Transverse field Ising model on the checkerboard lattice: a plaquette-operator approach

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We study the effect of quantum fluctuations by means of a transverse magnetic field ($\Gamma$) on the antiferromagnetic $J_1 - J_2$ Ising model on the checkerboard lattice, the two dimensional version of pyrochlore lattice. A plaquette operator formalism has been implemented to bosonise the model, in which a single boson is associated to each eigenstate of a plaquette and the inter-plaquette interactions define an effective Hamiltonian. The excitations of a plaquette would represent an-harmonic fluctuations of the model, which lead not only to lower the excitation energy compared with a single spin flip but also to lift the extensive degeneracy in favor of a plaquette ordered state, which breaks lattice rotational symmetry for $J_2 > J_1$ (the collinear phase). The bosonic excitation gap vanishes at the critical boundary to Néel ($J_2 < J_1$) and collinear ordered ($J_2 > J_1$) phases, respectively. At the homogeneous coupling ($J_1 = J_2$) a (canted) resonating plaquette state (RPS) is established from an-harmonic fluctuations, which lasts for low fields, $\Gamma/J_1 \lesssim 0.4$, followed by a crossover to the fully polarized phase. We will show that our results predict an order-by-disorder as a results of transverse field at the critical point ($J_2 = 0.5J_1$) of the antiferromagnetic $J_1 - J_2$ Ising square lattice.

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Frustrated magnetic systems imply large degenerate classical configurations as a groundstate subspace, which could lead to novel phases and exotic features like emergent magnetic monopoles in spin ice $^1$. Quantum fluctuations as perturbations may select one of these degenerate states as a unique quantum ground-state of the system representing unusual ordering. Besides the magnetic properties, which are described by models of frustrated systems, such models mimic some features of unconventional superconductor in terms of resonating valence bond (RVB) phase on the triangular lattice $^{12,13}$ governed by quantum dimer model (QDM). The RVB scenario has received a great impact to elucidate the plaquette RVB phase in the s=1/2 honeycomb $J_1 - J_2$ Heisenberg model $^{8,9}$, which is justified by the two-dimensional approach of density matrix renormalization group, recently $^{10,11}$. It gives the impression that the plaquette type ordered phase is a result of strong correlation and frustration, which has also been observed in the square lattice $^{14,15}$.

The three-dimensional pyrochlore lattice is a fascinating example of geometrically frustrated lattices, which has a two-dimensional (2D) version called checkerboard lattice (see Fig.3 middle). Quantum Heisenberg model has been widely studied on checkerboard lattice, where degeneracy of the groundstate is lifted toward a unique non-magnetic ordered state, which is called a plaquette ordered state or plaquette ordered phase (PSP), e.g. $^4$. This state does not break SU(2) symmetry and is gapped but breaks the space symmetry of the lattice $^{12,13}$. However, the reduction of symmetry from SU(2) to Z2 renders the antiferromagnetic Ising model on the checkerboard lattice as a prototype of frustrated systems, which gives interesting features.

At the isotropic coupling $J_1 = J_2$, the Ising model on checkerboard lattice has extensive degenerate ground states defined by ice-rule manifold, i.e. ‘two-in-two-out’ on crossed plaquettes, known as square ice. Quantum fluctuations lift the degeneracy of the manifold toward a single magnetic or non-magnetic plaquette ordered state $^{8,9}$. More precisely, the ice-rule manifold is mapped to quantum six-vertex model where quantum fluctuations in terms of the kinetic term of a QDM of flippable plaquettes stabilizes a plaquette phase at zero chemical potential $^{8,9}$. Here, we show explicitly the existence of a resonating plaquette state (RPS) in terms of its corresponding order parameter, which will be introduced. Moreover, we indicate the region, where an RPS is being formed in the neighborhood of $J_1 = J_2$ of our phase diagram.

