Transverse field effects on the competition between antiferromagnetic and cluster spin-glass phases

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We investigate a disordered cluster Ising antiferromagnet in the presence of a transverse field. By adopting a replica cluster mean-field framework, we analyze the role of quantum fluctuations in a model with competing short-range antiferromagnetic and intercluster disordered interactions. The model exhibits paramagnetic (PM), antiferromagnetic (AF), and cluster spin-glass (CSG) phases, which are separated by thermal and quantum phase transitions. A scenario of strong competition between AF and CSG unveils a number of interesting phenomena induced by quantum fluctuations, including a quantum PM state and quantum driven criticality. The latter occurs when the thermally driven PM-AF discontinuous phase transition becomes continuous at strong transverse fields. Analogous phenomena have been reported in a number of systems, but a description of underlying mechanisms is still required. Our results indicate that quantum driven criticality can be found in a highly competitive regime of disordered antiferromagnets, which is in consonance with recent findings in spin models with competing interactions.

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I. INTRODUCTION

Quantum frustrated magnets are an endless source of challenging problems and interesting phenomena [1–9]. Understanding the role of interactions as well as thermal and quantum fluctuations on the magnetic phases and phase boundaries is of utmost importance for the description of these materials. For instance, antiferromagnets with competing interactions are a prominent class of systems that harbors exotic physics. An interesting example of this is the quantum annealed criticality—when classical discontinuous phase transitions become continuous due to the increase of quantum fluctuations—that can be driven by competing interactions [10,11]. Despite attracting significant attention, the underlying mechanisms of this unconventional phenomenon are still unclear [12,13]. In particular, a relevant subject is whether quantum annealed criticality can be found when frustration is introduced by other sources, such as disorder. For instance, when bond disorder leads to frustration, besides the antiferromagnetic (AF) phase, magnetic glassy states can also be observed. These randomly frozen states often exhibit signatures consistent with a collective freezing of spin clusters, suggesting the onset of a cluster spin-glass (CSG) phase. Moreover, the possible presence of quantum annealed criticality in these frustrated systems still lacks a proper investigation. Motivated by this issue, the present work aims to analyze the role of quantum fluctuations on cluster disordered antiferromagnets.

From the theoretical point of view, describing the competition between CSG and AF states in the presence of quantum fluctuations represents a unique task for numerical approaches, generally demanding significant computational efforts. Analytical approaches are, therefore, an alternative to provide insights on the magnetic phases and the nature of phase transitions hosted by quantum disordered antiferromagnets. A simple way to study quantum fluctuations on spin systems is to consider transverse field Ising models (TFIMs), which can be seen as the ideal platforms for the research of quantum phenomena [14]. Even the simplest version of the model, the one-dimensional ferromagnetic TFIM, is prototypical for the study of quantum criticality [15]. Moreover, very recent studies also suggest that the phase transitions nature is highly sensitive to quantum fluctuations when competing interactions are considered in the TFIM [10,11]. For instance, in the J_1-J_2 antiferromagnetic TFIM, discontinuous thermally driven phase transitions can become continuous when quantum fluctuations are increased [10]. In addition, describing the role of bond disorder on TFIMs have motivated several investigations [7,16–24]. It has been found, for instance, that tuning the ratio between disorder strength and AF couplings allows to modulate a competition between a canonical spin-glass phase and antiferromagnetism [7]. Moreover, a replica approach for cluster spin-glasses in a transverse field has been proposed within the context of random bond models [21]. However, the competition between antiferromagnetism and a CSG state in a transverse field still lacks a proper description.

