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Solvable model of the quantum spin glass in a transverse field

Yadin Y. Goldschmidt
Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
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The spin-glass model with p-spin interactions in the presence of a transverse field is solved in the limit $p \to \infty$. The phase diagram is obtained and consists of three phases: a spin-glass phase and two paramagnetic phases. The paramagnetic phases are distinguished by transverse ordering. The spin-glass phase is similar to that of the random-energy model.

In recent years there have been several studies of quantum effects in spin glasses.[1-10] In particular, there was much interest in the Ising infinite-range spin glass in a transverse field. Besides its theoretical interest, this model has some possible experimental applications.[3] The mixed hydrogen-bonded ferroelectric $Rb_{1-x}(NH_4)_xH_2PO_4$ has been reported to display a spin-glass-type phase for some range of x values. This system can be modeled by an Ising spin glass in a transverse field, since it contains a mixture of ferroelectric and antiferroelectric materials. The transverse field[11,12] represents the tunneling effect of the proton between the two minima of the hydrogen bond. On the theoretical side, this model stands in the middle of some controversy on the nature of the spin-glass phase: Are there many coexisting, thermodynamic states separated by infinitely large energy barriers as in the classical infinite-range model, or are quantum fluctuations strong enough, for some values of the parameters, to destroy this picture due to tunneling effects across barriers?

Thirumalai, Li, and Kirkpatrick claimed,[8] using the static approximation, that there is a small region in the spin-glass phase where a replica-symmetric (RS) solution is stable, unlike the conventional infinite-range model with no transverse field. On the other hand, Buttner and Usadel[9] showed recently that a full treatment, which does not utilize the static approximation, predicts that the RS solution is always unstable in the spin-glass phase. Finally Ray, Chakrabarti, and Chakrabarti[10] performed some Monte Carlo simulations which tend to support stability of the RS solution, although the size of their sample is small and the error bars too large to allow any firm conclusion. A RS-breaking (RSB) solution has been constructed by Parisi[13] for the Ising spin glass (SG) with no transverse field, but to our knowledge, no one has constructed such a solution for the Ising SG in a transverse field. Physically, RSB is usually associated with the coexistence of many thermodynamic states whereas a RS solution is interpreted as representing a single Gibbs state (up to a global inversion).

In order to clarify these issues it is always instructive to investigate an exactly solvable model whose properties can be investigated in some detail. For the case of the classical Ising SG, such an exactly solvable model is the so-called Derrida random-energy model[14] which consists of a collection of independent random-energy levels. This model also has been solved, using replicas by Gross and Mezard.[15] It is sometimes referred to as "the simplest SG."

It is our aim in this paper to generalize this model to the quantum case and then solve it and obtain a complete phase diagram. The model we propose is an Ising infinite-range model with p-spin interaction and a transverse field and the limit $p \to \infty$ is considered. The Hamiltonian is given by

$$\mathcal{H} = -\sum_{(i_1 \cdots i_p)} J_{i_1 \cdots i_p} \hat{\sigma}^z_{i_1} \cdots \hat{\sigma}^z_{i_p} - \Gamma \sum_{j=1}^{N} \hat{\sigma}^x_j , \quad (1)$$

where the sum $(i_1 \cdots i_p)$ runs over all distinct p-plets, N is the total number of sites, and $\hat{\sigma}^z_i$ and $\hat{\sigma}^x_i$ are the spin operators at site i. $J_{i_1 \cdots i_p}$ are the random interactions whose distribution is given by (in the following we set $J=1$)

$$P(J_{i_1 \cdots i_p}) = \left(\frac{N^{p-1}}{J^2 \pi p!} \right)^{1/2} \exp\left(-\frac{(J_{i_1 \cdots i_p})^2}{J^2 p!} N^{p-1} \right) . \quad (2)$$

Γ denotes the strength of the transverse field. It is well known that for $\Gamma = 0$ the Hamiltonian describes, in the limit of $p \to \infty$, the random-energy model. For $\Gamma > 0$ we also have been able to solve the model described by the Hamiltonian (1) in the limit $p \to \infty$. We have used the static approximation, but argue that this approximation becomes exact as $p \to \infty$. We have not constructed a rigorous proof yet, but we conjecture that this is indeed the case (see below).