Recently, the transverse field Ising model (TFIM) on the $J_1 - J_2$ checkerboard lattice has been studied within linear spin-wave theory (LSWT) $^{14,15}$. The phase diagram consists of three phases, Néel ordered for low magnetic field and $J_2 < J_1$, highly degenerate collinear phase at low field and $J_2 > J_1$ and fully polarized phase for high transverse fields ($\Gamma$). Based on harmonic fluctuations considered in Ref. $^{23}$ the boundary between Néel and collinear phases is at $J_2 = J_1$ for $0 \leq \Gamma \lesssim 0.7$ without an indication of an RPS phase, which is a witness for the break down of LSWT. Moreover, the border for the polarized-Néel and polarized-collinear phase transitions can not be determined accurately within LSWT due to strong quantum fluctuations, leading to instabilities close to the phase boundaries.

The first clue to solve the problem is to employ the proper building blocks, which incorporate the correct ingredients of the ground state structure and the elementary excitations of the model. In the intermediate regime, where the role of frustration is important the plaquette flip excitation has lower energy than a single spin-flip excitation for $J_2 < 2/3$, which suggests that the true excitations of the model is governed by a plaquette flip that is a representation of an-harmonic fluctuations (of the original spin model). Moreover, the zeroth-order calculations of the ground state energy immediately justify that a single plaquette gives lower value than a single parti-
cel classical background. We implement a plaquette-operator approach (POA)\textsuperscript{24,25}, which is an extension of bond-operator approach\textsuperscript{22} to obtain the zero temperature phase diagram of $J_1 - J_2$ TFIM on checkerboard lattice, accurately. We explicitly find the quantum phase boundary for polarized-Néel and polarized-collinear transitions, where the excitation energy of bosonic quasi-particles vanishes as the onset of a Bose-polarized-collinear transitions, where the excitation energy of bosonic quasi-particles vanishes as the onset of a Bose-Einstein condensation of $\epsilon_1$-bosons. This excitation energy is the quantum fluctuation around the classical value of GSE and the properties of the model within a self-consistent procedure.

We consider the fluctuations of those bosons with negative energies ($\epsilon_u < 0$), which accounts to five bosons. To preserve the Hilbert space, the constraint of one boson per plaquette, $\sum_{u=1}^{5} b_{i,u}^\dagger b_{i,u} = 1$ is imposed within a Lagrange multiplier $\mu$, which is applied on average, i.e. $\mu_i = \mu, \forall i$. Finally, $H = H - \mu(\sum_{i=1}^{5} b_{i,u}^\dagger b_{i,u} - N)$ have to be minimized,

$$\frac{\partial(H)}{\partial \mu} = 0, \quad \frac{\partial(H)}{\partial \bar{p}} = 0,$$

where $N$ is the total number of independent plaquettes of the two-dimensional lattice. Taking into account the inter-plaquette interactions, which leads to the hybridization of the $\epsilon_1$-bosons with higher energy bosons and after a diagonalization transformation in the momentum space representation, the Hamiltonian is

$$\hat{H} = N\mu + N\bar{p}(\epsilon_1 - \mu) - \frac{1}{2}N\sum_{u=2}^{5}(\epsilon_u - \mu) + \sum_{k} \sum_{\nu=1}^{4} \left(\frac{1}{2} + \gamma_{\nu,k}^\dagger \omega_{\nu,k}(\mu, \bar{p})\right)^2,$$

where $\omega_{\nu,k}$ defines the spectrum of the quasi-particles of the interacting model and $\gamma_{\nu,k}$ is the corresponding bosonic creation operator.

As the first indication, the zeroth order approximation gives lower energy than the corresponding one of the LSWT, i.e. $\epsilon_1 < \epsilon_{L_{SWT}}^{(0)}$, which justifies that a plaquette is the proper building block of the model. Taking into account the quantum fluctuations, we have plotted the ground-state energy per spin (GSE) versus $J_2/J_1$ for $\Gamma = 0.7$ in Fig. 2. The results of POA is accompanied by the classical value of GSE and the
results of LSWT based on Néel and collinear backgrounds, presented in Ref.\textsuperscript{23}. Obviously, the GSE of POA is lower than the corresponding classical and LSWTs ones, which is a justification that POA gives a more precise representation of the ground-state. Moreover, POA does not depend on a specific form of background and, hence, it does not suffer from the inconsistency of GSE and its corresponding background.

