A Novel Quantum Transition in a Fully Frustrated Transverse Ising Antiferromagnet

Anjan Kumar Chandra

Centre for Applied Mathematics and Computational Science, Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata-700064, India.

E-mail: `anjan.chandra@saha.ac.in`

Jun-ichi Inoue

Complex Systems Engineering, Graduate School of Information Science and Technology, Hokkaido University, N14-W9, Kita-ku, Sapporo 060-0814, Japan

E-mail: `j_inoue@complex.eng.hokudai.ac.jp`

Bikas K. Chakrabarti

Centre for Applied Mathematics and Computational Science and Theoretical Condensed Matter Physics Division, Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata-700064, India.

E-mail: `bikask.chakrabarti@saha.ac.in`

Abstract. We consider a long-range Ising antiferromagnet (LRIAF) put in a transverse field. Applying quantum Monte Carlo method, we study the variation of order parameter (spin correlation in Trotter time direction), susceptibility and average energy of the system for various values of the transverse field at different temperatures. The antiferromagnetic order is seen to get immediately broken as soon as the thermal or quantum fluctuations are added. We also discuss the phase diagram for the Sherrington-Kirkpatrick (SK) model with the same LRIAF bias, also in presence of a transverse field. We find that while the antiferromagnetic order is immediately broken as one adds an infinitesimal transverse field or thermal fluctuation to the system, an infinitesimal SK spin glass disorder is enough to induce a stable glass order in the antiferromagnet. This glass order eventually gets destroyed as the thermal or quantum fluctuations increased beyond their threshold values and the transition to para phase occurs. Indications of this novel phase transition are discussed. Because of the presence of full frustration, this surrogate property of the LRIAF for incubation of stable spin glass phase in it (induced by addition of a small disorder) should enable eventually the study of classical and quantum spin glass phases by using some perturbation theory with respect to the disorder .

1. Introduction

Quantum phases in frustrated systems are being intensively investigated these days; in particular in the context of quantum spin glass and quantum ANNNI models [1]. Here we study a fully-frustrated quantum antiferromagnetic model. Specifically, the long-range antiferromagnetic Ising model put under transverse field. The finite temperature properties of sub-lattice decomposed version of this model was already considered earlier [3, 4]. The quantum phase transition and entanglement properties of the full long-range model at zero temperature was studied by Vidal et al [5]. Here we present some results obtained by applying quantum Monte Carlo technique [6] to the same full long-range model at finite temperature. We observe indications of a quantum phase transition in the model, where the antiferromagnetically ordered phase gets destabilized by both infinitesimal thermal (classical) as well quantum fluctuations (due to tunneling or transverse field) and the system becomes disordered or goes over to the para phase.

The ordered phase of the long range Ising Antiferromagnet (LRIAF) seems to be extremely volatile and loses the order (freezing of spin orientations) at any finite fluctuation level; classical or quantum. However the LRIAF model has the required frustration of the Sherrington-Kirkpatrick (SK) model, which could support the spin glass order, but for any disorder. To check if this 'liquid'-like antiferromagnetic phase of LRIAF can get 'crystallized' into spin-glass phase if a little disorder is added, we study next this LRIAF Hamiltonian with a tunable coupling with the SK spin glass Hamiltonian and study this entire system's phase transitions induced by both thermal and tunneling field. Indeed, the stable SK spin glass phase is observed for thermal or quantum fluctuations below finite threshold values.

We employ the analytic (mean field) solution of the transverse Ising model with long-range interactions can be in presence of the special kind of quenched disorder appropriate for the SK spin glasses. With this, we study the phase diagram for the SK model with LRIAF bias in a transverse field. We again find that the antiferromagnetic order is immediately broken when one adds an infinitesimal transverse field or thermal fluctuation to the system. However, an infinitesimal SK-type disorder is enough to make the system 'crystallized' into a glass phase.

This paper is organized in the following manner. In Section 2, we introduce the pure quantum LRIAF model and then discuss the (finite temperature) quantum Monte Carlo results. In Section 3, we consider the SK model with antiferromagnetic bias in a transverse field, and discuss the (analytic) mean field phase diagram. In Section 4, we present some discussions on our results.