In this paper, we investigate the competition between AF ordering and cluster freezing by adopting a disordered version of the TFIM with focus on the role of AF correlations and

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quantum fluctuations in the onset of a CSG state and the nature of phase transitions. In order to describe the collective freezing of clusters, we adopt a model with random intercluster interactions, introducing a relevant degree of freedom, the cluster magnetic moment, for the description of the CSG state. In other words, our model embodies a competitive scenario by including AF first-neighbor interactions and random bonds between clusters. To incorporate effects of both quantum and thermal fluctuations, we adopted a cluster mean-field (CMF) approximation. This method has been used extensively in the study of frustrated and disordered spin systems, often yielding a suitable description of phase diagrams and thermodynamic quantities [25–27]. In addition, we incorporate the replica formalism within the CMF theory, allowing us to describe both the collective freezing of clusters and the AF ordering and, therefore, providing a framework able to account for the competitive nature of this quantum spin model. Moreover, we found evidence of a change in the nature of phase boundaries, namely, the thermally driven discontinuous transitions can become continuous when the transverse field is increased. It means that the model adopted can belong to a class of systems with competing interactions that host quantum annealed criticality.

The rest of the paper is organized as follows. In Sec. II we present the model and the replica CMF formalism. The results, including phase diagrams and the thermal dependence of order parameters, are presented and discussed in Sec. III. Our conclusion is given in Sec. IV.

II. MODEL AND METHOD

We adopt the quantum Ising model defined by

$$H = -\sum_{i<j} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z - \Gamma\sum_i \hat{\sigma}_i^x, \tag{1}$$

where $\hat{\sigma}_i^z$ and $\hat{\sigma}_i^x$ represent Pauli matrices, J_{ij} is the exchange interaction between the sites i and j, and Γ corresponds to the transverse magnetic field. We consider a square lattice divided into N_{cl} identical clusters with n_s sites each:

$$H = \sum_{\nu}^{N_{cl}} H_{\text{intra}}^{\nu} - \sum_{\nu<\lambda}^{N_{cl}} \sum_{\substack{i,\, j \\ i\,\in\,\nu \\ j\,\in\,\lambda}} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z, \tag{2}$$

with H_{intra}^{ν} representing the intracluster couplings. We assume two types of interaction: short-range and long-range, which are AF and disordered, respectively. The long-range interactions introduce a cluster-cluster coupling between all pairs of nearest-neighbor clusters ($J_{\nu\lambda}$) and the short-range ones are spin-spin couplings $J_{ij} = -J_0$ between all pairs of first-neighbor sites. This approach results in the following Hamiltonian:

$$H = \sum_{\nu}^{N_{cl}} H_{\text{intra}}^{\nu} - \sum_{(\nu,\lambda)}^{N_{cl}} \left(J_{\nu\lambda}\hat{S}_\nu^z\hat{S}_\lambda^z - J_0 \sum_{\substack{(i,\, j) \\ i\,\in\,\nu \\ j\,\in\,\lambda}} \hat{\sigma}_i^z\hat{\sigma}_j^z \right), \tag{3}$$

where $\hat{S}_\nu^z = \sum_{i\in\nu}^{n_s}\hat{\sigma}_i^z$,

$$H_{\text{intra}}^{\nu} = \sum_{(i,j\in\nu)} J_0\hat{\sigma}_i^z\hat{\sigma}_j^z - \Gamma\sum_{i\in\nu}^{n_s}\hat{\sigma}_i^x, \tag{4}$$

where $(\cdots)$ imply a sum over nearest-neighbors, and $J_{\nu\lambda}$ is a random variable that follows a Gaussian probability distribution with mean zero and variance $J/\sqrt{z_{cl}}$, in which z_{cl} is the number of neighbor clusters. It means that, for $J = 0$ and $J_0 > 0$, the model reproduces the Ising model in the square lattice. In this limit case, the exact solution for the model is known. On the other hand, a nonzero J introduces clusters in the model, also leading to a competition between disorder and AF couplings.

