The Ising spin glass in a transverse field.

Results of two fermionic models.

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Abstract

We analyze the long range Ising spin glass in a transverse field $\Gamma$ by using Grassmann variables in a field theory where the spin operators are represented by bilinear combinations of fermionic fields. We compare the results of two fermionic models. In the four state (4S)-model the diagonal $S_i^z$ operator has two vanishing eigenvalues, that are suppressed by a restraint in the two states (2S)-model. Within a replica symmetric theory and in the static approximation we obtain similar results for both models. They both exhibit a critical temperature $T_c(\Gamma)$ that decreases when $\Gamma$ increases, until it reaches a quantum critical point (QCP) at the same value of $\Gamma_c$ and they are both unstable under replica symmetry breaking in the whole spin glass phase.
1 Introduction

The Ising model in a transverse field is widely studied for being the simplest system of interacting spins with quantum dynamics. The most striking feature is that the competition between thermal and quantum fluctuations reduce the critical temperature up to a point when a quantum phase transition occurs at $T = 0$, at a quantum critical point (QCP) \(^1\). We will not discuss here the extensive literature on results for several versions of the model, but we will concentrate instead in the quantum Ising spin glass in a transverse field. This is represented by a Hamiltonian in which only one component of the spins, say the $z$-component, interact among themselves with a random interaction while a uniform, constant field $\Gamma$ is applied in the transverse $x$-direction. The experimental realizations of this model are the $LiHo_xY_{1-x}F_4$ compounds\(^2\).

In the calculation of the quantum mechanical partition function special tools are needed to deal with the non-commuting operators forming the Hamiltonian. The method more currently used in the study of short-range \(^3\) and infinite range \(^4\) spin glasses in a transverse field is the Trotter-Suzuki formula \(^5\), that maps a system of quantum spins in $d$-dimensions to a classical system of spins in $(d + 1)$-dimensions, and it is suited to perform numerical studies. Another way of dealing with the non-commutativity of quantum mechanical spin operators is to use Feynman’s path integral formulations \(^6, 7\) and to introduce time-ordering by means of an imaginary time $0 \leq \tau \leq \beta$, where $\beta$ is the inverse temperature. The work by Bray and Moore\(^8\) established the basis for recent developments in the theory of the
quantum Heisenberg spin glass[8].

A still different functional integral formulation consists in using Grassmann variables to write a field theory with an effective action where the spin operators in the Hamiltonian are expressed as bilinear combinations of fermions[8, 10]. The advantage of the fermionic formulation is that it has a natural application to problems in condensed matter theory, where the fermion operators represent electrons that also participate in other physical processes, like superconductivity[11, 12] and the Kondo effect[13]. In the present paper we use two fermionic models within a grassmannian field theory[9] to analyze the long range Ising spin glass in a transverse field. The novelty resides in the method, as all previous results rely on the Trotter-Suzuki approximation[4]. A criticism to the fermionic formulation may be that the spin eigenstates at each site do not belong to one irreducible representation \( S^z = \pm \frac{1}{2} \), but they are labeled instead by the fermionic occupation numbers \( n_\sigma = 0 \) or \( 1 \), giving two more states with \( S^z = 0 \). We call this the "four states" (4S) model, and despite the presence of these two unwanted states the 4S-Ising spin glass model describes a spin glass transition with the same characteristics as the Sherrington-Kirkpatrick (SK) model[14] in a replica symmetric theory. A way to get rid of the unwanted states was introduced before by Wiethege and Sherrington[15] for non-random interactions and it consists in fixing the occupation number \( n_{\uparrow} + n_{\downarrow} \) by means of an integral constraint at every site. We refer to this as the "two states" (2S)-Ising model.