2. The pure LRIAF model

The Hamiltonian of the infinite-range quantum Ising antiferromagnet (without any spin glass disorder) is

$$H \equiv H^{(C)} + H^{(T)} = \frac{J_0}{N} \sum_{i,j(>i)=1}^{N} \sigma_i^z \sigma_j^z - h \sum_{i=1}^{N} \sigma_i^z - \Gamma \sum_{i=1}^{N} \sigma_i^x, \tag{1}$$

where J_0 denotes the long-range antiferromagnetic ($J_0 > 0$) exchange constant; for convenience, we fix the value $J_0 = 1$ in this section. Here σ^x and σ^z denote the x and z component of the N Pauli spins

$$\sigma_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \sigma_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad i = 1, 2, ..., N.$$

h and Γ denote respectively the longitudinal and transverse fields. We have denoted the co-operative term of H (including the external longitudinal field term) by $H^{(C)}$ and the transverse field part as $H^{(T)}$. As such the model has a fully frustrated (infinite-range or infinite dimensional) co-operative term. At zero temperature and at zero longitudinal and transverse fields, the $H^{(C)}$ would prefer the spins to orient in $\pm z$ directions only with zero net magnetization in the z-direction. This antiferromagnetically ordered state is completely frustrated and highly degenerate. Switching on the transverse field Γ would immediately induce all the spins to orient in the x-direction (losing the degeneracy), corresponding to a maximum of the kinetic energy

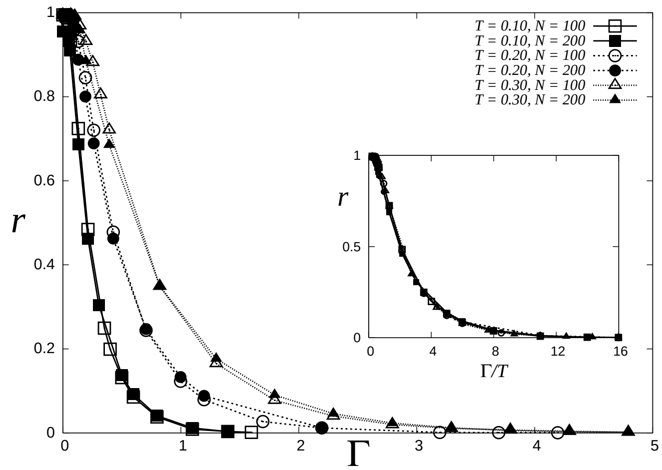

Figure 1. Variation of the order parameter r (correlation in the Trotter direction) with transverse field Γ for $T = 0.10, 0.20$ and 0.30 ($h = 0$) for two different system sizes ($N = 100$ and 200). $r = 0$ for large Γ. The inset shows the plot of r against the scaled variable Γ/T.

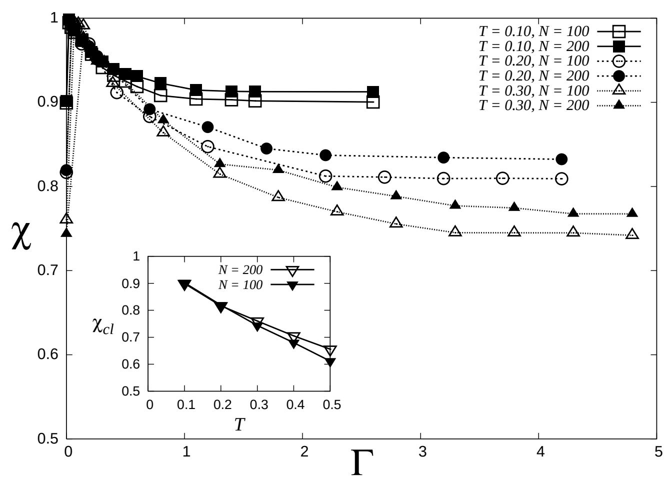

Figure 2. Variation of the susceptibility χ with transverse field Γ for $T = 0.10, 0.20$ and 0.30 ($h \leq 0.1$) for two different system sizes ($N = 100$ and 200). The corresponding susceptibility χ_{cl} for various temperatures for $N = 100$ and 200 for the classical system are shown in the inset. χ converges to the classical values χ_{cl} for large Γ.

term and this discontinuous transition to the para phase occurs at $\Gamma = 0$. However, at any finite temperature the entropy term coming from the extreme degeneracy of the antiferromagnetically ordered state and the close-by excited states does not seem to induce a stability of this phase.