The replica method is used to get the disorder-averaged free energy per cluster $f = -1/(\beta N_{cl})\overline{\ln Z} = -1/(\beta N_{cl})\lim_{n\to 0}\frac{\ln \overline{Z^n}}{n}$, where the overline denotes an average over the quenched intercluster disorder $J_{\nu\lambda}$ and $\beta = 1/k_BT$ (k_B is the Boltzmann constant and T is temperature). The computation of this average leads to the following replicated partition function within the imaginary time formalism [28]:

$$\overline{Z^n} = \mathrm{Tr}\mathcal{T}\exp\left(-\beta\int d\tau\left[\sum_\alpha H_{\text{intra}}^{\alpha}(\tau) + \sum_{(\nu,\lambda)}\left\{\sum_\alpha\sum_{\substack{(i,\, j) \\ i\,\in\,\nu \\ j\,\in\,\lambda}} J_0\hat{\sigma}_i^{z\alpha}(\tau)\hat{\sigma}_j^{z\alpha}(\tau) - \frac{\beta J^2}{2N_{cl}} \times \int d\tau'\sum_{\alpha,\gamma}\hat{S}_\nu^{z\alpha}(\tau)\hat{S}_\lambda^{z\alpha}(\tau)\hat{S}_\nu^{z\gamma}(\tau')\hat{S}_\lambda^{z\gamma}(\tau')\right\}\right]\right), \tag{5}$$

where τ is the imaginary time, $\mathcal{T}$ is the time ordering operator, and α (γ) represents the replica index.

The intercluster coupling terms of Eq. (5) can be analytically computed in a CMF approximation. For instance, Figure 1 illustrates the lattice divided into clusters of four sites ($n_s = 4$) with the mean fields replacing the intercluster interactions. Formally, this approach is achieved by introducing the variational parameters $Q^{\alpha\gamma}(\tau,\tau')$ and $m_i^{\alpha}(\tau)$, which can lead to the following free energy:

$$\beta f = \lim_{n\to 0}\left[\frac{\beta^2 J^2}{4n}\int d\tau\int d\tau'\sum_{\alpha,\gamma}[Q_{\alpha\gamma}(\tau,\tau')]^2 + -\frac{\beta J_0}{2n}\int d\tau\sum_\alpha\sum_{(i,j)'}^{n_s} m_i^{z\alpha}(\tau)m_j^{z\alpha}(\tau) - \frac{\ln\mathcal{Z}_{\text{eff}}}{n}\right], \tag{6}$$

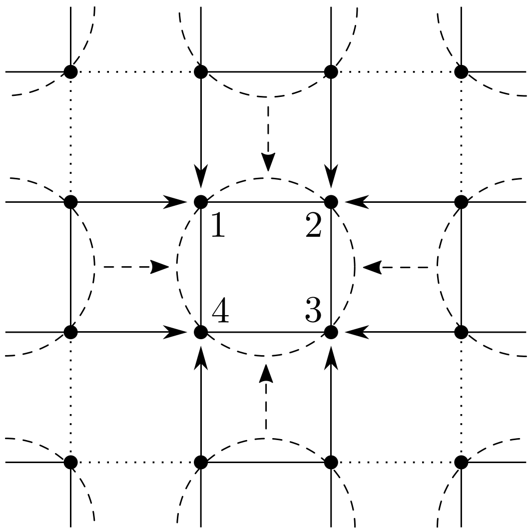

FIG. 1. The $n_s = 4$ cluster considered in the mean-field treatment. The solid lines represent the antiferromagnetic couplings and the arrows indicate the mean fields related to the short-range antiferromagnetic (solid lines) and the disordered (dashed lines) interactions.

where $(i, j)'$ refers to nearest-neighbor sites belonging to different clusters,

$$\mathcal{Z}_{\text{eff}} = \text{Tr}\mathcal{T} \exp\Bigg(-\beta \int d\tau \Bigg\{ \sum_{\alpha} [H^{\alpha}_{\text{intra}}(\tau) + J_0 \sum_{(i,j)'}^{n_s} \sigma_i^{z\alpha}(\tau) m_j^{z\alpha}(\tau)] + -\frac{\beta J^2}{2} \int d\tau' \sum_{\alpha,\gamma} Q^{\alpha\gamma}(\tau, \tau') \hat{S}^{z\alpha}(\tau) \hat{S}^{z\gamma}(\tau') \Bigg\}\Bigg) \quad (7)$$