In order to proceed and calculate the free energy of the model we use the Suzuki-Trotter formula[16,17] to cast the problem into an equivalent classical one and we use the replica trick[18] to be able to carry out the average over the random bonds. We find (denoting $\gamma \equiv \beta\Gamma$)

$$\begin{aligned} \overline{Z^n} &= \int dJ_{i_1 \cdots i_p} P(J_{i_1 \cdots i_p}) \operatorname{Tr} \exp\left[\beta \sum_{a=1}^{n} \left(\sum_{(i_1 \cdots i_p)} J_{i_1 \cdots i_p} \hat{\sigma}^{za}_{i_1} \cdots \hat{\sigma}^{za}_{i_p} + \gamma \sum_i \hat{\sigma}^{xa}_i \right) \right] \\ &= \left(\frac{1}{2} \sinh \frac{2\gamma}{M} \right)^{MNn/2} \int dJ_{i_1 \cdots i_p} P(J_{i_1 \cdots i_p}) \operatorname*{Tr}_{\sigma^a(k) = \pm 1} \exp\left(\frac{\beta}{M} \sum_{k=1}^{M} \sum_a \sum_{(i_1 \cdots i_p)} J_{i_1 \cdots i_p} \sigma^a_{i_1}(k) \cdots \sigma^a_{i_p}(k) \right. \\ &\qquad \left. + B \sum_k \sum_a \sum_j \sigma^a_j(k) \sigma^a_j(k+1) \right) , \end{aligned} \quad (3)$$

where we defined

$$B \equiv \tfrac{1}{2}\ln\coth(\gamma/M)\,. \tag{4}$$

In Eq. (3) the variable $k=1,\dots,M$ is a label for the Trotter direction and the limit $M\to\infty$ must be taken.

Integrating out over the bond distribution we obtain

$$\overline{Z^n}=\left(\frac{1}{2}\sinh\frac{2\gamma}{M}\right)^{MNn/2} e^{\beta^2 Nn/4M}\,\mathrm{Tr}\exp\left(\frac{1}{4}\frac{\beta^2 N}{M^2}\sum_{(ka)\neq(k'a')}[Q_{kk'}^{aa'}(\sigma)]^p+B\sum_{kaj}\sigma_j^a(k)\sigma_j^a(k+1)\right), \tag{5}$$

with

$$Q_{kk'}^{aa'}(\sigma)=\frac{1}{N}\sum_i \sigma_i^a(k)\sigma_i^\beta(k')\,. \tag{6}$$

The spin trace can be performed by constraining $Q_{kk'}^{aa'}(\sigma)$ to equal $Q_{kk'}^{aa'}$ using a Lagrange-multiplier matrix $\lambda_{kk'}^{aa'}$. One gets

$$\overline{Z^n}=\int_{-\infty}^{\infty}\prod_{(ak)\neq(a'k')} dQ_{kk'}^{aa'}\int\prod d\lambda_{kk'}^{aa'}e^{-NG}\,, \tag{7}$$

$$G=-\frac{1}{4}\frac{\beta^2}{M^2}\sum_{ka\neq k'a'}[Q_{kk'}^{aa'}]^p+\frac{1}{2}\frac{\beta^2}{M^2}\sum Q_{kk'}^{aa'}\lambda_{kk'}^{aa'}$$
$$-\ln\mathop{\mathrm{Tr}}_{\sigma^a(k)}\exp\left[\frac{1}{2}\frac{\beta^2}{M^2}\sum_{ka\neq k'a'}\lambda_{kk'}^{aa'}\sigma^a(k)\sigma^{a'}(k')+B\sum_{ka}\sigma^a(k)\sigma^a(k+1)+\frac{Mn}{2}\ln\left(\frac{1}{2}\sinh\frac{2\gamma}{M}\right)\right], \tag{8}$$

where contributions vanishing in the limit $M\to\infty$ have been discarded. Denoting

$$\chi_{kk'}^a\equiv Q_{kk'}^{aa}\,,\quad v_{kk'}^a\equiv\lambda_{kk'}^{aa}\,,\quad k\neq k'\,, \tag{9}$$

we can write G in the form

$$G=-\frac{1}{4}\frac{\beta^2}{M^2}\sum_{k,k'}\sum_{a\neq a'}[Q_{kk'}^{aa'}]^p-\frac{1}{4}\frac{\beta^2}{M^2}\sum_{k\neq k'}\sum_a[\chi_{kk'}^a]^p+\frac{1}{2}\frac{\beta^2}{M^2}\sum_{k\neq k'}\sum_a\chi_{kk'}^a v_{kk'}^a+\frac{1}{2}\frac{\beta^2}{M^2}\sum_{k\neq k'}\sum_{a\neq a'}Q_{kk'}^{aa'}\lambda_{kk'}^{aa'}-\ln\mathrm{Tr}\exp\mathcal{H}_{\mathrm{eff}}\,, \tag{10}$$