2.1. Monte Carlo simulation

2.1.1. Suzuki-Trotter mapping and simulation This Hamiltonian (1) can be mapped to a $(\infty + 1)$-dimensional classical Hamiltonian [6] using the Suzuki-Trotter formula. The effective Hamiltonian can be written as

$$\mathcal{H} = \frac{1}{NP} \sum_{i,j(>i)=1}^{N} \sum_{k=1}^{P} \sigma_{i,k}\sigma_{j,k} - \frac{h}{P} \sum_{i=1}^{N} \sum_{k=1}^{P} \sigma_{i,k} - \frac{J_p}{P} \sum_{i=1}^{N} \sum_{k=1}^{P} \sigma_{i,k}\sigma_{i,k+1},$$

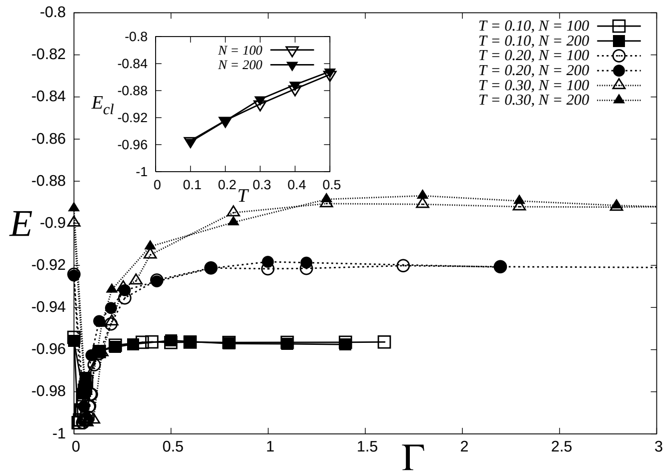

Figure 3. Variation of average energy E with transverse field Γ for $T = 0.10, 0.20$ and 0.30 ($h = 0$) for two different values of $N(= 100, 200)$. The corresponding average energy E_{cl} for various temperatures for $N = 100$ and 200 for the are shown in the inset. E converges to the classical values E_{cl} for large Γ .

where

$$J_p = -(PT/2)\ln(\tanh(\Gamma/PT)). \tag{2}$$

Here P is the number of Trotter replicas and k denotes the k-th row in the Trotter direction. J_p denotes the nearest-neighbor interaction strength along the Trotter direction. We have studied the system for $N = 100$. Because of the diverging growth of interaction J_p for very low values of Γ and also for high values of P, and the consequent non-ergodicity (the system relaxes to different states for identical thermal and quantum parameters, due to frustrations, starting from different initial configurations), we have kept the value of P at a fixed value of 5. This choice of P value helped satisfying the ergodicity of the system up to very low values of the transverse field at the different temperatures considered $T = 0.10$ and 0.20. Starting from a random initial configurations (including all up or 50-50 up-down configurations) we follow the time variations of different quantities until they relax and study the various quantities after they relax.

2.1.2. Results We studied results for three different temperatures $T = 0.10, 0.20$ and 0.30 and all the results are for $N = 100$ and 200 and $P = 5$. We estimated the following quantities after relaxation :

(i) *Correlation along Trotter direction (r)* : We studied the variation of the order parameter

$$r = \frac{1}{NP}\sum_{i=1}^{N}\sum_{k=1}^{P}\langle\sigma_{i,k}\sigma_{i,k+1}\rangle, \tag{3}$$

which is the first neighbor correlation along Trotter direction. Here, $\langle ...\rangle$ indicate the average over initial spin configurations. This quantity r shows a smooth vanishing behavior. We consider this correlation q as the order parameter for the transition at Γ_c. A larger transverse field is needed for the vanishing of the order parameter for larger temperature. The observed values (see Figure 1) of Γ_c are $\simeq 1.6, 2.2$ and 3.0 for $T = 0.1, 0.2$ and 0.3 respectively. As shown in the inset, an unique data collapse occurs when r is plotted against Γ/T and one seems to get the complete disorder immediately as the scaling dos not involve any finite value T_c. This is consistent with the observations in the next section.