In sect. 2 we analyse the 4S-Ising and 2S-Ising spin glass models in a transverse field, within the static approximation in a replica symmetric the-
ory. The static ansatz neglects time fluctuations and may be considered an approximation similar to mean field theory. Numerical Monte Carlo solutions of Bray and Moore’s equations indicate that the static approximation reproduces the correct results at finite temperatures\cite{16}. When $\Gamma = 0$ the static approximation reproduces the exact results obtained by other methods, in particular for the 2S-Ising spin glass model we recover SK equations \cite{14}. The results in both models are very similar; they both exhibit a critical spin glass temperature $T_c(\Gamma)$ that decreases when the strength $\Gamma$ of the transverse field increases, until it reaches a quantum critical point (QCP) at $\Gamma_c$, $T_c(\Gamma_c) = 0$. The value of $\Gamma_c$ is the same for both models and the 4S-Ising and 2S-Ising models are identical close to the QCP. We obtained for both models that the replica symmetric solution is unstable \cite{17} in the whole spin glass phase, in agreement with previous results with the Trotter-Suzuki method\cite{4}. We left sect. 3 for discussions.
2 The model and results

The Ising spin glass in a transverse field is represented by the Hamiltonian

\[ H = -\sum_{ij} J_{ij} S_i^z S_j^z - 2\Gamma \sum_i S_i^x \]  

where the sum is over the N sites of a lattice and \( J_{ij} \) is a random coupling among all pairs of spins, with gaussian probability distribution:

\[ P(J_{ij}) = e^{-J_{ij}^2 N / 16 J^2} \sqrt{N / 16\pi J^2}. \]  

The spin operators are represented by auxiliary fermions fields:

\[ S_i^z = \frac{1}{2}[n_i \uparrow - n_i \downarrow] \]
\[ S_i^x = \frac{1}{2}[a_i \uparrow a_i \downarrow + a_i \downarrow a_i \uparrow] \]

where the \( a_i \uparrow, a_i \downarrow \) are creation (destruction) operators with fermion anticommutation rules and \( \sigma = \uparrow, \downarrow \) indicates the spin projections. The number operators \( n_i \sigma = a_i \uparrow a_i \sigma = 0 \) or 1, then \( S_i^z \) in Eq.(3) has two eigenvalues \( \pm \frac{1}{2} \) corresponding to \( n_i \downarrow = 1 - n_i \uparrow \), and two vanishing eigenvalues when \( n_i \downarrow = n_i \uparrow \).

We shall use the Lagrangian path integral formulation in terms of anticommuting Grassmann fields described in previous publications \[9, 10\], so we avoid giving repetitious details. We consider two models: the unrestrained, four states model that has been used previously \[9, 11, 12, 13\], and also the two states model of Wiethege and Sherrington where the number operators satisfy the restraint \( n_i \uparrow + n_i \downarrow = 1 \), what gives \( S_i^z = \pm \frac{1}{2} \), at every site \[15\].

The partition function in the 4S-model is given by
\[ Z_{4S} = T_r e^{-\beta H} \] (4)

while in the restrained model it takes the form:

\[ Z_{2S} = T_r [e^{-\beta H} \prod_j \delta(n_{j\uparrow} + n_{j\downarrow} - 1)] \] (5)

where \( \beta = \frac{1}{T} \) is the inverse temperature.

By using the integral representation for the Kronecker \( \delta \)-function:

\[ \delta(n_{j\uparrow} + n_{j\downarrow} - 1) = \frac{1}{2\pi} \int_0^{2\pi} dx_j e^{ix_j [n_{j\uparrow} + n_{j\downarrow} - 1]} \] (6)

we can express \( Z_{4S} \) and \( Z_{2S} \) in the compact functional integral form

\[ Z\{\mu\} = \int D(\varphi^*\varphi) \prod_j \frac{1}{2\pi} \int_0^{2\pi} dx_j e^{-\mu_j e^{A}\{\mu\}} \] (7)

where:

\[
A\{\mu\} = \int_{\beta} \sum_{j,\sigma} \left[ \varphi_{j\sigma}^*(\tau) \frac{d}{d\tau} \varphi_{j\sigma}(\tau) + \mu_j \varphi_{j\sigma}^*(\tau) \varphi_{j\sigma}(\tau) \right] - H(\varphi_{j\sigma}^*(\tau), \varphi_{j\sigma}(\tau))
\] (8)

and \( \mu_j = 0 \) for the 4S-model while \( \mu_j = ix_j \) for the 2S-model. Going to Fourier representation we introduce the spinors:

\[ \psi_i(\omega) = \begin{pmatrix} \varphi_{i\uparrow}(\omega) \\ \varphi_{i\downarrow}(\omega) \end{pmatrix} \] (9)

and the Pauli matrices:

\[ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \] (10)
to write the spin glass part of the action

\[ A_{SG} = \sum_{\Omega} \sum_{i,j} \beta J_{ij} S_i^z(\Omega) S_j^z(\Omega) \]  