$$\mathcal{H}_{\mathrm{eff}}=\frac{1}{2}\frac{\beta^2}{M^2}\sum_{k\neq k'}\sum_a v_{kk'}^a\sigma^a(k)\sigma^a(k')+\frac{1}{2}\frac{\beta^2}{M^2}\sum_{kk'}\sum_{a\neq a'}\lambda_{kk'}^{aa'}\sigma^a(k)\sigma^{a'}(k')+B\sum_{ka}\sigma^a(k)\sigma^a(k+1)+\frac{1}{2}Mn\ln\left(\frac{1}{2}\sinh\frac{2\gamma}{M}\right). \tag{11}$$

The free energy will be given in the thermodynamic limit $N\to\infty$ by the dominant saddle-point solution of G:

$$\beta f=\lim_{n\to 0}G/n\,. \tag{12}$$

In order to evaluate G explicitly we must impose some ansatz on the structure of $Q_{kk'}^{aa'}$ and $\chi_{kk'}^{aa'}$. In the high-temperature phase it is reasonable to use the RS ansatz

$$Q_{kk'}^{aa'}=Q_{kk'}\,,\quad \lambda_{kk'}^{aa'}=\lambda_{kk'}\,,\quad a\neq a'\,, \tag{13}$$

$$v_{kk'}^a=v_{kk'}\,,\quad \chi_{kk'}^a=\chi_{kk'}\,. \tag{14}$$

In addition, we will also use the static approximation, and later we will give arguments concerning why it seems to be exact in the large p limit. The static hypothesis or ansatz is that all the order parameters displayed in Eqs. (13) and (14) are independent of k, k'; i.e., of the values of the Trotter indices. In that case we find

$$\lim_{n\to 0}\frac{1}{n}G=\tfrac{1}{4}\beta^2Q^p-\tfrac{1}{4}\beta^2\chi^p+\tfrac{1}{2}\beta^2\chi v-\tfrac{1}{2}\beta^2 Q\lambda-\frac{1}{n}\ln\int Dz_1\left[\int Dz_2\,\mathrm{Tr}\exp\left(h\sum_k\sigma(k)+B\sum_k\sigma(k)\sigma(k+1)+C_1\right)\right]^n, \tag{15}$$

with

$$Dz\equiv\frac{dz}{\sqrt{2\pi}}e^{-(1/2)z^2}\,, \tag{16}$$

$$h=\frac{b}{M}\equiv\frac{\beta}{M}[z_1\sqrt{\lambda}+z_2(v-\lambda)^{1/2}]\,, \tag{17}$$

$$C_1=\tfrac{1}{2}M\ln\left(\sinh\frac{\gamma}{M}\cosh\frac{\gamma}{M}\right). \tag{18}$$

One can use the solution of the one-dimensional Ising model to obtain finally

$$\beta f=\tfrac{1}{4}\beta^2Q^p-\tfrac{1}{4}\beta^2\chi^p+\tfrac{1}{2}\beta^2\chi v-\tfrac{1}{2}\beta^2Q\lambda-\int Dz_1\ln\int Dz_2\,2\cosh(\gamma^2+b^2)^{1/2}\,. \tag{19}$$

The stationary conditions for the free energy are

$$\lambda = \tfrac{1}{2} p Q^{p-1} , \tag{20a}$$

$$v = \tfrac{1}{2} p \chi^{p-1} , \tag{20b}$$

$$Q = \int Dz_1 \left[\frac{\int Dz_2 \sinh(\Xi) b/\Xi}{\int Dz_2 \cosh\Xi} \right]^2 , \tag{20c}$$

$$\chi = \int Dz_1 \frac{\int Dz_2 [b^2/\Xi^2 \cosh\Xi + \gamma^2/\Xi^3 \sinh\Xi]}{\int Dz_2 \cosh\Xi} , \tag{20d}$$

where

$$\Xi = (\gamma^2 + b^2)^{1/2} . \tag{21}$$

In the high-temperature phase we expect no SG ordering, hence $Q=0$ and $\lambda=0$ which is a consistent solution of Eq. (20). In that case