(ii) *Susceptibility (χ)* : The longitudinal susceptibility $\chi = (1/NP)\partial[\sum_{i,k}\langle\sigma_{i,k}\rangle]/\partial h$, where h ($\rightarrow 0$) is the applied longitudinal field, has also been measured. We went up to $h = 0.1$ and estimated the χ values. As we increase the value of the transverse field Γ from a suitably chosen low value, χ initially starts with a value almost equal to unity and then gradually saturates at lower values (corresponding to the classical system where $J_p = 0$ in Eq.(2)) as Γ is increased. Also at $\Gamma = 0$, the classical values are indicated in Figure 2. This saturation value of χ decreases with temperature. Again the field at which the susceptibility saturates are the same as for the vanishing of the order parameter for each temperature.

(iii) *Average energy (E)* : We have measured the value of the co-operative energy for each Trotter index and then take its average E i.e. $E = \langle H^{(C)}\rangle$ of Eq. (1) with $J_0 = 1$. It initially begins with -1.0 and after a sharp rise the average energy saturates, at large values of Γ, to values corresponding to the classical equilibrium energy (E_{cl} for $J_p = 0$ in Eq.(2)) at those temperatures. Again it takes larger values of Γ at higher temperatures to achieve the classical equilibrium energy. At $\Gamma = 0$, the corresponding classical values of E are plotted in Figure 3. The variations of all these quantities indicate that the 'quantum order' disappears and the quantities reduce to their classical values (corresponding to $J_p = 0$ in for large values of the transverse field Γ.

2.2. A mean field analysis

First, Let us consider the case of pure LRIAF model and rewrite our Hamiltonian H in Eq.(1) for $\tilde{J} = 0$ as

$$H = \frac{1}{2N}\left(\sum_{i=1}^{N}\sigma_i^z\right)^2 - \frac{1}{N}\sum_{i=1}^{N}(\sigma_i^z)^2 - h\sum_{i=1}^{N}\sigma_i^z - \Gamma\sum_{i=1}^{N}\sigma_i^x \tag{4}$$

If we now denote the total spin by $\vec{\sigma}_{tot}$ i.e. $\vec{\sigma}_{tot} = \frac{1}{N}\sum_{i=1}^{N}\vec{\sigma}_i$ (where $N|\vec{\sigma}| = 0, 1, 2, ..., N$), then the Hamiltonian H can be expressed as

$$\frac{H}{N} = \frac{1}{2}(\sigma_{tot}^z)^2 - h\sigma_{tot}^z - \Gamma\sigma_{tot}^x - \frac{1}{N}. \tag{5}$$

Let us assume the average total spin $\langle\vec{\sigma}\rangle$ to be oriented at an angle θ with the z-direction : $\langle\sigma_{tot}^z\rangle = m\cos\theta$ and $\langle\sigma_{tot}^x\rangle = m\sin\theta$. Hence the average total energy $E_{tot} = \langle H\rangle$ can be written as

$$\frac{E_{tot}}{N} = \frac{1}{2}m^2\cos^2\theta - hm\cos\theta - \Gamma m\sin\theta - \frac{1}{N}. \tag{6}$$

At the zero temperature and at $\Gamma = 0$, for $h = 0$, the energy E_{tot} is minimised when $\theta = 0$ and $m = 0$ (complete antiferromagnetic order in z-direction). As soon as $\Gamma \neq 0$ ($h = 0$) the minimisation of E_{tot} requires $\theta = \pi/2$ and $m = 1$ (the maximum possible value); driving the system to paramagnetic phase. This discontinuous transition at $T = 0$ was also seen in [5]. As observed in our Monte Carlo study in the previous section, $\Gamma_c(T) \rightarrow 0$ as $T \rightarrow 0$. This is consistent with this exact result $\Gamma_c = 0$ at $T = 0$. For $T = 0$ (and $h = 0$), therefore, the transition from antiferromagnetic ($\theta = 0 = m$) to para ($\theta = \pi/2, m = 1$) phase, driven by the transverse field Γ, occurs at $\Gamma = 0$ itself.

One can also estimate the susceptibility χ at $\Gamma = 0 = T$. Here $E_{tot}/N = \frac{1}{2}m^2\cos^2\theta - hm\cos\theta - \frac{1}{N}$ and the minimisation of this energy gives $m\cos\theta = h$ giving the (longitudinal) susceptibility $\chi = m\cos\theta/h = 1$. This is consistent with the observed behaviour of χ shown in Figure 2 where the extrapolated value of χ at $\Gamma = 0$ increases with decreasing T and approaches $\chi = 1$ as $T \to 0$.

