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Fermionic Ising glasses with BCS pairing interaction. Tricritical behaviour

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Abstract. We have examined the role of the BCS pairing mechanism in the formation of the magnetic moment and henceforth a spin glass (SG) phase by studying a fermionic Sherrington-Kirkpatrick model with a local BCS coupling between the fermions. This model is obtained by using perturbation theory to trace out the conduction electrons degrees of freedom in conventional superconducting alloys. The model is formulated in the path integral formalism where the spin operators are represented by bilinear combinations of Grassmann fields and it reduces to a single site problem that can be solved within the static approximation with a replica symmetric ansatz. We argue that this is a valid procedure for values of temperature above the de Almeida-Thouless instability line. The phase diagram in the T–g plane, where g is the strength of the pairing interaction, for fixed variance J^2/N of the random couplings J_{ij}, exhibits three regions: a normal paramagnetic (NP) phase, a spin glass (SG) phase and a pairing (PAIR) phase where there is formation of local pairs.The NP and PAIR phases are separated by a second order transition line $g = g_c(T)$ that ends at a tricritical point $T_3 = 0.9807J$, $g_3 = 5,8843J$, from where it becomes a first order transition line that meets the line of second order transitions at $T_c = 0.9570J$ that separates the NP and the SG phases. For $T < T_c$ the SG phase is separated from the PAIR phase by a line of first order transitions. These results agree qualitatively with experimental data in $Gd_xTh_{1-x}RU_2$.

PACS. 05.50.+q Lattice theory and statistics; Ising problems – 64.60.Cn Order disorder transformations; statistical mechanics of model systems

1 Introduction

Experimental evidence in cuprate superconductors [1] exhibit a very rich phase diagram that includes structural, antiferromagnetic, insulator-metal, superconducting and spin glass transitions, that depend strongly on the dopant concentration. The coexistence of spin glass ordering and superconductivity has been also observed in conventional superconductors doped with magnetic impurities [2]. Theoretical studies of conventional spin glass superconductors have focused in calculations of the superconducting density of states in the presence of localized magnetically ordered impurities. These systems are well described [3] by a Hamiltonian where the superconducting electrons are represented by a conventional BCS Hamiltonian and they interact with the localized magnetic impurities *via* the *s-d* exchange interaction. Theoretical studies of superconductive glass models that describe random arrays of Josephson junctions have been performed both for classical [4] and recently in a quantum model [5].

Our motivation in this paper is to study the interplay of the mechanisms that lead to spin glass ordering and BCS pair formation in a fermionic Ising spin glass model with BCS pairing among localized fermions of opposite spins. We argue in the Appendix that this effective Hamiltonian is obtained from the model of reference [3] by tracing out the degrees of freedom of the superconducting electrons to second order in the $s-d$ exchange interaction, when the localized spin operators are represented by bilinear combinations of fermions. In this case, besides the known RKKY interaction between localized spins we obtain an exchange induced pairing interaction between localized fermions, mediated by the superconducting electrons. This model allow us to investigate the competitions between frustration and double occupation of the sites in a half-filling situation.

Since the introduction of the Sherrington-Kirkpatrick [6] (SK) model to describe infinite-ranged Ising spin glasses, a vast amount of work was devoted to the study of analogous quantum spin glass (QSG) models with different and interesting low temperatures properties.

In an early seminal paper [7], Bray and Moore used Feynman's functional integrals formalism with a fictitious time $0 < \tau < \beta$, $\beta = \frac{1}{T}$, to analyze the quantum

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Heisenberg spin glass model. By using the static approximation to evaluate the spin-spin correlation functions, they established the existence of a phase transition at finite temperatures. This formalism has been extended recently to the study of quantum fluctuations in related spin glass models [8–10]. The authors in references [8,9] report on unconventional time(frequency) behaviour of the correlation functions at $T = 0$. In a remarkable later work [10] Grempel and Rozenberg found the exact numerical solution of Bray and Moore's equations [7] for $S = 1/2$, and they demonstrate the existence of an ordered spin glass phase below a finite critical temperature. Also the spin-spin correlation function $Q(\tau)$ is found to be roughly constant and equal to its classical value within a range of temperatures around the critical point, what it seems to justify the use of the static ansatz of reference [7] at not very low temperatures in the Heisenberg spin glass. Other functional integral techniques have been used earlier to study QSG models where the spin operators are represented by bilinear combinations of fermionic (anticommuting) Grassmann fields, both in the anisotropic (Ising) [11] and the isotropic (Heisenberg) [12] limits within a replica symmetric (RS) theory.

The static approximation was used, and it turned out to be exact, in the fermionic Ising model, while the fermionic Heisenberg model was solved by combining the static approximation for the order parameter with an instantaneous approximation for the retarded susceptibility.

Recent work [13] demonstrated the existence of several characteristic temperatures in both models, with the de Almeida-Thouless [14] instability occurring at a temperature T_1 lower than the spin glass transition T_{SG}. In the isotropic fermionic model [12] there exists still a lower temperature $T_2 < T_1$, at which the replica symmetry stability is restored. The region of RS instability is characterized by a negative entropy in the anisotropic [11] fermionic model, while the entropy remains positive in the isotropic model [12] but the specific heat changes sign in the RS instability region.

The anisotropic (Ising) QSG model [11,15] deserves some special discussion. In this particular case, the spin operator S_i^z commutes with the particle number operator $n_{is} = 0$ or 1, and thus it would not be necessary to employ the functional integral formulation since the Hamiltonian is diagonal in occupation number operators. However, there still remains an important difference between the fermionic and classical SK spin glass: in the quantum case the diagonal component of the order parameter in replica space is no longer constrained to unity. Consequently, the susceptibility χ emerges in the problem with an important new role and the spin glass order parameter has to be determined coupled to χ. By adding to the fermionic Ising [11,13] a term that favors BCS pairing, the use of functional integrals becomes necessary as the Hamiltonian does not commute with the particle occupation number operators.