$$f = \frac{1}{4T}(p-1)\chi^p - T \ln \int dZ\, 2\cosh[(1/T)(\Gamma^2 + \tfrac{1}{2} p\chi^{p-1} z^2)^{1/2}] , \tag{22}$$

where χ is a solution of the equation

$$\chi = \left[\int Dz \frac{\tfrac{1}{2} p\chi^{p-1} z^2}{\Gamma^2 + \tfrac{1}{2} p\chi^{p-1} z^2} \cosh[(1/T)(\Gamma^2 + \tfrac{1}{2} p\chi^{p-1} z^2)^{1/2}] + \frac{T\Gamma^2}{(\Gamma^2 + \tfrac{1}{2} p\chi^{p-1} z^2)^{3/2}} \sinh[(1/T)(\Gamma^2 + \tfrac{1}{2} p\chi^{p-1} z^2)^{1/2}] \right] \times \left[\int Dz \cosh[(1/T)(\Gamma^2 + \tfrac{1}{2} p\chi^{p-1} z^2)^{1/2}] \right]^{-1} . \tag{23}$$

In the limit of large p, there are two possible solutions for Eq. (23) which give rise to two different high-temperature phases.

Phase I. For large p, $\chi^p = 1$. More precisely, a possible solution of (23) is

$$\chi = 1 - \frac{4\Gamma^2 T^2}{p^2} + \cdots . \tag{24}$$

Plugging this solution into Eq. (22) and evaluating the integral using the saddle-point method in the limit $p \to \infty$ we obtain

$$f_I = -\frac{1}{4T} - T \ln 2 + O\left(\frac{1}{p}\right) , \tag{25}$$

where only the $O(1/p)$ correction depends on Γ. Thus in this phase the free energy is the same as in the ordinary random-energy model with $\Gamma = 0$.

Phase II. For large p, $\chi^p = 0$. This arises from another possible solution of Eq. (23) which is given for large p by

$$\chi = \frac{T}{\Gamma} \tanh \frac{\Gamma}{T} , \tag{26}$$

which is always smaller than 1. In this phase the free energy is given by

$$f_{II} = -T \ln 2 - T \ln \cosh \frac{\Gamma}{T} . \tag{27}$$

It is easy to calculate the entropy associated with the free energy (22) by using the relation $S = -\partial f/\partial T$. One finds that the free energy f_I given by Eq. (25) is not acceptable for $T < (2\sqrt{\ln 2})^{-1}$ since in that case the entropy becomes negative. In order to find a solution in the SG phase we returned to Eqs. (10) and (11), not assuming RS but using the static ansatz. We also assumed that for the saddle-point solutions χ and v are independent of α. For $Q_{aa'}$ and $\lambda_{aa'}$ we introduced a first stage RSB. This means that if we put $a=(L,\delta)$ where $L=1,\ldots,n/m$, $\delta=1,\ldots,m$ we define

$$Q_{L\delta,L\delta'} = q_2 , \quad Q_{L\delta,L'\delta'} = q_{11} , \quad L \neq L' , \tag{28}$$

and similarly for λ. After some algebra, the free energy is found to be

$$\beta f = \tfrac{1}{4}\beta^2[m q_{11}^p + (1-m) q_2^p] - \tfrac{1}{4}\beta^2\chi^p + \tfrac{1}{2}\beta^2 \chi v - \tfrac{1}{2}\beta^2[m q_{11}\lambda_{11} + (1-m) q_2 \lambda_2] - \frac{1}{m}\int Dz_1 \ln \int Dz_2 \left[\int Dz_3 2\cosh(b^2+\gamma^2)^{1/2} \right]^m , \tag{29}$$