Moreover, POA does not depend on a specific form of background and, hence, it does not suffer from the inconsistency of GSE and its corresponding background close to $J_2 = J_1$, which exists for LSWT\textsuperscript{22}. A remark is in order here, the quantum fluctuations in our approach are anharmonic in terms of the original spin model though we consider the quadratic term in Eq.\textsuperscript{3}. These are the excitations of a plaquette, which includes interactions of the original spins. Moreover, our POA gives $0.9 \lesssim \Gamma \lesssim 1$, which verifies our primary assumption of condensed plaquettes. However, by changing $J_2/J_1$ the critical boundary of the Néel or collinear phases is approached, where the gap vanishes. Going beyond the critical boundary into the Néel or collinear phases the constraint on the Hilbert space $\partial \mathcal{H}/\partial \mu = 0$ is not satisfied, which we avoid in our calculations.

In the phase diagram presented in Fig.\textsuperscript{1}, there are two solid-black curves, which represent the critical lines between polarized-Néel, polarized-collinear, RPS–Néel and RPS-collinear phases. On the critical line, the excitation gap of bosonic quasi-particles vanishes, which manifests a BE-condensation of $\epsilon_1$-bosons. For instance, at $\Gamma = 0.7$, the quantum critical point, which separates polarized and Néel phases is at $J_2/J_1 = 0.80$ that is denoted by A in Fig.\textsuperscript{2}. Similarly, the quantum phase transition from polarized to collinear phase takes place at $J_2/J_1 = 1.23$, which is pointed out by B in Fig.\textsuperscript{2}.

Fig.\textsuperscript{2}-left: We have plotted in the top part the density plot of the lowest spectrum of bosonic excitations at point A, where the gap vanishes at $(k_x = 0, k_y = 0)$. Its corresponding plaquette formation and the classical representation of spins are depicted in the middle and bottom of Fig.\textsuperscript{3} respectively. The whole lattice is covered by the $(0, 0)$ ordering of a single plaquette, which demonstrates a Néel ordered phase according to the classical representation of spins (bottom part).

Fig.\textsuperscript{3}-right: The top part shows the density plot of the lowest bosonic excitations, where the gap vanishes at the corners of Brillouin zone $(k_x = \pm \pi, k_y = \pm \pi)$ on the polarized-collinear critical point (B), which results in a staggered plaquette formation on the whole lattice that is shown in the middle part. The blue-plaquette represents the spin-flipped of a red-plaquette. The whole structure constitutes the collinear ordered phase as shown in a classical configuration in the bottom part. It has to be emphasized that the collinear phase comes out of the soft modes of bosonic excitations, which are a representation of an-harmonic fluctuations of the original spins. Hence, an-harmonic quantum fluctuations lift the classical degeneracy and lead to a quantum state, which has collinear long-range order.

