properties of such systems a nontrivial task.

The best known example of a frustrated magnetic system is the antiferromagnetic Ising model on a triangular lattice, in which each triangular plaquette has to contain at least one frustrated bond with higher than minimal energy. It is well known from the exact solution[2] that this classical model is disordered at any positive temperature $T > 0$, whereas at $T = 0$ it is characterized by a finite residual entropy and an algebraic decay of correlations.[3] A quantum analog of this model can be defined by the Hamiltonian

$$\hat{H} = J \sum_{(jj')} \hat{\sigma}^z_j \hat{\sigma}^z_{j'} - \Gamma \sum_j \hat{\sigma}^x_j , \tag{1}$$

where $J > 0$ is the coupling constant of the nearest-neighbor interaction, $\Gamma > 0$ is proportional to the magnitude of the transverse magnetic field inducing quantum fluctuations, $\hat{\sigma}^x$ and $\hat{\sigma}^z$ are the Pauli matrices, and the summation in the first term is performed over all pairs of nearest neighbors (jj') on a triangular lattice. The classical antiferromagnetic Ising model is recovered in the case $\Gamma = 0$.

Besides being applicable for the description of an easy-axis antiferromagnet with spin 1/2 and a triangular lattice, the quantum antiferromagnetic Ising model defined by Eq. (1) is also of interest as a representative of a wider class of the fully frustrated transverse-field Ising models, in which coupling constants can have both signs ($J_{jj'} = \pm J$), but on each plaquette of the lattice the number of the antiferromagnetic bonds (with $J_{jj'} = J > 0$) is odd.[4] The quantum fully frustrated Ising models on various lattices have been investigated[5–10] mostly in view of their relation to the quantum dimer models[11] with vanishing potential energy term. A method for constructing more general models implementing a continuous crossover between a frustrated Ising model and a dimer model (on the dual lattice) whose Hamiltonian includes both the kinetic and potential terms has been proposed recently in Ref. 12.

The first investigation of the finite-temperature phase diagram of the quantum antiferromagnetic Ising model on a triangular lattice was undertaken by Isakov and Moessner.[13] Relying on the analogy with the classical antiferromagnetic Ising model on a layered triangular lattice[14] in a system with a finite size in the direction perpendicular to the layers, they argued that at $0 < \Gamma < \Gamma_c$ (where $\Gamma_c \propto J$ is the critical value of Γ at zero temperature) this model has to have two finite-temperature phase transitions of the Berezinskii-Kosterlitz-Thouless type with a critical phase between them (as in the classical six-state clock model) and confirmed these conclusions with the help of numerical simulations. Soon after that, Jiang and Emig[15] proposed a derivation (based on a renormalization-group analysis) demonstrating that the temperatures of these two transitions T_1^c and T_2^c should behave themselves as

$$T^c_{1,2} \propto \Gamma \ln^\nu(\Gamma_c/\Gamma) , \tag{2}$$

where ν is the critical exponent of the three-dimensional XY model and $T_2^c/T_1^c = 9/4$.

However, the prediction of Ref. 15 was based on the renormalization-group analysis assuming the possibility of describing the evolution of the system in Euclidean time in the framework of the continuous approximation. This approach requires the size of the system in the time direction $\beta = 1/T$ to be much larger than the typical time between spin flips (inversely proportional to Γ), which at temperatures given by Eq. (2) is fulfilled only for $\Gamma_c - \Gamma \ll \Gamma_c$.

The main aim of the present work is to study the behavior of T_1^c and T_2^c in the quantum antiferromagnetic Ising model on a triangular lattice at $\Gamma \ll J$, where the continuous approximation is not applicable. Our result consists of finding that in this range of parameters both transition temperatures are just proportional to Γ and do not diverge with the increase of J as predicted by Eq. (2). We also demonstrate that in the fully frustrated transverse-field Ising model on a square lattice the situation is the basically the same: the ordered and disordered phases are separated by the critical phase with both transition temperatures being proportional to the magnitude of the field in weak fields. Up to now, the investigation of this model has been focused on its zero-temperature properties.[5–7]

II. ANTIFERROMAGNETIC MODEL ON A TRIANGULAR LATTICE

A. The case of the infinite coupling constant

We start by considering the quantum antiferromagnetic Ising model on a triangular lattice in the special case of the infinite coupling constant, $J = \infty$. In such a case, the

Hilbert space of the model is restricted to the states with only one frustrated bond in each triangular plaquette (that is, the ground states of the classical antiferromagnetic Ising model labeled below by index a) and their linear combinations. The finite-temperature partition function can be then written as

$$Z = \sum_a W_a \tag{3}$$

with

$$W_a = \langle a|\exp(-\beta\hat{H})|a\rangle \tag{4}$$

and $\beta \equiv 1/T$. The summation in Eq. (3) is performed over all ground states of the classical model.

