One-step replica symmetry breaking solution for fermionic Ising spin glass in a transverse field

F. M. Zimmer, S.G. Magalhaes*

Lab. de Mecânica Estatística e Teoria da Matéria Condensada, Dep. Física, UFSM, 97105-900 Santa Maria, RS, Brazil

Abstract

The fermionic Ising spin glass models in a transverse field are investigated in a Grassmann path integral formalism. The Parisi’s scheme of one-step replica symmetry breaking (RSB) is used within the static ansatz. This formalism has already been applied in a theory in which \( m \) (Parisi’s block-size parameter) is taken as a constant [13]. Now, it is extended to consider \( m \) as a variational parameter. In this case, the results show that RSB is present when \( T \to 0 \), in which the system is driven by quantum fluctuations.

The infinite range Ising spin glass (ISG) in a transverse field has been extensively studied as a theoretical quantum spin glass model. The strength of quantum fluctuations is adjusted by the transverse magnetic field. An experimental realization of this model is the quantum spin glass system \( LiHo_xY_{1-x}F_4 \) [1]. Moreover, there are now several disordered Cerium and Uranium alloys [2] in which it is possible to find a spin glass phase (SG) as well as a Kondo behavior around a quantum critical point (QCP). It is not our intention to discuss this particular complicated problem. However, a proper fermionic formulation of the SG problem in a transverse field can also be useful for this mentioned class of strongly correlated problems [3].

Several techniques have been used to treat the ISG in a transverse field. Nevertheless, they show some controversial results concerning the local stability of replica symmetry solution [4, 5, 6, 7, 8, 9]. For instance, it is an open question whether or not the quantum tunneling through the barriers between the many degenerated thermodynamic states in the free energy landscape is able to restore the replica symmetry (RS). The quantum ISG model treated by the Trotter-Suzuki formalism in the static approximation [10] has shown stable RS solutions in a small region close to freezing temperature \( T_c \) [4]. However, the replica symmetry breaking (RSB) is found in whole SG phase when the Trotter-Suzuki formalism is used without the static approximation, in which the dynamic spin self-interaction is treated by a numerical calculation [5]. For this case, the ordered SG phase has been investigated by one-step RSB solution, [6, 7] in which it is suggested that the quantum tunneling does not restore the RS. On the other hand, this quantum problem has also been investigated by using imaginary-time

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*ggarcia@ccne.ufsm.br
replica formalism under the static ansatz. This approach has shown that the RS quantum SG phase is stable in almost whole SG phase \[8\]. Furthermore, the SG quantum rotors as well as the transverse field ISG have been studied within a Landau theory in which the dynamic effects are considered in an analytical approximation near the critical temperature \[11\]. In this treatment, the RSB occurs in the SG phase at finite temperatures and it suggests suppression of the RSB when \( T \to 0 \).

Recently, the fermionic ISG in a transverse field \( \Gamma \) has been studied using functional integral formalism with Grassmann variables \[9\]. This problem has been treated within the static approximation. The phase diagram found in Ref. \[9\] shows that the \( T_c \) decreases toward a QCP when \( \Gamma \) reaches a critical value. In this formalism, the RS solution is unstable in whole SG phase \[9\] in disagreement with Ref. \[8\]. In a subsequent work still using the static approximation, the replica symmetry has been broken within the one-step RSB like-Parisi’s scheme \[12\]. Nonetheless, the block-size parameter \( m \) has been taken as a temperature independent \[13\]. The results within this particular RSB treatment suggest that the RS is restored at \( T = 0 \) when \( \Gamma > 0 \) \[13\]. However, it arises some questions whether \( m \) is taken as a variational parameter as in the original Parisi’s scheme \[12\] for \( \Gamma > 0 \). Are the results using the original Parisi’s scheme of RSB changed significantly when compared with those obtained in Ref. \[13\] for \( \Gamma > 0 \)? Are the quantum effects able to restore the RS in this fermionic formulation?

The purpose of the present work is to investigate the one-step RSB in the fermionic ISG in a transverse field using the original Parisi’s scheme. In particular, we compare it with the alternative procedure of the same problem proposed in Ref. \[13\]. The problem is formulated in a path integral formalism as in Ref. \[13\]. The static approximation is used to treat the spin-spin correlation functions. However, the parameter \( m \) is taken as a saddle-point equation, which is the main difference between this work and Ref. \[13\]. In our quantum spin glass treatment, the static approximation is an important point. It is recognized that the static approximation can yield inaccurate quantitative results at very low temperature. However, because of a lack of a suitable analytical method to go beyond the static ansatz in whole SG phase in this fermionic formalism, there are still several quite recent papers studying the ISG in transverse field within this particular level of approximation \[9, 13\]. This paper reports results for the one-step RSB order parameters, free energy and entropy. Our results agree partially with those of Ref. \[13\]. Nevertheless, the RS is not restored at \( T \to 0 \), which is in agreement with Refs. \[6, 7\].