There is a crucial aspect that characterizes the representation of spin operators in Fock space, because there are four quantum states at every site [12], two of them non-magnetic, and the quantum statistics that controls number occupation can induce unusual phase transitions. In other words, the QSG frustration can be disrupted as long as we have access with equal probability to the magnetic and the non-magnetic states at each site. In fact, a recent paper [16] has reported tricritical behaviour in the fermionic Ising QSG model, within the static approximation, by varying the electronic concentration. This raises the question if the effects that come from the relative occupation of magnetic and non-magnetic states can be properly exploited, and consequently to produce unusual phase transitions even if the average occupation per site is kept constant and equal to one. The main difference between reference [16] and ours resides in the mechanism that controls the magnetic moment formation on the sites. They achieve that by varying the electronic concentration while we have a pairing mechanism that energetically favors the double occupation and therefore non-magnetic states in the half-filling situation.

This paper is structured as follows: in Section 2 we study the model derived in the Appendix and find the thermodynamic potential, together with the saddle point equations for the order parameters. In Section 3 we discuss the nature of the phase transitions in the resulting phase diagram in the $T-g$ plane, where g is the strength of the pairing interaction, for fixed variance of the random couplings J_{ij}. Lowering the temperature, for high values of g, there is a line of second order transitions from normal to the pair formation phase, that ends at a tricritical point $T = T_3$ and $g = g_3$, characterized by the simultaneous vanishing of the two first coefficients in the Landau expansion of the free energy [17]. From there on, the line becomes one of first order transitions until it meets the line of second order spin glass transitions at $T = T_c$. For $T < T_c$ the first order transition line separates the spin glass and pair formation phases. All these results were obtained by using the static approximation. As we discussed previously, we expect this to be a justifiable ansatz because all the relevant temperatures are of the order $\beta J \approx 1$ [7], and our theory is not applicable to very low temperatures due to the de Almeida-Thouless instability.

We reserve Section 4 for discussions and comparison with other models and the experimental data [2].

2 General formulation

Conventional spin glass superconductors are well represented by a Hamiltonian where the conduction electrons are described by a BCS Hamiltonian and they interact *via* an effective $s-d$ exchange term with randomly localized magnetic impurities [3]. We show in the Appendix that, when the localized spins are represented in terms of fermions, the degrees of freedom of the superconducting electrons can be integrated using second order perturbation theory in the exchange interaction J_{sd} to give rise to an effective BCS pairing interaction among the fermions, besides the very well-known RKKY interaction among

the localized spins. In the mean field spirit we are lead to consider the following Hamiltonian:

$$\overline{H} = H - \mu N = -\sum_{ij} J_{ij} S_i^z S_j^z - \mu \sum_i \sum_{s=\uparrow,\downarrow} c_{is}^\dagger c_{is} - \frac{g}{N} \sum_{i,j} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} \quad (1)$$

where the operator S_i^z is defined as

$$S_i^z = c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}, \quad (2)$$

μ is the chemical potential, $c_{is}^\dagger$ (c_{is}) are fermions creation (destruction) operators and $s =\uparrow$ or $\downarrow$ indicates the spin projection. The coupling J_{ij} is an independent random variable with the distribution

$$P(J_{ij}) = e^{-J_{ij}^2 N/2J^2} \sqrt{N/2\pi J^2}. \quad (3)$$

The first two terms in the Hamiltonian of equation (1) describe a fermionic Ising spin glass [11,13,15] while the last term is a BCS-like pairing interaction and corresponds to the mechanism that favors the double occupation of sites [18].

Our ultimate goal is to reduce this problem to a one-site problem. Functional integration techniques have proved to be a suitable approach for disordered quantum-mechanical many-site problems, as it has been for classical problems [19]. Furthermore, this formulation showed to be quite successful to describe the usual superconductive transition with a BCS coupling [20] and in the presence of transition metal impurities [21]. In that case, the particle-hole transformation introduced by the use of Nambu matrices within the static approximation made the problem with a BCS coupling solvable, because it becomes a mean field theory in momentum and frequency space. As the static approximation is exact for the BCS problem and is also exact for the fermionic Ising glass [11,12], we expect it to give reliable interpolation results here for finite temperatures [10]. Our theory is not valid at very low temperatures due to the de Almeida-Thouless instability, then we are not concerned with the singular behaviour found at $T = 0$ in other models [8,9].

In the Lagrangian formulation [11,19,21] the partition function is expressed as

$$Z = \int D(\phi^* \phi) e^A \quad (4)$$

where the action A is given by

$$A = \int_0^\beta \left[\sum_{is} \phi_{is}^*(\tau) \frac{d}{d\tau} \phi_{is}(\tau) - \overline{H}(\phi_{is}^*(\tau), \phi_{js}(\tau)) \right] d\tau. \quad (5)$$

In both expressions $\phi_{is}^*(\tau)$ and $\phi_{is}(\tau)$ are anticommuting Grassmann variables, τ is a complex time and β the inverse absolute temperature.