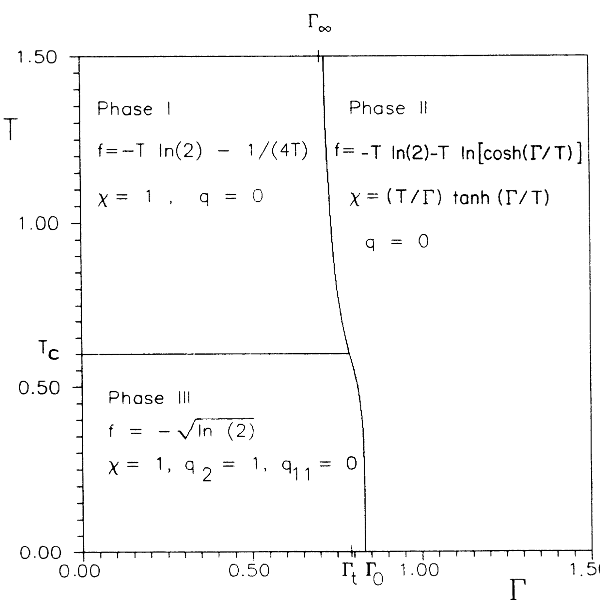

FIG. 1. Phase diagram of the model in the Γ-T plane in the limit $p \to \infty$. Phase III is the spin-glass phase and phases I and II are the paramagnetic phases. Phase II is characterized by transverse ordering. The special points have values given by $T_c = 1/(2\sqrt{\ln 2}) \approx 0.6006$, $\Gamma_0 = \sqrt{\ln 2} \approx 0.832$, $\Gamma_\infty = 1/\sqrt{2} \approx 0.707$, and $\Gamma_t = \ln(2+\sqrt{3})/(2\sqrt{\ln 2}) \approx 0.791$.

where

$$b=\beta[z_1(\lambda_{11})^{1/2}+z_2(\lambda_2-\lambda_{11})^{1/2}+z_3(\nu-\lambda_2)^{1/2}]\,. \tag{30}$$

We have found a consistent solution to the stationary conditions by assuming $q_{11}<1$, $q_2=1$, $\chi=1$ (in the large p limit). Plugging this solution in (29) and noticing that for large p, $\lambda_{11}=0$, $\lambda_2=\frac{1}{2}p$, $\nu=\frac{1}{2}p$, and evaluating the integral by steepest descent as $p\to\infty$ we find

$$f=-\tfrac{1}{4}\beta m-\frac{1}{\beta m}\ln 2 \tag{31}$$

and $q_{11}=0$. Using stationarity with respect to m one finds $m=\beta_c/\beta$ with $\beta_c=2\sqrt{\ln 2}$ and hence

$$f_{\rm III}=-\sqrt{\ln 2}\,. \tag{32}$$

Thus the free energy in the SG phase is independent of T and Γ, and the entropy vanishes identically. For the case $\Gamma=0$, it was argued[15] that one-stage RSB is enough to obtain the exact solution in the spin-glass phase, and the same arguments apply here. We see that at least for large p, the nature of the SG phase is similar to the classical model and RS has to be broken. The phase diagram of the model is depicted in Fig. 1. The transitions between phases I and II and III and II are first-order transitions. When crossing the first-order-transition boundary one chooses the *lower* free energy among the solutions which are locally stable—see discussion by Mottishaw[19] for a similar case. We see that quantum fluctuations have the effect of destroying the SG phase for large Γ rather than giving rise to a SG solution with no RSB.

One can calculate the amount of transverse ordering by evaluating $-\partial f/\partial\Gamma$. Thus one finds that while phase II is characterized by transverse order of magnitude $\tanh(\Gamma/T)$, in phases I and II there is no transverse ordering. Notice that for $p=2$ it was found[4–9] that there is only one high-temperature phase, thus the existence of two high-temperature phases is a property of large p. A similar situation happens in the classical model solved in Ref. 19 of $s=0,\pm 1$ spins where two paramagnetic phases were found for large p, whereas for $p=2$ only one paramagnetic phase is known to exist.[20]

Finally, we will comment on the validity of the static ansatz for the case $p\to\infty$. In the two paramagnetic phases we have tried to introduce dependence on the indices k,k' through their difference $\Delta=k-k'$. Thus we have introduced order parameters χ_Δ and ν_Δ, $|\Delta|=1,\ldots,M$, and we have rewritten the free energy in terms of these variables. We were able to solve the model for the case where part of $\chi_\Delta^\rho=1$ and the rest are zero, and we have found that the resulting free energy becomes higher compared to the isotropic case where all χ_Δ^ρ are zero or all are 1. We did not form a rigorous formal proof yet but the indication is that the static ansatz is justified for $p\to\infty$. To prove this conjecture remains a task for the future.[21] It will be also possible to calculate corrections to the $p\to\infty$ limit and thus to find how the phase diagram looks for large, but finite p and to find a solution with RSB in the SG phase that depends on Γ, unlike the infinite p case. It will also be very interesting to solve the model without the use of replicas. These are projects for future research

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[21]Notice that for $p\to\infty$ the entropy always tends to zero as $T\to 0$, unlike the $p=2$ case where a manifestation of the error in the static approximation is the nonvanishing of the entropy when $T\to 0$ in the paramagnetic phase (Ref. 8).