At finite temperatures $T \neq 0$, for $h = 0$, we have to consider also the entropy term and minimise the free energy $\mathcal{F} = E_{tot} - TS$ rather than E_{tot} where S denotes the entropy of the state. This entropy term will also take part in fixing the value of θ and m at which the free energy $\mathcal{F}$ is minimised. As soon as the temperature T becomes non-zero, the extensive entropy of the system for antiferromagnetically ordered state with $m \simeq 0$ (around and close-by excited states with $\theta = 0$) helps stabilisation near $\theta = 0$ and $m = 0$ rather than near the para phase with $\theta = \pi/2$ and $m = 1$, where the entropy drops to zero. While the transverse field tends to align the spins along x direction (inducing $\theta = \pi/2$ and $m = 1$), the entropy factor prohibits that and the system adjusts θ and m values accordingly and they do not take the disordered or para state values ($\theta = \pi/2$ and $m = 1$) for any non-zero value of Γ (like at $T = 0$). For very large values of Γ, of course, the free energy $\mathcal{F}$ is practically dominated by the transverse field term in H and again $\theta = \pi/2$ and $m = 1$, beyond $\Gamma = \Gamma_c(T) > 0$ for $T > 0$. However, this continuous transition-like behaviour may be argued [7] to correspond to a crossover type property of the model at finite temperatures (suggesting that the observed finite values of $\Gamma_c(T)$ are only effective numerical values). In fact, for $h = 0$ one adds the entropy term $-T\ln D_s$ to E_{tot} in Eq.(7) to get $\mathcal{F}$ and one can then get [7], after minimising the $\mathcal{F}$ with respect to m and θ, $m = \tanh(\Gamma/2T)$, which indicates an analytic variation of m and no phase transition at any finite temperature for $\tilde{J} = 0$ (antiferromagnetic phase occurs only at $\Gamma = T = 0$ as shown in Figure 4.

3. LRIAF with SK disorder: 'Liquid' phase of the SK spin glasses gets frozen

In the last part of this paper, we discuss the phase diagram for the Sherrington-Kirkpatrick model with antiferromagnetic bias in a transverse field. We find that the antiferromagnetic order is immediately broken when one adds an infinitesimal transverse field or thermal fluctuation to the system, whereas an infinitesimal SK-type disorder is enough to get the system 'crystallized' into the glass phase.

The model we discuss here is given by the following Hamiltonian

$$H = \frac{1}{N}\sum_{ij(j>i)} (J_0 - \tilde{J}\tau_{ij})\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x \tag{7}$$

where J_0 is a parameter which controls the strength of the antiferromagnetic bias and $\tilde{J}$ is an amplitude of the disorder τ_{ij} in each pair interaction. The Γ controls the quantum-mechanical fluctuation. When we assume that the disorder τ_{ij} obeys a Gaussian with mean zero and variance unity, the new variable $J_{ij} \equiv -J_0 + \tilde{J}\tau_{ij}$ follows the following distribution. $P(J_{ij}) = \exp[-(J_{ij} + J_0)^2/2\tilde{J}^2]/\sqrt{2\pi}\tilde{J}$. Therefore, we obtain the 'pure' antiferromagnetic Ising model with infinite range interactions when we consider the limit $\tilde{J} \to 0$ keeping $J_0 > 0$. On the other hand, for $J_0 < 0$ with $\Gamma = 0$ is identical to the classical SK model. In this paper, we investigate the condition for which the antiferromagnetic order survives.

For the Hamiltonian (7), we immediately obtain the saddle point equations under the static and replica symmetric approximations as follows (see e.g. [2, 8]).

$$m = \int_{-\infty}^{\infty} Dz \frac{(\tilde{J}\sqrt{q}z + K_0 m)}{\sqrt{(\tilde{J}\sqrt{q}z + K_0 m)^2 + \Gamma^2}} \tanh\beta\sqrt{(\tilde{J}\sqrt{q}z + K_0 m)^2 + \Gamma^2} \tag{8}$$

$$q = \int_{-\infty}^{\infty} Dz \left\{ \frac{(\tilde{J}\sqrt{q}z + K_0 m)}{\sqrt{(\tilde{J}\sqrt{q}z + K_0 m)^2 + \Gamma^2}} \right\}^2 \tanh^2\beta\sqrt{(\tilde{J}\sqrt{q}z + K_0 m)^2 + \Gamma^2}, \tag{9}$$