In the infinite-temperature limit ($\beta \to 0$) one gets $W_a \to 1$, that is, Z is reduced to the *zero-temperature* partition function of the classical antiferromagnetic Ising model. At $\beta > 0$ weights W_a become dependent on the structure of the state a. A convenient way of describing this dependence consists of introducing an effective classical Hamiltonian $\mathcal{H}_{\rm eff}(a)$ defined by the relation

$$W_a \equiv \exp[-\mathcal{H}_{\rm eff}(a)]. \tag{5}$$

At $\beta\Gamma \ll 1$ the spin flips induced by the second term in Eq. (1) are rare, which allows one to calculate the statistical weights W_a corresponding to different states perturbatively. In such a way, one obtains that, in the lowest order in $\beta\Gamma$, $\mathcal{H}_{\rm eff}(a)$ is just proportional to $M(a)$, the number of spins in state a that allow for flipping any of them without taking the system out of its Hilbert space,

$$\mathcal{H}_{\rm eff}(a) = -\tfrac{1}{2}(\beta\Gamma)^2 M(a). \tag{6}$$

The terms of the fourth and higher orders in β depend on the structure of the state a in a more complex way, but at $\beta\Gamma \ll 1$ the main role is played by the terms included into Eq. (6).

It is well known that the set of the ground states of the classical antiferromagnetic Ising model on a triangular lattice can be mapped onto the states of a solid-on-solid (SOS) model describing the [111] facet of a cubic crystal.[16] In terms of the SOS representation, each Ising spin $\sigma_j = \pm 1$ is replaced by integer height variable h_j in such a way that the relation

$$h_{j'} - h_j = -\frac{1 + 3\sigma_j\sigma_{j'}}{2} = \begin{cases} +1, \\ -2 \end{cases} \tag{7}$$

is satisfied for every pair of neighboring sites on the triangular lattice. Equation (7) assumes that one of the three basic vectors of the triangular lattice (whose sum is equal to zero) is directed from site j to site j' and not from j' to j (which would correspond to the opposite sign of $h_{j'} - h_j$).

When each triangular plaquette contains only one frustrated bond (with $\sigma_j\sigma_{j'} = +1$), Eqs. (7) unambiguously define the values of all integer variables h_j as soon as the value of h_j is chosen for one of the sites. On the other hand, any state of the SOS model with $h_{j'} - h_j = +1, -2$ corresponds to some ground state of the antiferromagnetic Ising model.

It follows from the known properties of the classical antiferromagnetic Ising model on a triangular lattice that, when all allowed states of such an SOS model enter the partition function with the same weight, this model is in the rough phase, in which correlations of heights diverge logarithmically,[17]

$$g_{jk} = \langle (h_j - h_k)^2 \rangle \approx \frac{K}{2\pi^2} \ln r_{jk}\,, \tag{8}$$

where r_{jk} is distance between sites j and k and $K = K_0 = 18$.

The same surface representation can be used for interpreting the quantum spin model (1) with $J = \infty$ as a quantum SOS model in which the amplitude of height jumps, $h_j \to h_j \pm 3$, compatible with restrictions imposed by Eqs. (7) is given by Γ. Alternatively, the use of Eq. (4) allows one to speak about the classical SOS model in which now the weights corresponding to different configurations of the surface are no longer equal to each other and depend on the configuration. Since in terms of the height representation flippable spins correspond to points where the surface has no local slope, in terms of the SOS representation functional $M(a)$ is a measure of the flatness of the surface. Then it is clear from the negative sign in Eq. (6) that the interaction described by this equation suppresses the fluctuations of the surface.

It has to be emphasized that the classical SOS model defined by the Hamiltonian $\mathcal{H}_{\rm eff}(a)$ is exactly equivalent to the original quantum spin model. The price one has to pay for the reduction of a quantum model at a finite temperature to a purely classical one is that it is impossible to write down the explicit form of $\mathcal{H}_{\rm eff}(a)$, Eq. (6) being applicable only at $\beta\Gamma \ll 1$. However, a number of properties of the classical SOS model defined by $\mathcal{H}_{\rm eff}(a)$ can be discussed without knowing the exact form of $\mathcal{H}_{\rm eff}(a)$.

In particular, it is clear that the decrease of T (increase of $\beta \equiv 1/T$) leads to the suppression of the factor K in the correlation function (8) and finally has to induce a phase transition into the ordered (flat) state. Note that, at $T = 0$, a surface described by a quantum SOS model always has to be in the ordered (flat) phase[18] with a well defined value of $\langle h \rangle$ and saturation of correlation function g_{jk} at large distances.