In order to apply the particle-hole transformation within the static approximation and to make explicit our central approximation, we work with time Fourier transformed quantities. Therefore, the pairing part of the action becomes

$$A_{pairing} = \frac{\beta g}{N} \sum_{\Omega} \sum_{ij} \rho_i^*(\Omega) \rho_j(\Omega) \quad (6)$$

where

$$\rho_i(\Omega) = \sum_{\omega} \phi_{i\downarrow}(-\omega) \phi_{i\uparrow}(\Omega + \omega) \quad (7)$$

with Matsubara's frequencies $\omega = (2m+1)\pi$ and $\Omega = 2m\pi$, ($m = 0, \pm 1, ...$). In the static approximation, we retain just the term $\Omega = 0$ in the sum over the frequency Ω. Hence we get for $A_{pairing}$

$$A_{pairing}^{st} = \frac{\beta g}{4N} \sum_{p=1}^{2} \left[\sum_{i\omega} \underline{\psi}_i^\dagger(\omega) \underline{\sigma}_p \underline{\psi}_i(\omega) \right]^2 \quad (8)$$

where we introduced the Nambu matrices

$$\underline{\psi}_i^\dagger(\omega) = (\phi_{i\uparrow}^*(\omega) \;\; \phi_{i\downarrow}(-\omega))$$
$$\underline{\psi}_i(\omega) = \begin{pmatrix} \phi_{i\uparrow}(\omega) \\ \phi_{i\downarrow}^*(-\omega) \end{pmatrix} \quad (9)$$

and the Pauli matrices

$$\underline{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \underline{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
$$\underline{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (10)$$

The spin part of the action can also be written within the static approximation as:

$$A_{SG} = \sum_{ij} \beta J_{ij} S_i^z S_j^z \quad (11)$$

where, from equation (2),

$$S_i = \sum_{\omega} \underline{\psi}_i^\dagger(\omega) \, \underline{\psi}_i(\omega). \quad (12)$$

Finally, the free action is expressed in terms of Nambu matrices

$$A_0 = \sum_i \underline{\psi}_i^\dagger(\omega) \, \underline{G_0}^{-1}(\omega) \, \underline{\psi}_i(\omega). \quad (13)$$

where the free inverse propagator is

$$\underline{G_0^{-1}}(\omega) = \imath \, \omega + \mu \, \underline{\sigma}_3. \quad (14)$$

and the total action can be rebuild as $A = A_0 + A_{pairing}^{st} + A_{SG}$. We are now able to follow the standard procedures to get the configurational averaged thermodynamic potential by using the replica formalism

$$\Omega = -\frac{1}{\beta} \lim_{n \to 0} \frac{\langle Z^n \rangle_{ca} - 1}{n} \quad (15)$$

where the configurational averaged replicated partition function, after averaging over J_{ij}, becomes

$$Z(n) \equiv \langle Z^n \rangle_{ca} = \int D(\phi^*_\alpha, \phi_\alpha) \exp\left[\sum_{i\alpha\omega} \underline{\psi}_i^{\dagger\alpha}(\omega)\underline{G_0^{-1}}(\omega)\underline{\psi}_i^{\alpha}(\omega) + \frac{\beta g}{4N}\sum_\alpha \sum_{p=1}^{2}\left[\sum_{i\omega}\underline{\psi}_i^{\dagger\alpha}(\omega)\underline{\sigma}_p\underline{\psi}_i^{\alpha}(\omega)\right]^2 + \frac{\beta^2 J^2}{2N}\sum_{\alpha\beta}\left[\sum_i S_i^\alpha S_i^\beta\right]^2\right]. \quad (16)$$

The notation $\underline{\psi}_i^{\alpha}(\omega)$ means that a replica index $\alpha = 1, 2, ..., n$ has been associated to each matrix element. We introduce replica dependent auxiliary fields η_α and $q_{\alpha\beta}$ to linearize the action in equation (16), and get

$$Z(n) = \frac{1}{\aleph^n}\int_{-\infty}^{+\infty}\prod_{\alpha\beta} dq_{\alpha\beta}\int_{-\infty}^{+\infty}\prod_\alpha d\eta_{\alpha R} d\eta_{\alpha I} \times e^{-N\left[\frac{\beta^2 J^2}{2}\sum_{\alpha\beta} q_{\alpha\beta}^2 + \beta g\sum_\alpha \eta_\alpha^*\eta_\alpha - ln\Lambda(q_{\alpha\beta},\eta_\alpha)\right]} \quad (17)$$

where $\eta_\alpha = \eta_{\alpha R} - i\eta_{\alpha I}$, $\aleph = (\frac{2\pi}{N\beta^2 J^2})(\frac{\pi}{N\beta g})$ and

$$\Lambda(q_{\alpha\beta}, \eta_\alpha) = \int D(\phi^*_\alpha, \phi_\alpha)\exp\left[\sum_\alpha\sum_\omega \underline{\psi}^{\dagger\alpha}(\omega)\underline{G_0}^{-1}(\omega)\underline{\psi}^{\alpha}(\omega) + \beta g\sum_\alpha\sum_\omega \underline{\psi}^{\dagger\alpha}(\omega)\underline{\eta}_\alpha\underline{\psi}^{\alpha}(\omega) + \beta^2 J^2\sum_{\alpha\beta} q_{\alpha\beta} S_i^\alpha S_i^\beta\right] \quad (18)$$

while the matrix $\underline{\eta_\alpha}$ is defined as

$$\underline{\eta}_\alpha = \begin{pmatrix} 0 & \eta_\alpha \\ \eta_\alpha^* & 0 \end{pmatrix}. \quad (19)$$