with the variational parameters corresponding to the cluster spin-glass order parameter $Q^{\alpha\gamma}(\tau, \tau') = \langle \hat{S}^{z\alpha}(\tau) \hat{S}^{z\gamma}(\tau') \rangle_{H_{\text{eff}}}$ (for $\alpha \neq \gamma$), the cluster magnetic moment self-interaction $Q^{\alpha\alpha}(\tau, \tau') = \langle \hat{S}^{z\alpha}(\tau) \hat{S}^{z\alpha}(\tau') \rangle_{H_{\text{eff}}}$, and the site magnetization $m_i^{\alpha}(\tau) = \langle \sigma_i^{z\alpha}(\tau) \rangle_{H_{\text{eff}}}$, where $\langle \cdots \rangle_{H_{\text{eff}}}$ expresses the thermal average over the effective model in Eq. (7).

In this work, we consider the static approximation [28] and replica symmetry ansatz, which neglect the time dependence and the replica index of the order parameters: $Q^{\alpha\alpha}(\tau, \tau') = \bar{q}$, $Q^{\alpha\gamma}(\tau, \tau') = q$ and $m_i^{\alpha}(\tau) = m_i$. It is worth mentioning that despite the static approximation for the intercluster couplings, the intracluster dynamic is fully preserved. This procedure results in the following effective problem:

$$f = \frac{\beta J^2}{4}(\bar{q}^2 - q^2) - \frac{J_0}{2} \sum_{(i,j)'}^{n_s} m_i^z m_j^z + -\frac{1}{\beta} \int Dz \ln \int Dx \, \text{Tr}\, e^{-\beta \hat{H}_{\text{eff}}(z,x)}, \quad (8)$$

where the effective single-cluster Hamiltonian is

$$\hat{H}_{\text{eff}}(z, x) = J_0 \sum_{(i,j)}^{n_s} \hat{\sigma}_i^z \hat{\sigma}_j^z + J_0 \sum_{(i,j)'}^{n_s} \hat{\sigma}_i^z m_j^z + - \Gamma \sum_{i}^{n_s} \hat{\sigma}_i^x - J\big[x\sqrt{\bar{q} - q} + z\sqrt{q}\big] \sum_{i}^{n_s} \hat{\sigma}_i^z, \quad (9)$$

with

$$\bar{q} = \int Dz \frac{\int Dx \, \text{Tr} \int d\tau \hat{S}^z \hat{S}^z(\tau) e^{-\beta \hat{H}_{\text{eff}}(z,x)}}{\int Dx \, \text{Tr}\, e^{-\beta \hat{H}_{\text{eff}}(z,x)}}, \quad (10)$$

$$q = \int Dz \left[\frac{\int Dx \text{Tr} \sum_{i}^{n_s} \sigma_i^z \exp(-\beta \hat{H}_{\text{eff}}(z, x))}{\int Dx \text{Tr} \exp(-\beta \hat{H}_{\text{eff}}(z, x))} \right]^2, \quad (11)$$

$$m_i^z = \int Dz \frac{\int Dx \text{Tr}\, \sigma_i^z \exp(-\beta \hat{H}_{\text{eff}}(z, x))}{\int Dx \text{Tr} \exp(-\beta \hat{H}_{\text{eff}}(z, x))}, \quad (12)$$

and $D\xi = d\xi \exp(-\xi^2/2)/\sqrt{2\pi}$ ($\xi = x$ or z).

III. RESULTS

The numerical results are obtained by computing Eqs. (9), (10), (11), and (12) in a self-consistent procedure, where the single-cluster effective model is evaluated by exact diagonalization. The AF long-range order is characterized by a nonzero staggered magnetization ($m_{AF} = |m_1^z - m_2^z + m_3^z - m_4^z|/4$) calculated using the local magnetizations [Eq. (12)] and the CSG phase occurs when $q \neq 0$. The cluster magnetic moment self-interaction $\bar{q}$, given by Eq. (10), is a relevant mean-field order parameter related to disorder and quantum fluctuations. We note that this internal field can be nonzero even in the paramagnetic (PM) state, being dependent on Γ, J_0/J, and temperature. In addition, first-order phase transitions can be located by comparing the free-energy (Eq. (8)) of the phases under transformation.