More interesting features appear in the isotropic case, $J_2 = J_1$, where the bosonic quasi-particle spectrum becomes flat. It might be interpreted as an equal opportunity of all modes to participate in the formation of the quantum state. However, our results advocate a contribution of $(0, 0)$ and $(\pm \pi, \pm \pi)$ modes for small magnetic fields, which leads to an RPS phase. Having in mind that for $0 < \Gamma \leqslant 0.4$, the region around $J_2 = J_1$ is surrounded by the $(0, 0)$ soft modes on the left side and $(\pm \pi, \pm \pi)$ soft modes on the right side, it is rational to have dominant contribution from these modes, which have lower energies. Accordingly, we introduce an order parameter to represent a resonating formation of plaquettes. We define $|\varphi\rangle = |\uparrow \downarrow \uparrow \downarrow \rangle$ and its corresponding flipped plaquette...
which manifests the existence of the RPS phase whenever its expectation value is close to one. The expectation value of RPO, $\langle \hat{O} \rangle$, is plotted in the right part of Fig. 4. It clearly confirms the existence of RPS phase for $0 < \Gamma/J_1 \lesssim 0.4$ around $J_2 = J_1$. Increasing the transverse field decreases the RPO expectation value, which indicates the annihilation of the RPS phase. We have also plotted the field induced magnetization, $\langle S_z \rangle/S$ in the left part of Fig. 4. $\langle S_z \rangle$ starts from zero at $\Gamma = 0$ and increases almost linearly with the magnetic field. It means that we have a small amount of field induced magnetization in the RPS phase, which is called canted RPS phase.

To gain more insight on the behavior of order parameters for the isotropic case $J_2 = J_1$, both order parameters are plotted versus $\Gamma/J_1$ in Fig. 5-left. For $0 < \Gamma/J_1 \lesssim 0.4$, $\langle \hat{O} \rangle > 0.75$ and $\langle S_z \rangle/S < 0.5$, which is denoted by (canted) RPS phase. A classical representation of the canted RPS phase is shown in Fig. 6 which shows a plaquette type ordering in addition to considerable inclination along the magnetic field. For larger magnetic fields, $\Gamma/J_1 \geq 0.5$, a polarized configuration is dominant as shown in Fig. 6. The spin configurations are consistent with an extrapolation to zero temperature of the recent Monte-Carlo simulation at the isotropic coupling of the checkerboard lattice while we observe no sharp phase transition between (canted) RPS and polarized phases.

The quasi-particle excitation gap versus $\Gamma/J_1$ at the isotropic coupling $J_2 = J_1$ is plotted in Fig. 5-right. It is important to mention that the gap only vanishes at $\Gamma = 0$, which states that the transitions along $\Gamma$ between (canted) RPS and polarized phases is not a phase transition, rather, a cross over. The signature of the two mentioned phases of Fig. 6 can be observed on the trend of energy gap in Fig. 5-right. In the (canted) RPS phase, $0 < \Gamma/J_1 \lesssim 0.4$, the gap is nonzero and slightly increases with $\Gamma$, while the trend changes around $\Gamma = 0.5$, which is non-linear in $\Gamma$. The gap increases linearly with $\Gamma$ in the polarized phase, for $\Gamma/J_1 \gtrsim 0.5$.

Finally, we introduce how to map our model to the $\hat{J}_1 - \hat{J}_2$ TFIM on square lattice. We consider non-corner sharing plaquettes with crossed terms as a unit cell of our transformation. A quasi-spin 1/2 is associated to each crossed plaquette as a unit cell of our transformation. A quasi-spin 1/2 is associated to each crossed plaquette as a unit cell of our transformation. A quasi-spin 1/2 is associated to each crossed plaquette as a unit cell of our transformation.

FIG. 4. (color online) Left: The density plot of transverse magnetization $(S_z)/S$. Right: The density plot of plaquette order parameter, $\langle \hat{O} \rangle$. The black part is the region where the constraint of one boson per plaquette is not satisfied that contains no data.

FIG. 5. (color online) Left: Plaquette and transverse magnetization order parameters versus transverse field $(\Gamma/J_1)$ for $J_2 = J_1$. Right: The excitation gap versus transverse field for $J_2 = J_1$, which shows a linear behavior for $\Gamma/J_1 > 0.5$. The inset shows the low fields behavior.

FIG. 6. (Color online) Schematic spin configurations of the RPS, canted RPS and polarized phases. The RPS phase breaks lattice translational symmetry and contains decoupled plaquettes that resonate between two Néel configurations. The canted RPS contains seemingly decoupled plaquettes that have a considerable inclination along the magnetic field.

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