We analyze the problem within the replica-symmetric ansatz

$$q_{\alpha\neq\beta} = q \quad q_{\alpha\alpha} = q + \overline{\chi} \quad \eta_\alpha(\eta_\alpha^*) = \eta(\eta^*) \quad (20)$$

where q is the spin glass order parameter and $\overline{\chi}$ is related to the static susceptibility [11] by $\overline{\chi} = \frac{\chi}{\beta}$. The complex order parameter η gives the number of particle-hole pairs of opposite spin at each site, as is obtained extremizing $Z(n)$, that is, solving $\frac{\partial}{\partial\eta}\langle Z^n\rangle = 0$ in equation (17) and the corresponding equation for η^*. This yields

$$\eta = \sum_\omega \langle \phi^*_{i\uparrow}(\omega)\phi^*_{i\downarrow}(-\omega)\rangle = \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}\rangle$$
$$\eta^* = \sum_\omega \langle \phi_{i\downarrow}(-\omega)\phi_{i\uparrow}(\omega)\rangle = \langle c_{i\downarrow} c_{i\uparrow}\rangle, \quad (21)$$

where the brackets indicate both, a statistical average and average over disorder.

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

$$\Lambda(q, \overline{\chi}, \eta) = \int_{-\infty}^{+\infty} dz \frac{e^{\frac{-z^2}{2}}}{\sqrt{2\pi}}\left[\int_{-\infty}^{+\infty} d\xi \frac{e^{\frac{-\xi^2}{2}}}{\sqrt{2\pi}} I(\xi, z)\right]^n \quad (22)$$

$$I(\xi, z) = \int D(\phi^*, \phi) e^{\sum_\omega \underline{\psi}^\dagger(\omega)\underline{G}^{-1}(\omega)\underline{\psi}(\omega)} \quad (23)$$

where the matrix $\underline{G}^{-1}(\omega)$ is given by:

$$\underline{G}^{-1}(\omega) = \begin{pmatrix} i\omega + \lambda(z,\xi) + \beta\mu & \beta g\eta \\ \beta g\eta^* & i\omega + \lambda(z,\xi) - \beta\mu \end{pmatrix} \quad (24)$$

and

$$\lambda(z, \xi) = \beta J\sqrt{2q}z + \beta J\sqrt{2\overline{\chi}}\xi. \quad (25)$$

In equation (23), the differential $D(\phi^*, \phi)$ stands for $\prod_\omega\prod_s d\phi^*_s(\omega)d\phi_s(\omega)$ and the functional integral over Grassmann variables separates into a product of integrals over exponentials of quadratic forms, that can be readily performed with the result [19]:

$$\ln I(\xi, z) = \sum_\omega \ln \mid \underline{G}^{-1} \mid = \sum_\omega \ln[(i\omega + \lambda(z,\xi))^2 - \beta^2\mu^2 - \beta^2 g^2 \mid \eta \mid^2]. \quad (26)$$

To perform the frequency sum in equation (26) one should have in mind that the Nambu formalism introduces a particle-hole transformation in the fermions of spin down. Then from equation (14, 16) we have that

$$\frac{1}{N}\frac{\partial\Omega}{\partial\mu} = \langle c^\dagger_\uparrow c_\uparrow\rangle - \langle c_\downarrow c^\dagger_\downarrow\rangle = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle - 1, \quad (27)$$

and the converging factors in the frequency sums should be adjusted to these prescriptions, with the result

$$I(\xi, z) = \cosh(\lambda(z,\xi)) + \cosh(\beta\mu') \quad (28)$$

where

$$\mu' = \sqrt{\mu^2 + g^2\eta^2}. \quad (29)$$

Not giving rise to confusion, from now on we write η in place of $|\eta|$. Introducing equation (28) in equation (22) and using equation (17) we finally obtain for the thermodynamic potential in equation (15) at the saddle point:

$$\frac{\beta\Omega}{N} = \frac{1}{2}\beta^2 J^2\overline{\chi}(2q + \overline{\chi}) + \beta g\eta^2 - \int_{-\infty}^{+\infty} Dz \ln\left[e^{\beta^2 J^2\overline{\chi}}\cosh(\beta J\sqrt{2q}z) + \cosh(\beta\mu')\right]. \quad (30)$$

where $Dz = dz\frac{e^{\frac{-z^2}{2}}}{\sqrt{2\pi}}$. We want, on the average, to insure the half-filling situation of one-electron per site, thus fixing $\mu = 0$ in equations (28, 30). The saddle point equations

for the order parameters that follow from equation (30) are:

$$\overline{\chi} = \int Dz \frac{\cosh(\beta J\sqrt{2q}z)}{\cosh(\beta J\sqrt{2q}z) + e^{(-\beta^2 J^2 \overline{\chi})}\cosh(\beta g\eta)} - q \tag{31}$$

$$q = \int Dz \frac{\sinh^2(\beta J\sqrt{2q}z)}{[\cosh(\beta J\sqrt{2q}z) + e^{(-\beta^2 J^2 \overline{\chi})}\cosh(\beta g\eta)]^2} \tag{32}$$

$$\eta = \frac{1}{2}\int Dz \frac{e^{(-\beta^2 J^2 \overline{\chi})}\sinh(\beta g\eta)}{\cosh(\beta J\sqrt{2q}z) + e^{(-\beta^2 J^2 \overline{\chi})}\cosh(\beta g\eta)} \cdot \tag{33}$$

The replica symmetric solution described here is unstable at low temperatures, when the de Almeida-Thouless [14] eigenvalue λ_{AT} becomes negative. The calculation of λ_{AT} in this model follows as in a previous work [13], with the result:

$$\lambda_{AT} = 1 - \beta^2 J^2 \times \int_{-\infty}^{\infty} Dz \frac{[1 + e^{(-\beta^2 J^2 \overline{\chi})}\cosh(\beta g\eta)\cosh(\beta J\sqrt{2q}z)]^2}{[e^{(-\beta^2 J^2 \overline{\chi})}\cosh(\beta g\eta) + \cosh(\beta J\sqrt{2q}z)]^4}. \tag{34}$$