The infinite range ISG in a transverse magnetic field \( \Gamma \) is described by the Hamiltonian:

\[
\hat{H} = -\sum_{i \neq j} J_{ij} \hat{S}_i^z \hat{S}_j^z - 2\Gamma \sum_i \hat{S}_i^x
\]  

(1)

where the sums are run over the \( N \) sites of a lattice. The exchange interaction \( J_{ij} \) among all pairs of spins is a random variable that follows a Gaussian probability distribution with mean equal to zero and variance \( 16J^2 \). The spin operators in Eq. (1) are defined in terms of fermion operators \[9\]: \( \hat{S}_i^z = \frac{1}{2} [\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}] \), \( \hat{S}_i^x = \frac{1}{2} [c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow}] \) where \( \hat{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) gives the number of fermions at site \( i \) with spin projection \( \sigma = \uparrow \) or \( \downarrow \). \( c_{i\sigma}^\dagger \) and \( c_{i\sigma} \) are respectively the fermion creation and annihilation operators.

The Hamiltonian (1) is defined on a fermionic space where the operator \( S^z \)
has two magnetic eigenvalues and two non-magnetic eigenvalues (empty and
double occupied site). Therefore, there are two states that do not belong to the
usual spin space. However, it is possible to express the partition function of a
spin system (2S-model) in terms of the partition function of a corresponding
fermionic system by using a restriction that considers only sites occupied by
one fermion \[^{[15]}\]. This work considers two models: the 4S-model without any
restriction about the non-magnetic states and the 2S-model in which the non-
magnetic states are forbidden. The restriction in the 2S-model is obtained by
using the Kronecker delta function \[^{[15]}\]. Therefore, the partition functions for
both models are written in a compact form as \[^{[9]}\]:

\[
Z\{y\} = \int D(\phi^* \phi) \prod_j \frac{1}{2\pi} \int_0^{2\pi} dx_j e^{-y_j A(y)}
\]  \(^{(2)}\)

with the action

\[
A\{y\} = \int_0^\beta d\tau \left\{ \sum_{j,\sigma} \phi^*_{j\sigma}(\tau) \frac{\partial}{\partial \tau} + y_j \phi_{j\sigma}(\tau) \right\}
\]  \(^{(3)}\)

\[\beta = 1/T \ (T \text{ is the temperature}), \ y_j = ix_j \text{ for the 2S-model or } y_j = 0 \text{ for the} \]
4S-model, which corresponds to the half-filling situation.

In Eq. \(^{(3)}\), the Fourier decomposition of the time-dependent quan-
tities is employed. The configurational averaged free energy per site is ob-
tained by using the replica method:

\[
\beta F = -\frac{1}{n} \lim_{n \to 0} \left( \langle Z\{y\}^n \rangle_{J_{ij}} - 1 \right) / n
\]  \(^{(4)}\)

where the replicated partition function is

\[
\langle Z\{y\}^n \rangle_{J_{ij}} = \int dU \exp\left\{ -N \left( \frac{\beta^2 J^2}{2} \sum_{\alpha,\gamma} q_{\alpha,\gamma}^2 + \ln \Lambda\{y\} \right) \right\}
\]  \(^{(4)}\)

with \[
\int dU = \int_\infty^- \prod_{\alpha,\gamma} dq_{\alpha,\gamma}(\beta J \sqrt{N/2\pi}) \]
where \(\alpha\) and \(\gamma\) are replica indices running from 1 to \(n\). It is assumed the static approximation, therefore:

\[
\Lambda\{y\} = \prod_{\alpha} \int_0^{2\pi} \frac{dx_{\alpha}}{2\pi} e^{-y_{\alpha}} \int D[\phi^*_{\alpha}, \phi_{\alpha}] \exp[\bar{H}],
\]  \(^{(5)}\)

\[
\bar{H} = \sum_{\alpha} A_{0\Gamma}^\alpha + 4\beta^2 J^2 \sum_{\alpha,\gamma} q_{\alpha,\gamma} S_{\alpha}^z S_{\gamma}^z
\]  \(^{(6)}\)