However, for $\beta\Gamma \ll 1$ the suppression of factor K has to be small, whereas the phase transition to the ordered state will take place when this factor is suppressed from $K_0 = 18$ down to $K_1^c = 4$ (see Ref. 17). Note that this has to be so independently of whether in the ordered phase the spins on all three sublattices are magnetically ordered or if on one of them the average magnetization is zero (see the discussion in Refs. 13 and 15). In terms of the SOS representation, the first case corresponds to $\langle h \rangle$ being an integer and the second one to $\langle h \rangle$ being a half-integer, but in both cases the periodicity of the h-dependent effective potential is the same, and the critical value of K is determined by this periodicity.[19]

Apparently such a pronounced suppression of K cannot happen while $\beta\Gamma \ll 1$ and requires $T \sim \Gamma$, whereas at $T \gg \Gamma$ the system has to remain in the critical phase. One can conclude that at $J = \infty$ the phase transition between the critical and the ordered states of the original spin model takes place at a finite temperature T_1^c proportional to Γ whose value follows from the relation $K(T_1^c) = K_1^c$.

B. The case $J < \infty$

When $J < \infty$, the Hilbert space of the model is substantially extended because now all configurations of the Ising spins $\sigma_j = \pm 1$ are allowed. In terms of the SOS representation, this corresponds to the appearance of the possibility of the formation of screw dislocations.[17] A screw dislocation is an object on going around which the integer variable h_j, interpreted as height, instead of returning to the same value changes by the so-called Burgers number $b = \pm 6$. Each dislocation is centered around a plaquette containing not one but three[20] frustrated bonds with $\sigma_j\sigma_{j'} = +1$, which therefore can be identified with the dislocation core. In the framework of the path-integral description of a quantum system, dislocations are linear topological excitations and must either form closed loops in space-time or cross the whole system in the direction of the Euclidean time.

In terms of the original spin variables, the closed dislocation loops in space-time correspond to the spin flips which are prohibited at $J = \infty$. At $\Gamma \ll J$ such processes can be taken into account in the framework of the perturbation theory. The most important of them is the second-order process, which leads to a decrease of the system's energy by an amount proportional to Γ^2/J for each spin that cannot be flipped without increasing the energy of the system. At $T \sim \Gamma \ll J$ this gives a correction to K of the order of Γ/J and therefore leads only to a small shift of T_1^c with respect to its value at $J = \infty$.

On the other hand, the dislocations crossing the whole system in the time direction can lead to the disordering of the critical phase. At $\Gamma/J \to 0$, when the system does not experience evolution in the Euclidean time, these dislocations can be identified with that of the classical SOS model. The core energy of such dislocations is proportional to J, which makes their fugacities at $T \ll J$ exponentially small. The main difference which appears at $\Gamma/J \ll 1$ is that quantum fluctuations lead to a small negative correction to the core energy, but this is irrelevant for further reasoning.

When logarithmic interaction of dislocations is strong enough, they are bound in neutral pairs and the system has the same properties as in the absence of dislocations.[17] The strength of this interaction is determined by the same parameter K as the amplitude of the fluctuations of h. The dislocations with Burgers number b remain bound in neutral pairs only for

$$K < K_2^c = \frac{b^2}{4}, \tag{9}$$

whereas at $K > K_2^c$ there appear free dislocations whose proliferation leads to the disordering of the critical phase. In the antiferromagnetic Ising model on a triangular lattice, dislocations have $b = \pm 6$ and, accordingly, $K_2^c = 9$ (as found in Ref. 17).

Since $K_2^c = 9$ is smaller than $K_0 = 18$ but larger than $K_1^c = 4$, one can conclude that, at $\Gamma \ll J$, the dissociation of dislocation pairs leading to disordering of the critical phase takes place at temperature $T_2^c \sim \Gamma$, which is higher than T_1^c and therefore there exists a finite interval of temperatures $T_1^c < T < T_2^c$ where the system remains critical. The value of T_2^c is determined by the relation $K(T_2^c) = K_2^c = 9$. As T_1^c, the transition temperature T_2^c is basically proportional to Γ and remains finite when J is taken to infinity at a finite Γ, with the difference between the values of T_2^c at $J = \infty$ and at $\Gamma \ll J < \infty$ being exponentially small in J/Γ. Note that there are no reasons to expect the ratio T_2^c/T_1^c to be equal to $K_2^c/K_1^c = 9/4$ (as was proposed in Ref. 15) because factor K is not proportional to T but depends on the ratio Γ/T in a more complicated way.