For the entropy we obtain:

$$\frac{S}{K} = \frac{-3}{2}\beta^2 J^2 \overline{\chi}(2q + \overline{\chi}) - 2\beta g\eta^2 + \int_{-\infty}^{+\infty} Dz \ln[e^{\beta^2 J^2 \overline{\chi}}\cosh(\beta J\sqrt{2q}z) + \cosh(\beta g\eta)]. \tag{35}$$

We show in Figure 5 the behaviour of λ_{AT} and S/K as a function of the temperature for a value of $g > g_c$. We observe a discontinuity in the derivative of the entropy from the normal to pairing phase typical of the second order transition. For lower temperatures λ_{AT} and S/K become negative due to replica symmetry breaking.

A detailed discussion of the numerical solutions of the saddle point equations, as well as the Landau expansion of the thermodynamic potential in equation (30) in powers of order parameters q and η is performed in Section 3.

3 Phase diagram and tricritical point

The numerical analysis of the equations for the order parameters q, η and $\overline{\chi}$ in equations (31–33) allow us to build a phase diagram (temperature *versus* pairing coupling g) where three regions can be identified (see Fig. 1):

i) For high T and small g, we get a normal phase with no long range order where $q = 0$ and $\eta = 0$.
ii) Enhancing the pairing coupling g, one gets a phase transition at $g = g_c(T)$ where there is a new order corresponding to the spin pairing on the sites. In terms of the order parameters, that means $\eta \neq 0$ while $q = 0$.
iii) As one lowers the temperature, for $g < g_c(T_c)$, the model exhibits a phase transition at $T = T_c$ where q starts to grow continuously but with η still equal to zero as shown in Figure 2. The behaviour of the order parameter q and the susceptibility $\chi = \beta\overline{\chi}$ shows a second order transition from a normal phase to a spin glass phase. Actually, that situation has been already analysed in [11] where an expansion of equations (31, 32) in powers of q for $\eta = 0$ gives $T_c = 0.9570J$.

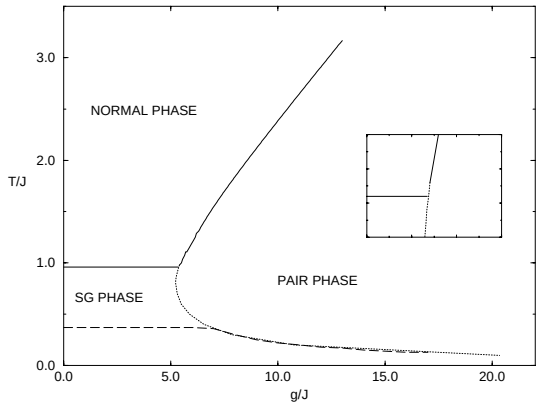

Fig. 1. Phase diagram as function of temperature and pairing coupling g/J. Solid lines indicate second order transitions while the dotted line indicates a first order transition. The tricritical point T_3, g_3 is shown in detail in the diagram. The points where λ_{AT} becomes negative are represented by the dashed line.

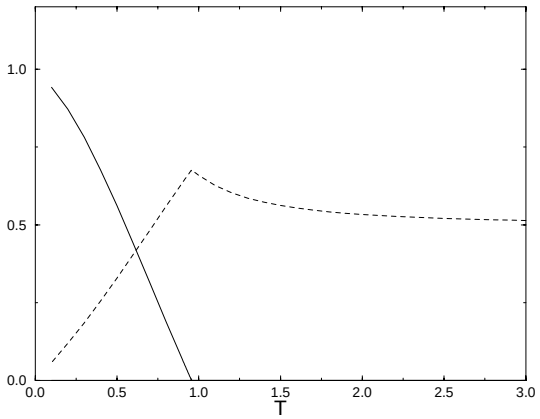

Fig. 2. Temperature behaviour of q (solid line), and $\overline{\chi} = \frac{\chi}{\beta}$ (dashed line) for $g = 0.5J < g_c$. Here $\eta = 0$.

The nature of the transition line given by the equation $g = g_c(T)$ is far more complex. If $T > T_c$, the numerical analysis shows that η grows continuously from zero as one crosses the transition line (see Fig. 3). This result suggests that we get a second order transition. However, when $T < T_c$, the numerical solution of the order parameter in Figure 4 seems to indicate that the transition line becomes first order at some point. To investigate this question further we perform a Landau expansion [22] of the thermodynamic potential $\beta\Omega$ in equation (30) in powers of the two order parameters η and q, that define the symmetries of the pairing and the spin glass phases, while $\overline{\chi}$ is taken at the saddle-point value in equation (31). We find it is more convenient to start expanding in powers

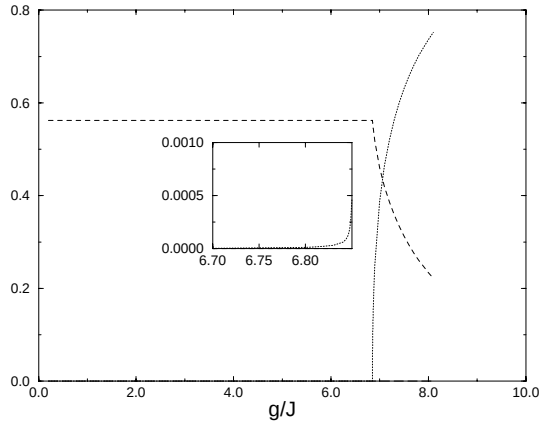

Fig. 3. Dependence of the order parameter η (dotted line) and the parameter $\overline{\chi}$ (dashed line) with the coupling g/J for $T > T_c$, where $T = 1.5J$. We show in detail the continuous behaviour of η around g_c.