where $K_0 \equiv -\mathrm{sgn}(J_0)|J_0|$ and $m \equiv N^{-1}\sum_i \sigma_i^z$ is a magnetization and $q \equiv N^{-1}\sum_i \langle\sigma_i^z\rangle^2$ is a spin glass order parameter. We defined $Dz \equiv dz\, \mathrm{e}^{-z^2/2}/\sqrt{2\pi}$. The bracket $\langle\cdots\rangle$ denotes an expectation over the density matrix: $\rho = \mathrm{e}^{-\beta H}/\mathrm{tr}\, \mathrm{e}^{-\beta H}$. When J_0 is negative, (8) has the only solution $m = 0$. The general phase boundaries (see Figure 4) between the ferro (F), spin glass (SG), antiferro (AF) and para (P) phases can be obtained by solving the the above two equations in the limit $m \to o; q \neq 0$ for the F-SG boundary, $q \to 0$ for SG-P boundary and $m \to 0$ for the F-P boundary. In these limits, the P-SG boundary equations become (see e.g. [8])

$$\Gamma = \tilde{J} \tanh\left(\frac{\Gamma}{T}\right). \tag{10}$$

3.1. Classical system

In the classical limit, the equations of state are simplified as $m = \int_{-\infty}^{\infty} Dz \tanh \beta(\tilde{J}\sqrt{q}z - J_0 m)$, $q = \int_{-\infty}^{\infty} Dz \tanh^2 \beta(\tilde{J}\sqrt{q}z - J_0 m)$. For $J_0 > 0\,(K_0 < 0)$, we find that $m = 0$ is only physical solution for all temperature regimes. This fact means that there are three possible phases, namely, the antiferromagnetic phase, the paramagnetic phase and the spin glass phase. In these three phases, the magnetization m is zero. To determine the critical point T_{SG} at which the spin glass transition takes place, we expand the equation with respect to q for $q \simeq 0$ and $m = 0$. Then, we have $T_{SG} = \tilde{J}$ and the critical point is independent of the antiferromagnetic bias J_0.

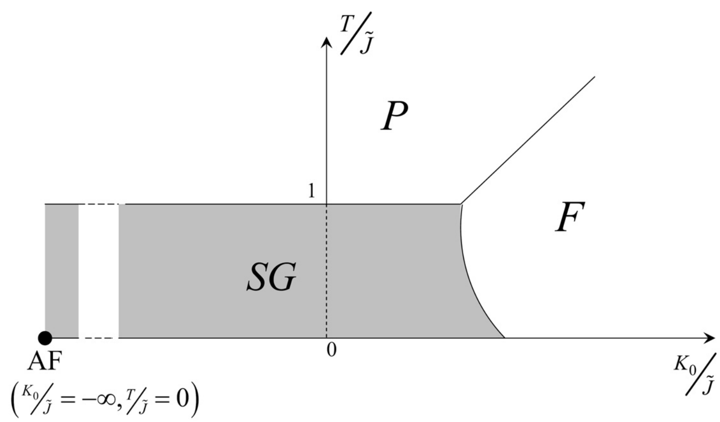

Figure 4. The phase diagram of classical SK model [9] extended for antiferromagnetic bias. For $J_0 > 0\,(K_0 < 0)$, there exist spin glass phase below $T/\tilde{J} = 1$ and the critical temperature is independent of the strength of the antiferromagnetic bias J_0. For finite temperature $T > 0$, the anti-ferromagnetic order disappears and the system changes to the paramagnetic phase. When we add an infinitesimal disorder $\tilde{J} > 0$, the antiferromagnetic order is broken down and the system suddenly gets 'crystallized' into a spin glass (SG) phase.

This result means that the antiferromagnetic order can appear if and only if we set $J_0 > 0$ and $T/\tilde{J} = 0, J_0/\tilde{J} = \infty\,(K_0/\tilde{J} = -\infty)$. On the other hand, for $0 < J_0 < \infty$ at low temperature regime $T < T_{SG}$, the spin glass phase appears. We plot the phase diagram in Figure 4. We also conclude that the system described by the Hamiltonian (7) with $\Gamma = 0$ is immediately 'crystallized' when we add any infinitesimal disorder $\tilde{J} > 0$.