(11)

where

\[ S_i^z(\Omega) = \frac{1}{2} \sum_\omega \psi_\omega^\dagger(\omega + \Omega) \sigma^z \psi_\omega(\omega) \]  

(12)

with Matsubara’s frequencies \( \omega = (2n + 1)\pi \) and \( \Omega = 2m\pi \). In the static approximation, we retain just the term \( \Omega = 0 \) in the sum over the frequency \( \Omega \).

The transverse part of the action is given by:

\[ A_{\Gamma} = \sum_j \psi_j^\dagger(\omega) \gamma_j^{-1}(\omega) \psi_j(\omega) \]

(13)

where the inverse propagator is

\[ \gamma_j^{-1} = i\omega + \mu_j + \Gamma \sigma_x \]

(14)

and the total action can be redefined as

\[ A\{\mu\} = A_{\Gamma} + A_{SG}^{st} \]

(15)

where \( A_{SG}^{st} \) is the static component of Eq. (11). We are now able to follow the standard procedures to get the configurational averaged free energy per site by using the replica formalism:

\[ F = -\frac{1}{\beta N} \lim_{n \to 0} \frac{Z(n) - 1}{n} \]

(16)

where the configurational averaged, replicated, partition function \( < Z^n >_{c,a} = Z(n) \) becomes, after averaging over \( J_{ij} \):
\[ Z(n) = \int_{-\infty}^{\infty} \prod_{\alpha\beta} dq_{\alpha\beta} e^{-N \frac{q_{\alpha\beta}^2}{q}} \prod_{j} \left\{ \prod_{\alpha} \frac{1}{2\pi} \int_{0}^{2\pi} dx_{j\alpha} e^{-\mu_{j\alpha} \Lambda_{j}(q_{\alpha\beta})} \right\} \] (17)

with the replica index \( \alpha = 1, 2, ..., n \), and

\[ \Lambda_{j}(q_{\alpha\beta}) = \int D(\varphi_{\alpha}^\dagger \varphi_{\alpha}) \exp \left[ \sum_{\alpha} \sum_{\omega} \bar{\psi}^{\dagger \alpha}_{\omega} \gamma_{-1}^{-1}(\omega) \bar{\psi}_{\alpha}(\omega) + \beta^2 J^2 \sum_{\alpha\beta} q_{\alpha\beta} S_{z\alpha} S_{z\beta} \right] \] (18)

We indicate by \( S_{z} \) the static component \( S_{z}(\Omega = 0) \) of Eq.(12). We assume a replica symmetric solution of the saddle point equations:

\[ q_{\alpha\beta} = q \quad \quad q_{\alpha\alpha} = q + \bar{\chi} \] (19)

where \( q \) is the spin glass order parameter and \( \bar{\chi} \) is related to the static susceptibility by \( \bar{\chi} = T \chi \).

The sums over \( \alpha \) in the spin part of the action produce again quadratic terms that can be linearized by introducing new auxiliary fields, with the result

\[ \Lambda_{j}(q, \bar{\chi}) = \int_{-\infty}^{\infty} Dz \prod_{\alpha} \int_{-\infty}^{\infty} D\xi_{\alpha} I_{j\alpha}(q, \bar{\chi}, \mu_{j\alpha}, z, \xi_{\alpha}) \] (20)

where \( Dy = \frac{1}{\sqrt{2\pi}} dy e^{-\frac{1}{2}y^2} \) and

\[ I_{j\alpha} = \int D(\varphi_{\alpha}^\dagger \varphi_{\alpha}) e^{\sum_{\omega} \bar{\psi}^{\dagger}_{\omega} \gamma_{j^{-1}}^{-1}(\omega) \bar{\psi}_{\alpha}(\omega)} \] (21)

with

\[ \gamma_{j^{-1}}^{-1}(\omega) = \gamma_{j}^{-1}(\omega) + h_{\alpha} \bar{\xi}_{\alpha} \] (22)
\[ h_\alpha = \beta J \sqrt{2qz} + \beta J \sqrt{2\bar{\chi}_\alpha} \] (23)