The presence of both short-range interactions ($J_0 > 0$) and long-range disorder ($J > 0$) introduces a competition between AF ordering and CSG freezing. In the absence of transverse field, the low-temperature magnetic state for weak AF couplings ($J_0/J < 1$) is a CSG, as shown in Fig. 2(a). In this phase, the cluster magnetic moments are randomly frozen and the replica symmetry is broken. An increase in the J_0/J strength reduces the freezing temperature by favoring AF spin pairs inside the cluster. The AF pairs lead to a low cluster magnetic moment, introducing an unfavorable scenario for the CSG state. For a strong enough J_0/J, the CSG state disappears and the onset of antiferromagnetism is observed at low temperatures. We notice that tuning the ratio J_0/J could be an intricate task in physical systems. However, changing the system ground-state from antiferromagnetism to CSG has been achieved in several systems, often by chemical doping [29–34]. For instance, in the $La_{2-x}Sr_xCuO_4$ compound an AF state is observed at very low Sr contents, but this long-range order is suppressed as $x \to 0.02$. For $x \gtrsim 0.02$, a cluster spin-glass phase is found at low temperatures. We note that this competing scenario holds for both bulk and thin films of $La_{2-x}Sr_xCuO_4$ [30]. Moreover, a

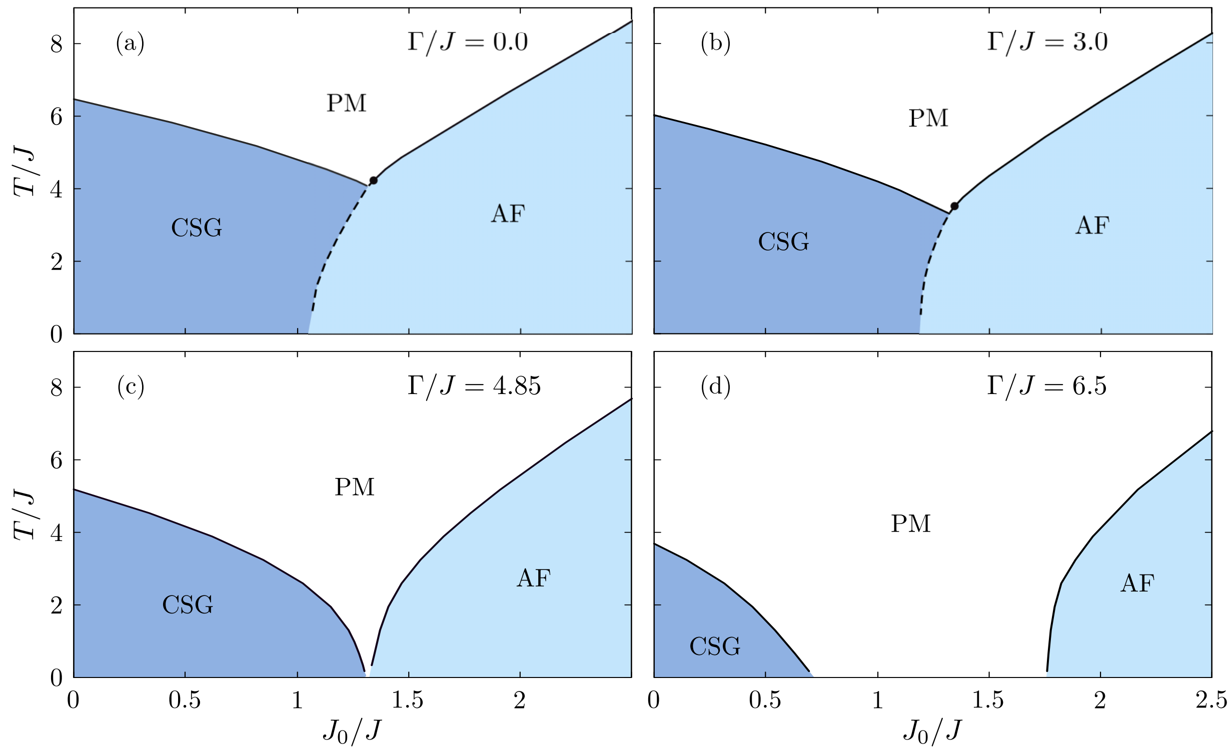

FIG. 2. Phase diagrams of the disordered TFIM in the temperature-coupling plane for several transverse field strengths. Solid and dashed curves indicate continuous and discontinuous phase transitions, respectively. The circle indicates the tricritical point.

similar change in the low temperature phases were observed for $(Sr_{1-x}Ca_x)_3Ru_2O_7$ (at $x \approx 0.4$) [31], $TbMn_{1-x}Sc_xO_3$ (at $x \approx 0.3$) [32], and $CeNi_{1-x}Cu_x$ (at $x \approx 0.7$) [33]. Therefore, our theoretical framework provides phase diagrams resembling those obtained for several disordered antiferromagnets, suggesting that tuning J_0/J can mimic some doping effects on the magnetism of these materials. It is also worth mentioning that the results of Fig. 2(a) are analogous to those found for the CSG model proposed in Ref. [35], in which van Hemmen-like disordered couplings were adopted. In this way, the classical limit of the present model is in agreement with both theoretical and experimental expectations for a system with competing CSG and AF states.