From the view point of the degeneracy of the spin configurations, we easily estimate the number of solution for the antiferromagnetic phase as $2^{N/2} = \mathrm{e}^{0.346N}$, which is larger than the number of the SK model $\mathrm{e}^{0.199N}$ [9]. However, for the infinite range antiferromagnetic model, the energy barrier between arbitrary configurations which gives the same lowest energy states is of order 1 and there is no ergodicity breaking.

3.2. Quantum system

We next consider the case of presence of transverse field $\Gamma \neq 0$ for $J_0 > 0\,(K_0 < 0)$. In this case, we also find that the saddle point equation (8) has a solution $m = 0$ and the phase boundary between the spin glass and paramagnetic phases is given by setting $m = 0$ and $q \simeq 0$ and we get (10). Obviously, the boundary at $T = 0$ gives $\Gamma_{SG} = \tilde{J}$. On the other hand, when we consider the case of $\Gamma \simeq 0$, we have $T_{SG} = \tilde{J}$. These fact means that there is no antiferromagnetic nor the spin glass phase when we consider the pure case $\tilde{J} = 0$ because the critical point leads to $T_{SG} = \Gamma_{SG} = 0$. Therefore, we conclude that the antiferromagnetic phase can exist if and only if $T = \Gamma = 0$.

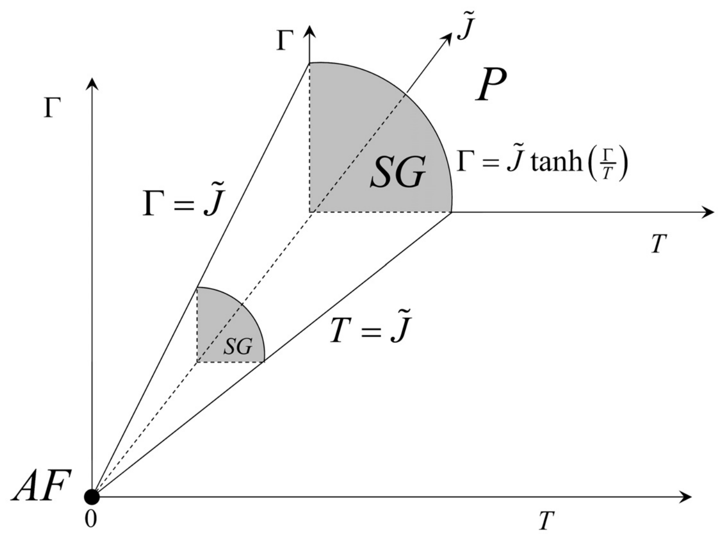

Figure 5. Phase diagram for the quantum system. The antiferromagnetic order exists if and only if we set $T = \Gamma = 0$. As the $\tilde{J}$ decreases, the spin glass phase gradually shrinks to zero and eventually ends up at an antiferromagnetic phase at its vertex (for $\Gamma = 0 = T = \tilde{J}$) as discussed in Section 2.

4. Discussion

We considered here a long-range Ising antiferromagnet at a finite temperature and put in a transverse field. The antiferromagnetic order is seen to get immediately broken as soon as the thermal or quantum fluctuations are added. However, when we add the Sherrington-Kirkpatrick Hamiltonian as perturbation we find that an infinitesimal SK spin glass disorder is enough to induce a stable glass order in this LRIAF antiferromagnet. This glass order eventually gets destroyed as the thermal or quantum fluctuations increased beyond their threshold values and the transition to para phase occurs. As shown in the phase diagram in Figure 5, the antiferromagnetic phase of the LRIAF (occurring only at $\tilde{J} = 0 = \Gamma = T$), can get 'crystallized' into spin-glass phase if a little SK-type disorder is added ($\tilde{J} \neq 0$); the only missing element in the LRIAF (which is fully frustrated, but lacks disorder) to induce stable order (freezing of random spin orientations) in it. As mentioned already, the degeneracy factor $\mathrm{e}^{0.346N}$ of the ground state of the LRIAF is much larger than that $\mathrm{e}^{0.199N}$ for the SK model. Hence, (because of the presence of full frustration) the LRIAF posses a surrogate incubation property of stable spin glass phase in it when induced by addition of a small disorder. This observation should enable eventually the study of classical and quantum spin glass phases by using some perturbation theory with respect to the disorder.

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