The gaussian integral over Grassmann variables is straightforward\[9, 11, 13\], giving the result:

\[ \ln(I_{j\alpha}) = \sum_\omega \ln[(i\omega + \mu_j)^2 - \Delta_\alpha] \] (24)

\[ \Delta_\alpha = [\beta J \sqrt{2qz} + \beta J \sqrt{2\bar{\chi}_\alpha}]^2 + (\beta \Gamma)^2 \] (25)

The sum over frequencies can be also easily performed\[1, 11, 13\] and we obtain

\[ I_{j\alpha} = 1 + e^{2\mu_{j\alpha}} + e^{\mu_{j\alpha}} 2 \cosh \sqrt{\Delta_\alpha} \] (26)

From Eq.(17), Eq.(20) and Eq.(26) we obtain at the saddle point:

\[ Z(n) = e^{-nN \frac{\beta^2 J^2}{2}(\bar{\chi}^2 + 2q\bar{\chi})} \prod_j \left\{ \int_{-\infty}^{\infty} Dz \int_{-\infty}^{\infty} D\xi_\alpha \frac{1}{2\pi} \right\}
\int_0^{2\pi} dx_{j\alpha}[e^{-\mu_{j\alpha}} + e^{\mu_{j\alpha}} + 2 \cosh \sqrt{\Delta_\alpha}] \} \] (27)

For the four states (4S) model there is no restraint and \( \mu_{j\alpha} = 0 \), then the integrals over \( x_{j\alpha} \) equal unity in Eq.(27). For the restrained two states (2S) model we have \( \mu_{i\alpha} = ix_{j\alpha} \) from Eq.(16), then the integrals over the exponential terms identically vanish in Eq.(27). We then obtain for the model with \( 2(p+1) \) states, \( p = 0 \) or 1:

\[ \beta F_p = \frac{1}{2}(\beta J)^2[\bar{\chi}^2 + 2q\bar{\chi}] - \int_{-\infty}^{\infty} Dz \log[2K_p(q, \bar{\chi}, z)] \] (28)

where

\[ K_p(q, \bar{\chi}, z) = p + \int_{-\infty}^{\infty} D\xi \cosh \sqrt{\Delta} \] (29)
The saddle point equations for the order parameters are:

\[ \chi_p = \int_{-\infty}^{\infty} Dz \frac{1}{K_p} \int_{-\infty}^{\infty} D\xi \{ \frac{h^2}{2 \Delta} \cosh \sqrt{\Delta} + \frac{\beta^2 \Gamma^2}{\Delta^2} \sinh \sqrt{\Delta} \} - q_p \]  

(30)

\[ q_p = \int_{-\infty}^{\infty} Dz \frac{1}{K_p^2} \{ \int_{-\infty}^{\infty} D\xi \frac{h}{\sqrt{\Delta}} \sinh \sqrt{\Delta} \}^2 \]  

(31)

where \( h(\xi, z) \) is given in Eq.(23). We obtain for the de Almeida-Thouless eigenvalue [17] and entropy in both models:

\[ \lambda_p^{AT} = 1 - 2(\beta J)^2 \int_{-\infty}^{\infty} Dz \frac{1}{K_p^4} \{ K_p \int_{-\infty}^{\infty} D\xi \{ \frac{h^2}{2 \Delta} \cosh \sqrt{\Delta} + \frac{(\beta \Gamma)^2}{\Delta^2} \sinh \sqrt{\Delta} \} - [ \int_{-\infty}^{\infty} D\xi \frac{\lambda}{\sqrt{\Delta}} \sinh \sqrt{\Delta} ]^2 \} \]  