The behavior of order parameters can help us discuss the coupling effects on the present model. Figures 3(a) and 3(b) exhibit the order parameters for different regimes of AF couplings in the absence of transverse field. In particular, while a large $\bar{q}$ is observed within the CSG phase, this parameter approaches zero within the AF long-range order as a consequence of the cluster compensation introduced by the AF couplings. Moreover, thermal fluctuations can increase $\bar{q}$, by activating uncompensated cluster states even when the AF couplings rule the low temperature magnetism, as shown in Fig. 3(b) for $J_0/J = 2$.

It should be noted that the CSG and AF states are separated by a discontinuous phase transition, which is a consequence of the competing nature of the two phases. In addition, continuous phase transitions occur between the PM and CSG states. A more interesting scenario occurs in the PM-AF phase boundary, in which a tricritical point separates the continuous and discontinuous phase transition lines. The presence of the PM-AF discontinuous phase transitions can also be related to the competition between compensation/uncompensation mechanisms. It should be noted that the nonzero $\bar{q}$ near the PM-AF phase transition [see Fig. 3(b)], indicates that disorder affects the system not only in the CSG state. As a consequence, in a highly competitive regime (i.e., $J_0/J \approx 1.25$) a discontinuous phase transition can be found between PM and AF phases. Analogous phenomena has been reported in other spin systems with competing interactions, such as the J_1-J_2 Ising model, in which tricriticality also occurs [36].

The presence of a transverse field introduces quantum fluctuations in the Ising spin system. These quantum fluctuations reduce the ordering temperatures of both AF and CSG phases. The temperature dependence of the order parameters for $\Gamma/J = 4.85$ are depicted in Figs. 3(c) and 3(d). Comparing these results with the zero-field limit, one can note that Γ reduces both the staggered magnetization and the CSG order parameter q [Figs. 3(a) and 3(b)]. Quantum fluctuations also reduce the z component of the cluster magnetic moment, as evidenced by the temperature dependence of $\bar{q}$ for $\Gamma/J = 0$ [Figs. 3(a) and 3(b)] and $\Gamma/J = 4.85$ [Figs. 3(c) and 3(d)]. In particular, an increase in $\bar{q}$ can be driven by thermal fluctuations even within the CSG state, as evidenced by the results for $J_0/J = 0.5$ and $\Gamma/J = 4.85$. It should be stressed that despite the fact that the increase of Γ can eliminate both the AF and CSG states, as shown in Fig. 4, it also can favor the glassy state at very low temperatures. In particular, the phase diagrams in Figs. 2(b) and 2(c) show that the CSG state can be observed at larger values of J_0/J as the transverse field is increased. In other words, increasing the strength of Γ/J can lead to replica symmetry breaking in a disordered antiferromagnet.