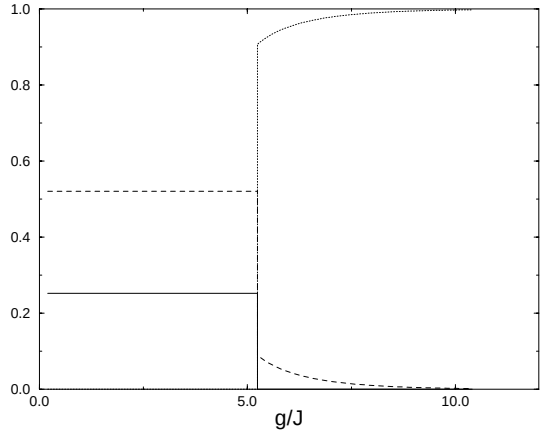

Fig. 4. Dependence of the order parameters η (dotted line), q (solid line), and the parameter $\overline{\chi}$ (dashed line) with the coupling g/J for $T < T_c$, where $T = 0.75J$. At the transition point both η and q have discontinuous behaviour indicating a first order transition.

of q and we write from equation (30):

$$\beta\Omega = \sum_{k=0}^{3} f_k(\eta, \overline{\chi}, T) q^k \tag{36}$$

where $\overline{\chi}(q, \eta, T)$ is the solution of the saddle point equation

$$\sum_{k=0}^{3} \frac{\partial}{\partial \overline{\chi}} f_k(\eta, \overline{\chi}, T) q^k = 0. \tag{37}$$

We look for a solution of equation (37) also in the form of a series

$$\overline{\chi} = \overline{\chi}_0 + \overline{\chi}_1 q + \overline{\chi}_2 q^2 \tag{38}$$

with the result that $\overline{\chi}_0$ is given by

$$\frac{1}{\beta^2 J^2} \frac{\partial}{\partial \overline{\chi}} f_0(\eta, \overline{\chi}_0, T) = \overline{\chi}_0 - \frac{1}{D} = 0 \tag{39}$$

where

$$D = 1 + e^{(-\beta^2 J^2 \overline{\chi}_0)} \cosh(\beta g \eta) \tag{40}$$

and

$$\overline{\chi}_1 = -\left[\left(\frac{\partial}{\partial \overline{\chi}} f_1\right)\left(\frac{\partial^2}{\partial \overline{\chi}^2} f_0\right)^{-1}\right]_{\eta, \overline{\chi}_0, T}, \tag{41}$$

$$\overline{\chi}_2 = -\left[\left(\frac{\partial}{\partial \overline{\chi}} f_2 + \overline{\chi}_1 \frac{\partial^2}{\partial \overline{\chi}^2} f_1 + \frac{1}{2}\overline{\chi}_1^2 \frac{\partial^3}{\partial \overline{\chi}^3} f_0\right) \times \left(\frac{\partial^2}{\partial \overline{\chi}^2} f_0\right)^{-1}\right)\Bigg]_{\eta, \overline{\chi}_0, T}. \tag{42}$$

Introducing equation (38) into equation (36) by expanding the f_k's in powers of q, we finally obtain after some lengthy calculations the compact result:

$$\beta\Omega = \frac{\beta^2 J^2 \overline{\chi}_0^2}{2} - \ln(e^{\beta^2 J^2 \overline{\chi}_0} + 1) + A_1 \eta^2 + A_2 \eta^4 + A_3 \eta^6 - B_1 q^2 - B_2 q^3 \tag{43}$$

where

$$A_1 = \frac{1}{2!}(\beta g)^2 \left[\frac{2}{\beta g} - \frac{1}{\tilde{D}_0}\right],$$

$$A_2 = \frac{1}{4!}(\beta g)^4 \left[\frac{3}{\tilde{D}_0^2} - \frac{1}{\tilde{D}_0}\right], \tag{44}$$

$$A_3 = \frac{1}{6!}(\beta g)^6 \left[-\frac{1}{\tilde{D}_0} + \frac{15}{\tilde{D}_0^2} - \frac{30}{\tilde{D}_0^3}\right],$$

$$B_1 = \beta^4 J^4 \left[\frac{1}{2\beta^2 J^2} - \frac{1}{D_0^2}\right]$$

$$B_2 = \frac{2}{3}\frac{\beta^6 J^6}{D_0^3}(3D_0 + 1). \tag{45}$$

$$\tilde{D}_0 = e^{\beta^2 J^2 \overline{\chi}_0} D_0 = e^{\beta^2 J^2 \overline{\chi}_0} + 1. \tag{46}$$