III. FULLY FRUSTRATED MODEL ON A SQUARE LATTICE

The same approach can be applied to the fully frustrated transverse-field Ising model on a square lattice. In the case $J = \infty$, the Hilbert space of any fully frustrated transverse-field Ising model is defined by the set of the ground states of the classical fully frustrated Ising model on the same lattice, which is isomorphic to the full set of states of the classical dimer model on the dual lattice.[4] On a square lattice, the classical dimer model without any interaction of dimers is exactly solvable[21] and allows for a mapping onto a SOS model[22] with integer height variables h_j defined on the sites of the same square lattice. For a given configuration of Ising spins σ_j, the values of h_j can be defined by the relation analogous to Eq. (7),

$$h_{j'} - h_j = -(1 + 2\tau_{jj'}\sigma_j\sigma_{j'}) = \begin{cases} +1, \\ -3 \end{cases} \tag{10}$$

where $\tau_{jj'} = J_{jj'}/J = \pm 1$. Equation (10) assumes that the square lattice is divided into two equivalent square sublattices (A and B) and site j belongs to sublattice A and site j' to sublattice B. In the opposite case, the sign of $h_{j'} - h_j$ naturally has to be the opposite.

When each square plaquette contains only one frustrated bond (with $J_{jj'}\sigma_j\sigma_{j'} = J > 0$), Eqs. (10) unambiguously define the values of all integer variables h_j as soon as the value of h_j is chosen for one of the sites. On the other hand, any state of the SOS model on a square lattice with $h_{j'} - h_j = +1, -3$ corresponds to some ground state of the fully frustrated Ising model on the same lattice.

Since the classical system of noninteracting dimers on a square lattice is in the critical phase,[23] the corresponding SOS model is in the rough phase with the asymptotic behavior of the height-height correlation function given by Eq. (8), where according to Ref. 22 $K = K_0 = 32$. As in the case of a triangular lattice, the description in terms of the classical SOS model, in which all allowed configurations enter the partition with the same weight, is applicable to the fully frustrated transverse-field Ising model with $J = \infty$ in the classical limit $\beta = 0$ (that is, $T = \infty$).

Having $T < \infty$ decreases the fluctuations of the surface. In the lowest order in $\beta\Gamma$ the Hamiltonian of the classical SOS model describing the system is again given by Eq. (6). In terms of the dimer representation, this Hamiltonian corresponds to having an attraction between parallel dimers belonging to the same plaquette. The classical dimer model with such an interaction has been studied in Ref. 24. In our system, the effective Hamiltonian has this form only at the highest temperatures, whereas with the decrease of temperature the interaction of the more distant dimers also starts to play a role. However, since variables h_j are integers, the phase transition to the ordered phase takes place at the temperature at which factor K has decreased down to $K_1^c = 4$ (exactly as in the case of a triangular lattice), independently of the exact form of the dimer-dimer interaction. In accordance with that, at $J = \infty$ the temperature of the phase transition to the ordered phase is proportional to Γ, and for $\Gamma \ll J < \infty$ the correction to the value of this quantity is small.

The second phase transition is related to the appearance of free (unpaired) dislocations crossing the whole system in the direction of Euclidean time. As in the case of a triangular lattice, dislocations can be associated with the plaquettes which contain not one but three frustrated bonds.[20] For $K < K_2^c$ [where K_2^c is given by Eq. (9)] they are bound in neutral pairs which dissociate when the value of K reaches K_2^c. In the SOS model describing the ground states of the fully frustrated Ising model on a square lattice, Burgers numbers b are equal to ± 8 and, accordingly, $K_2^c = 16$ (cf. with Ref. 24). Since $K_2^c = 16$ is smaller than $K_0 = 32$ but larger than $K_1^c = 4$, one can again make a conclusion that the critical phase exists in a finite interval of temperatures $T_1^c < T < T_2^c$, whereas the phase transition leading to the disordering of the critical phase takes place at temperature T_2^c at which $K(T_2^c) = K_2^c = 16$. For $\Gamma \ll J$ this temperature, like T_1^c, is proportional to Γ.

IV. CONCLUSION

In the present work we have demonstrated that in the quantum antiferromagnetic transverse-field Ising model on a triangular lattice, as well as in the fully frustrated Ising model on a square lattice, the temperatures of the phase transitions separating the critical phase from the ordered and disordered phases in weak fields are proportional to the magnitude of the field. The analysis of Jiang and Emig[15] leading to a different conclusion fails in weak fields ($\Gamma \ll J$) because the continuous approximation used in Ref. 15 for the description of the spin fluctuations in Eucledean time requires the size of the system in the time direction β to be much larger than the typical time between spin flips, which is inversely proportional to Γ. For $T \sim T_{1,2}^c$, this condition is fulfilled only when $\Gamma_c - \Gamma \ll \Gamma_c$, whereas out of this range the continuous approach cannot be trusted. The results of the numerical simulations of the antiferromagnetic model on a triangular lattice[13] are consistent with T_1^c and T_2^c being proportional to Γ at small Γ.

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