with the definitions:

\[
A_{0\Gamma}^\alpha = \sum_\omega \varphi_\alpha^\dagger(\omega)(i\omega + y_{\alpha} + \beta \Gamma \sigma^z)\varphi_\alpha(\omega),
\]  \(^{(7)}\)

\[
S_{\alpha}^z = \frac{1}{2} \sum_\omega \varphi_\alpha^\dagger(\omega)\sigma^z \varphi_\alpha(\omega),
\]  \(^{(8)}\)

\[
\varphi_\alpha^\dagger(\omega) = \begin{pmatrix} \phi_{1\alpha}^*(\omega) & \phi_{2\alpha}^*(\omega) \end{pmatrix}
\] is a Grassmann spinor, \(\sigma^x\) and \(\sigma^z\) are the Pauli matrices, and \(\omega\) denotes fermionic Matsubara frequencies.
The set of integrals in $\int dU$ has been exactly performed in the thermodynamic limit by the steepest descent method. The simplest conjecture to the replica matrix $\{Q\}$ for overlaps in the spin space is the replica symmetry ansatz (RS). However, it produces an unstable solution in the ordered spin glass phase \[13\]. An attempt to solve this problem is the so called method of replica symmetry breaking (RSB) \[12\].

In the Parisi’s scheme of one-step RSB (1S-RSB), the replica matrix $\{Q\}$ is parameterized dividing the $n$ replicas into $n/m$ groups with $m$ replicas in each one, such as:

$$q_{\alpha\gamma} = r \quad \text{if} \quad I(\alpha/m) = I(\gamma/m)$$

$$q_{\alpha\gamma} = q_0 \quad \text{if} \quad I(\alpha/m) \neq I(\gamma/m) \quad (9)$$

where $I(x)$ gives the smallest integer which is greater than or equal to $x$. The parameter $r$ is the replica-diagonal spin-spin correlation $r = \langle S_\alpha S_\alpha \rangle$. The physical meaning of $m$ is that two different spin glass order parameters $q_0$ and $q_1$ are mixed up in the ratio $m : 1 - m$.

The parametrization (9) is used to sum over the replica index. It produces quadratic terms in Eq. (6) that are linearized introducing new auxiliary fields in Eq. (5). The functional Grassmann integral is now performed and the sum over the Matsubara frequencies can be evaluated like references \[9, 13\]. Finally, the restriction condition over the number of states admitted in each model is explicitly adopted. This procedure results in the following expression to the free energy:

$$\beta F_s = \frac{\beta^2 J^2}{2} \left[ m(q_1^2 - q_0^2) + r^2 - q_0^2 \right] - \frac{1}{m} \int_{-\infty}^{\infty} Dz \ln \int_{-\infty}^{\infty} Dv (2K_s)^m$$

with

$$K_s = s - 2 + \int_{-\infty}^{\infty} D\xi \cosh(\beta\sqrt{\Delta})$$

where $s (= 2$ or 4) represents the number of states admitted in each model, $dx = dx e^{-x^2/2}/\sqrt{2\pi} (x = z, v$ or $\xi)$, $\Delta = \hbar^2 + \Gamma^2$, $h = J(\sqrt{2q_0}z + \sqrt{2}(q_1 - q_0)v + \sqrt{2}(r - q_1)\xi)$ and the parameters $q_0$, $q_1$, $r$ and $m$ are given by the extreme condition of the free energy \[10\].

The set of saddle-point equations for the parameters $q_0$, $q_1$, $r$ and $m$ can numerically be solved. Here, the equation for $m$ is self-consistently solved with the parameters $q_0$, $q_1$ and $r$ \[12\] instead of Ref. \[13\] where $m$ is taken as a constant value belong to the interval $0 < m < 1$. The 2S model recovers the classical results for 1S-RSB \[12\] when $\Gamma = 0$. When $\Gamma > 0$, the replica-diagonal correlation $r$ becomes temperature dependent and $r$ must be evaluated together with the other parameters ($q_0$, $q_1$, $m$). The results are shown in Fig. 1. The parameters $q_0$, $q_1$, $m$ and $\delta = q_1 - q_0$ (which gives 1S-RSB parameter) are zero at $T > T_c$ where the replica symmetry solution is valid. The transverse field reduces $T_c$ and the order parameters as well. The thermodynamic quantities are less sensitive on variations of $m$ at $T$ near $T_c$ than at lower temperatures. For example, the results obtained using the original Parisi’s scheme show that $\delta$ increases when $T$ decreases from $T_c$. 