(32)

\[ \frac{S}{K} = -\frac{3}{2} (\beta J)^2 (\bar{\chi}^2 + 2 \bar{\chi} q) + \int_{-\infty}^{\infty} Dz \log (2K_p) - \]  

\[ \frac{(\beta \Gamma)^2}{\Delta^2} \int_{-\infty}^{\infty} Dz \frac{1}{K_p^2} \int_{-\infty}^{\infty} D\xi \frac{\sinh \sqrt{\Delta}}{\sqrt{\Delta}} \]  

(33)

The Landau expansion of the free energy in powers of q gives:

\[ \beta F_p = \beta F_p^0 + B_p q^2 + C_p q^3 \]  

(34)

where the coefficients are:

\[ B_p = [D_p - 1]|D_p - 2| \]

\[ C_p = -\frac{4}{3} [D_p - 1] \{ 2(D_p - 1)^2 + 3(D_p - 2) \} \]  

(35)

and

\[ D_p = \frac{p + J_1}{p + J_0} \]

(36)

\[ J_l = \int_{-\infty}^{\infty} D\xi \xi^{2l} \cosh \sqrt{2\bar{\chi}_0 \beta^2 J^2 \xi^2 + \beta^2 \Gamma^2} \]  

(37)
In Eq.(37) we need also:

\[ \bar{\chi}(q = 0) = \bar{\chi}_0 = \frac{1}{\sqrt{2\beta J}} \sqrt{D_p - 1} \] (38)

As \( C_p < 0 \), the spin glass phase is characterized by \( B_p > 0 \), giving a maximum instead of a minimum [14] of the free energy. The critical temperature is obtained by solving simultaneously:

\[ D_p = \frac{p + J_1(\beta_c)}{p + J_0(\beta_c)} = 2 \]
\[ \bar{\chi}_0 = \frac{1}{\sqrt{2\beta_c J}} \] (39)

The numerical results for the critical temperature \( T_c(\Gamma) \) and the entropy \( S_0 = S(T_c, \Gamma) \) are shown in Fig. 1 for the 4S-model and Fig. 2 for the 2S-model. For large values of the transverse field \( \Gamma \) the 2S-model and 4S-model are undistinguishable. The analytic solution of Eq.(39) when \( T_c = 0 \) gives the critical value \( \Gamma_c = 2\sqrt{2} J \) for both models. When \( \Gamma = 0 \), the equations (30)-(33) for the 2S-model (\( p=0 \)) reproduce the Sherrington-Kirkpatrick [14] results, while for the 4S-model (\( p=1 \)), we recover our previous results [9].

Finally, we comment on the de Almeida-Thouless instability. The exact solution for \( \lambda^{AT} \) in Eq.(32) in both limits, \( \Gamma = 0 \) and \( \Gamma = \Gamma_c \), shows that \( \lambda^{AT} = 0 \) at the transition point both for the 2S-model and the 4S-model, while numerical results confirm that \( \lambda^{AT}(T_c) = 0 \) for both models on the critical line \( T_c(\Gamma) \). This is a correct result and A.T. acknowledges a flaw in a previous publication [18].
3 Discussion

We performed a new study of two quantum Ising spin glass models in a transverse field by means of a path integral formalism where the spin operators are represented by bilinear combinations of fermionic fields. All previous results in this problem were obtained with the Trotter-Suzuki approximation [4]. In the unrestricted four-states (4S)-model the fermionic representation gives for the diagonal $S^z_i$-operator two eigenvalues $S^z_i = \pm \frac{1}{2}$ and two vanishing eigenvalues, while in the state (2S)-model the vanishing eigenvalues are suppressed by means of an integral constraint. The results in both models were obtained with the static approximation and the phase diagram coincides with previous results with the Trotter-Suzuki method [4]. Regarding the de Almeida-Thouless instability [17], we obtained that the replica symmetric solution is unstable in the whole spin glass phase.

In future work we will apply the fermionic representation of the transverse Ising spin glass to problems in condensed matter theory and also the replica symmetry breaking in the ordered state will be investigated.

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5 Figure Captions

Fig1. Critical temperature $T_c(\Gamma)$ and entropy on the critical line $S_c(T_c, \Gamma)$ for the 4S-model.

Fig2. Same as Fig1, for the 2S-model
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