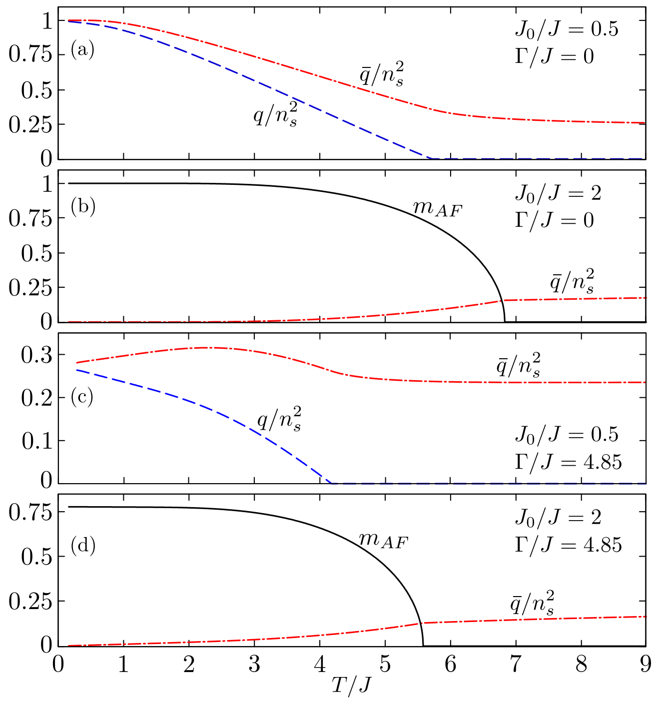

FIG. 3. Temperature dependence of the order parameters. In the absence of transverse field, panels (a) and (b) show the results for weak and strong AF interactions, respectively. Panels (c) and (d) exhibit the order parameters for weak and strong AF interactions, respectively, when quantum fluctuations are introduced by the transverse magnetic field.

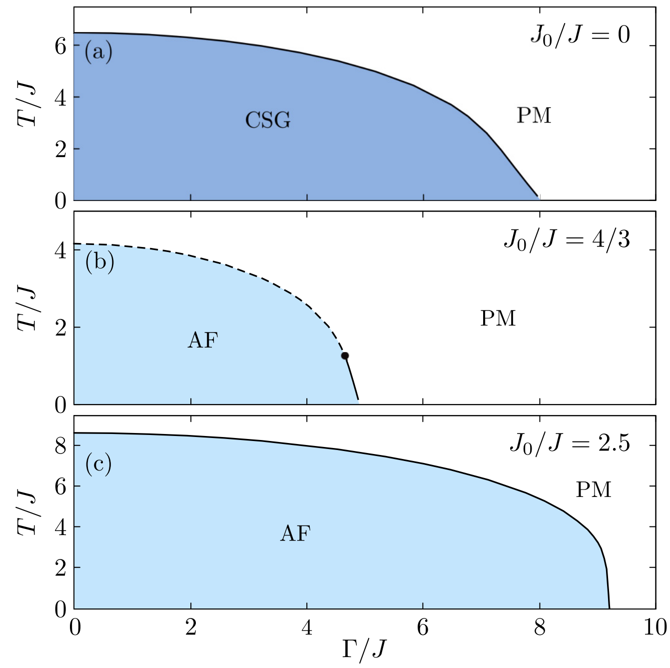

FIG. 4. Phase diagrams of the disordered TFIM in the temperature-transverse field plane for several antiferromagnetic couplings. Solid and dashed curves indicate continuous and discontinuous phase transitions, respectively. The circle indicates the tricritical point.