4
Figure 1: Parameters $q_0$, $q_1$, $\delta = q_1 - q_0$, $r$ and $m$ as a function of $T/J$ for the 2S model. The upper, the middle and the lower panels are, respectively, for $\Gamma/J = 0.0$, 0.5 and 1.0. The dotted lines show the RS solution for $r$.

in agreement with Ref. [13]. This occurs because right below the transition temperature the remaining RSB order parameters have very weak dependence on the solution of parameter $m$. On the other hand, at lower temperature, the original Parasi’s scheme shows that the parameter $m$ becomes increasingly important. For instance, the parameter $\delta$ is greater than zero and the difference between $r$ and $r_{RS}$ (for $\Gamma > 0$) is increased when $T$ decreases by contrast with Ref. [13] where $\delta$ becomes zero when $T \to 0$. Therefore, our results indicate that the validity range in temperature of RSB procedure proposed in Ref. [13] is restrained to a region quite close to the critical temperature $T_c$. As consequence, any conclusion about whether or not the RS is restored in Ref. [13] is limited by the procedure itself. On the contrary, our results obtained by the original Parisi’s scheme (in the same static approximation) suggest that the RSB effects are present even at $T \to 0$ as it can be seen by the extrapolation of curves in Fig. 1 to $T \to 0$. 

5
Fig. 2 shows the order parameters for the 4S model. The behavior of $q_0$, $q_1$, $\delta$ and $m$ is qualitatively the same as that one of the 2S model. However, $r$ is temperature dependent for all values of $\Gamma$ due to the presence of non-magnetic states. On the other hand, the ground state energy of the 4S model when $\Gamma = 0$ is the same as that of the classical 2S model [16]. The results of the 2S and the 4S models are converging to the same values when $T \to 0$ even for $\Gamma > 0$. Therefore, it could be expected that in the ground state of the 4S model every site carry a single fermion. Hence the empty and the double occupied sites do not contribute to the thermodynamic quantities at $T \to 0$.

The free energies for 2S and 4S models when $\Gamma = 0.5J$ and $1.0J$ are exhibited in Fig. 3. The 1S-RSB can be compared with the RS solution. The difference between these two approaches increases when $T$ decreases from $T_c$. The 1S-RSB ansatz gives higher values for the free energy, and its entropy ($S = -\partial F/\partial T$) is positive for the range of temperatures analyzed in Fig. 3. The increase of $\Gamma$ reduces the difference between the RS and the 1S-RSB. It could be conjectured...
Figure 3: Free energy as a function of $T/J$ for the 2S and 4S models. The upper and the lower panels are, respectively, for $\Gamma/J = 0.5$ and 1.0. The solid lines are results for the 1S-RSB, while the dotted lines are for the RS approach. The insert shows the entropy at lower temperatures.

that when the strength of $\Gamma$ is enhanced quantum fluctuations assume a relevant role inducing tunneling between the metastable spin glass valleys. Thereby, it could reduce the importance of the replica symmetry breaking. Nevertheless, it is still not able to restore the RS solution. Although these results are limited by the static ansatz that is expected to yield inaccurate quantitative results at very low temperature, they are in good qualitative agreement with those obtained by the Trotter-Suzuki formalism without the static ansatz \cite{6,7} when $T$ decreases from $T_c$ and by the Landau theory of quantum spin glass rotors \cite{11} when $\Gamma$ increases towards the QCP.

To conclude, it is studied the fermionic Ising spin glass model in a transverse field $\Gamma$ within a Grassmann path integral formalism. The static ansatz and the replica trick with one-step replica symmetry breaking scheme are used. Recently, this problem has been analyzed by the same formalism and the same static approximations, but within a theory in which the Parisi block size parameter $0 < m < 1$ is taken as an independent parameter of temperature \cite{13}. This method in Ref. \cite{13} for finite and fixed values of $m$ leads to the conclusion that the RSB parameter decreases towards zero at low temperature and the RS is restored at $T = 0$ when $\Gamma > 0$. We have compared the procedure proposed in Ref. \cite{13} with the original Parisi’s scheme which indicates that this alternative procedure is reliable mainly in the vicinity of the critical temperature. Therefore, any extrapolation to lower temperature is limited by the procedure itself besides the static approximation. Moreover, when quantum fluctuations become important, our results provide evidences that the original Parisi’s RSB scheme should be used to improve the physical description of the ordered spin glass phase treated.
by the replica method.
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