First we notice that the correct solution of equation (37) implies the exact cancelation of the term linear in q in $\beta\Omega$. The order parameter η and q minimize and maximize [6], respectively, $\beta\Omega$ in equation (43). We obtain then that the normal paramagnetic phase is characterized by $A_1 > 0$, $B_1 > 0$; the spin glass phase with $q \neq 0$, $\eta = 0$ by $A_1 > 0$, $B_1 < 0$; and the pairing phase with $q = 0$, $\eta \neq 0$ by $A_1 < 0$, $B_1 > 0$. Lowering the temperature for small values of g, B_1 changes sign first at $T_c = 0.9570J$ and as $B_2 > 0$ this is a second order transition line from paramagnetic to spin glass phase that was analyzed in detail elsewhere [11]. For $g > g_c(T)$ and $T > T_c$ we have $A_1 < 0$, $B_1 > 0$, and the line $A_1 = g - g_c(T) = 0$ is a second order transition line if $A_2 > 0$. A quick glance at A_2 shows that it is positive at high temperatures and negative at low temperatures, then we identify the point g_3, T_3 where $A_1 = A_2 = 0$ as a tricritical point, in agreement with the known criteria [13]. At this point, a line of second order transitions becomes a first order transition line. From equations (39, 43) we obtain $T_3 = 0.9807J$, $g_3 = 5.8843J$. The expansion of A_1 around the tricritical point gives for the critical line:

$$A_1 = -0.0566(g - g_3) + 0.02575(T - T_3) = 0 \tag{47}$$

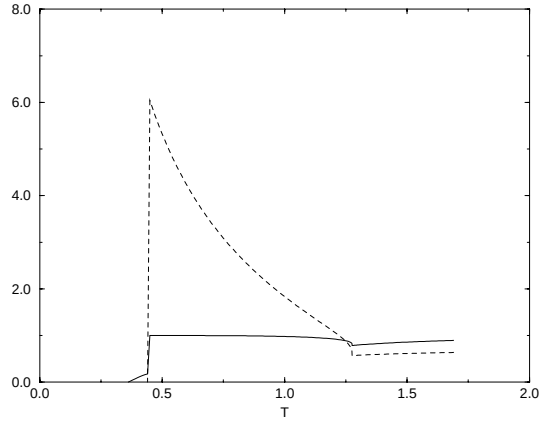

Fig. 5. The Almeida-Thouless eigenvalue (solid line) and entropy (dashed line) for $g = 6.2J$.

and $\eta \approx (T_P - T)^{1/2}$ for $T_3 < T < T_P$, where $T_P = T_3 + 2.2(g - g_3)$. For $T < T_3$ and $g < g_3$, the transition from the pairing to the spin glass phase becomes a first order transition. Tricritical behaviour has been found previously [16] in the fermionic Ising spin glass model with charge fluctuation, and a discussion of the relation between this model and ours is left for Section 4.

We show in Figure 5 the behaviour of λ_{AT} and S/K as a function of the temperature for a value of $g > g_c$. We observe a discontinuity in the derivative of the entropy from the normal to pairing phase typical of the second order transition. For lower temperatures λ_{AT} and S/K become negative due to replica symmetry breaking.

4 Conclusions

We study in this paper the interplay of the mechanisms that leads to spin glass ordering and BCS pair formation in a soluble mean field model Hamiltonian for a fermionic quantum spin glass with a BCS pairing between local fermions. As we show in the Appendix, this model would describe the spin dynamics of a superconductive spin glass [2,3] and allow us to study the role of the pairing mechanism as control of the site occupation and the local moment formation. Comparing our results with previous work that exhibit tricriticality [15,16], we can see that the pairing order parameter η enters in an effective chemical potential μ' in equation (29), and our equations would reduce to theirs if we make $g = 0$, $\mu \neq 0$. As we are insuring here half-filling on the average, we get $\mu' = g\eta$ and by varying g we change the site occupation by favouring doubly occupied states.

As a result we obtain the phase diagram in Figure 1 where we observe a normal paramagnetic (NP) phase at high temperatures with $q = \eta = 0$. By lowering the temperature for $g < g_c(T_c)$ we encounter a second order transition line from the NP phase to the SG (spin glass) phase at $T_c = 0.9570J$. For $g > g_c(T_c)$ the second order transition is from the NP phase to the PAIR (pairing formation) phase if $T_3 < T < T_P(g)$. At $T = T_3$, $g = g_3$ there is a tricritical point where the pairing transition becomes first order. This point is almost indistinguishable in Figure 1 from the point $T = T_c$, $g = g_c$. For $T < T_c$ the line $g_c(T)$ becomes a first order transition line separating the SG and PAIR phases. The phase diagram obtained in Figure 1 is in good qualitative agreement with the experimental results of reference [2] for $Gd_xTh_{1-x}RU_2$ samples, by assuming that the ratio J/g is proportional to the Gd concentration. This assumption is reasonable, as we show in the Appendix that the effective value of g is proportional to the number of superconductive pairs, that for a given temperature decreases drastically with the concentration of magnetic impurities, leading to an increase in J/g.

To conclude, we studied a model for a fermionic SK spin glass with BCS pairing among the local fermions that is soluble by reduction to a one site problem. Although this model originates in the description of the spin dynamics of conventional spin glass superconductors, we hope that these results may be also relevant for the study of strongly correlated fermions systems through the localized one site approximations [23]. It is possible to extend the analysis of reference [10] for the study of the time correlation functions in the present problem, but it will be the subject of a future work.