This result corroborates recent studies of disorder cluster antiferromagnets, in which field-induced cluster freezing is found [37,38]. In particular, in Ref. [38], the role of a longitudinal magnetic field on the competition between CSG and AF phases were investigated within a disordered Ising model with a rather different type of disordered coupling given by a van Hemmen-like interaction [39]. As a result, a glassy state is found even at very low levels of disorder for strong longitudinal fields. On the other hand, our findings in the present work suggest that the transverse field can favor a CSG state only at intermediate levels of disorder. It indicates that transverse and longitudinal fields have different effects on the competition between CSG and AF phases at low levels of disorder. This difference could be attributed to the quantum fluctuations introduced by the transverse field, which is absent when only a longitudinal field is considered [38]. We also note that, for strong enough Γ/J, only continuous phase transitions are found in the phase diagrams, as shown in Figs. 2(c) and 2(d).

Several interesting phenomena arise in the regime of strong competition between AF interactions and disorder. For instance, a quantum paramagnetic state arises at zero temperature [see Fig. 2(d)]. One can note that this disordered state occurs as a consequence of the presence of both quantum fluctuations—introduced by the transverse field—and the competition between couplings. For $J_0/J \approx 4/3$, an even more appealing result can be observed: the discontinuous PM-AF phase boundary becomes a continuous one when Γ/J increases, as shown in Fig. 4(b). In other words, continuous phase transitions emerge as a consequence of quantum fluctuations. Analogous findings have been reported in recent studies of other transverse field Ising models with competing interactions, such as the J_1-J_2 square lattice [10] and the J_1-J_2-J_3 honeycomb lattice [11]. Therefore, our results support the proposal that continuous phase transitions can be induced by quantum fluctuations in systems with competing interactions [10]. It is worth stressing that the PM-AF phase boundary is not affected by the replica-symmetric approximation, suggesting that the change in the phase boundary nature is not an artifact of the theoretical framework adopted.

IV. CONCLUSION

We studied a disordered AF Ising model in a transverse field, characterizing the role of thermal and quantum fluctuations on phase boundaries. By adopting a replica CMF formalism we were able to identify continuous and discontinuous phase transitions, as well as tricriticality. We found that strong competition between AF interactions and disorder supports discontinuous phase transitions driven by thermal fluctuations and continuous phase transitions induced by quantum fluctuations. We remark that this phenomenon occurs at the AF phase boundary and, therefore, is not affected by the replica-symmetric approach considered in this work. Analogous findings have been reported in a rather different context, namely ferroeletric materials, in which room temperature phase transitions are discontinuous, but signatures of quantum criticality are observed at very low temperatures [12]. Our results indicate that a similar phenomenon occurs in a highly competitive regime of disordered antiferromagnets, supporting the recent findings for other TFIMs with competing interactions [10,11]. In this way, our findings reinforce that competing interactions provide a suitable scenario for quantum annealed criticality in spin systems [10].

In addition, we found that the competition between cluster spin glass and antiferromagnetism can be affected by the transverse field. For instance, it is found that increasing Γ/J can favor the CSG state over the AF one in the highly competitive regime of J_0/J. It should be stressed that we considered a particular disordered AF model and further studies are required to corroborate our main findings in the context of quantum disordered antiferromagnets. We note that our calculations are based on a cluster approximation that goes a step beyond the standard single-site mean-field treatment. However, despite that we considered a square lattice and our approach retains some features of the lattice geometry, the intercluster interactions are still evaluated within a mean-field picture, allowing, for instance, a finite temperature CSG phase. Therefore, we hope our results motivate further investigations of the competition between cluster freezing and AF long-range order in the presence of quantum fluctuations. In particular, taking into account that geometrical frustration is known to favor spin-glass freezing [40,41], an interesting question regards the role of this type of frustration in disordered antiferromagnets under transverse field.

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