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Appendix

Conventional spin glass superconductors are usually represented by a system of conduction electrons with BCS coupling interacting with localized spins [3]. Using Gorkov's decoupling scheme the Hamiltonian is:

$$\overline{H}_{alloy} = \sum_{ks}(\epsilon_k - \mu)a^\dagger_{ks}a_{ks} - \sum_k [\Delta_k a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow} + \Delta^\dagger_k a_{-k\downarrow}a_{k\uparrow}] - J_{sd}\sum_i \mathbf{S}_i.\mathbf{s}_i \tag{A.1}$$

where $\mathbf{S}_i$ is the magnetic moment localized at the random site $\mathbf{R}_i$ and $\mathbf{s}_i$ is the local spin density of the conduction electrons

$$\mathbf{s}_i = \sum_{kk'}\sum_{ss'} e^{i(\mathbf{k}-\mathbf{k}').\mathbf{R}_i} a^\dagger_{ks}\sigma_{ss'}a_{k's'}, \tag{A.2}$$

where $\sigma_{ss'}$ indicates the elements of the vector Pauli matrices and $a^\dagger_{ks}(a_{ks})$ are the usual creation (annihilation) operators for superconducting electrons. The order parameters Δ_k, $\Delta^\dagger_k$ are to be determined self-consistently from

the equations of motion, but here we consider them to be phenomenological parameters. In this paper we choose to represent the localized moments by a bilinear combination of fermion operators [12]

$$\mathbf{S}_i = \sum_{ss'} c_{is}^\dagger \sigma_{ss'} c_{is'} \tag{A.3}$$

as we did in equation (2).

The partition function for the superconducting alloy may be written in terms of functional integrals as we did in equations (4, 5):

$$Z_{alloy} = \int \prod_{is} D(\phi_{is}^*, \phi_{is}) \int \prod_{ks} D(\phi_{ks}^*, \phi_{ks}) e^{A_{alloy}} \tag{A.4}$$

where the action is now given by

$$A_{alloy} = \int_0^\beta \left[\sum_{is} \phi_{is}^*(\tau) \frac{d}{d\tau} \phi_{is}(\tau) + \sum_{ks} \phi_{ks}^*(\tau) \frac{d}{d\tau} \phi_{ks}(\tau) - H_{alloy}(\phi^*(\tau), \phi(\tau)] \, d\tau \right] \tag{A.5}$$

and we introduced the Grassmann fields ϕ_{ks}^*, ϕ_{ks} for the conducting band. Using the Nambu formalism as we did in Section 2 we may write the partition function

$$Z_{alloy} = \int \prod_{is} D(\phi_{is}^*, \phi_{is}) e^{A_0} \int \prod_{ks} D(\phi_{ks}^*, \phi_{ks}) e^{A_{BCS} + A_{sd}} \tag{A.6}$$

where A_0 is the action for non-interacting fermions given in equation (13) and A_{BCS} is the action for the superconducting electrons:

$$A_{BCS} = \sum_{k\omega} \underline{\psi}_k^\dagger(\omega) \underline{G_k}^{-1}(\omega) \underline{\psi}_k(\omega) \tag{A.7}$$

where similarly to equations (9, 24)

$$\underline{\psi}_k^\dagger(\omega) = (\phi_{k\uparrow}^*(\omega) \;\; \phi_{-k\downarrow}(-\omega)) \quad \underline{\psi}_k(\omega) = \begin{pmatrix} \phi_{k\uparrow}(\omega) \\ \phi_{-k\downarrow}^*(-\omega) \end{pmatrix} \tag{A.8}$$

$$\underline{G}_k^{-1}(\omega) = \begin{pmatrix} i\omega - \beta(\epsilon_k - \mu) & \beta\Delta_k \\ \beta\Delta_k^* & i\omega + \beta(\epsilon_k - \mu) \end{pmatrix}. \tag{A.9}$$

The $s-d$ exchange part of the action is given by

$$A_{sd} = -J_{sd}\beta \sum_i \sum_\Omega \mathbf{S}_i(-\Omega).\mathbf{s}_i(\Omega) \tag{A.10}$$

where from equations (A.2, A.3)

$$\mathbf{S}_i(\Omega) = \sum_{ss'} \sum_\omega \phi_{is}^*(\omega + \Omega) \sigma_{ss'} \phi_{is'}(\omega) \tag{A.11}$$

$$\mathbf{s}_i(\Omega) = \sum_{ss'} \sum_{kk'} \sum_\omega e^{i(\mathbf{k}-\mathbf{k}').\mathbf{R}_i} \phi_{ks}^*(\omega + \Omega) \sigma_{ss'} \phi_{k's'}(\omega). \tag{A.12}$$

We indicate by $\omega = (2n+1)\pi$ and $\Omega = 2n\pi$ the fermionic and bosonic Matsubara frequencies, respectively. When we are interested in the localized spins dynamics, the conduction electrons degrees of freedom in equation (A.6) may be integrated out to second order perturbation theory in J_{sd} to give the result:

$$Z_{alloy} = \int \prod_{is} D(\phi_{is}^*, \phi_{is}) e^{A_0 + A_{eff}(\phi_{is}^*, \phi_{is})} \tag{A.13}$$

where

$$A_{eff}(\phi_{is}^*, \phi_{is}) = -\frac{1}{2}(\beta J_{sd})^2 \sum_{\Omega\alpha\beta} \sum_{ij} V_{ij}^{\alpha\beta}(\Omega) S_i^\alpha(\Omega) S_j^\beta(-\Omega) - \frac{1}{2}(\beta J_{sd})^2 \sum_\Omega \sum_{ij} W_{ij}(\Omega) [S_i^+(\Omega) S_j^-(\Omega) + S_i^-(\Omega) S_j^+(-\Omega)] \tag{A.14}$$

and the dynamic interactions $V_{ij}^{\alpha\beta}(\Omega)$, $W_{ij}(\Omega)$ are obtained from the correlation functions $\langle S_i^\alpha(\Omega) S_j^\beta(-\Omega)\rangle$. By performing the frequency sums as indicated in Section 2 and approximating $\Delta_k \approx \Delta$, we obtain for the static part with $\Omega = 0$:

$$V_{ij}^{\alpha\beta}(0) = \delta_{\alpha\beta} \sum_{\mathbf{q}} e^{i\mathbf{q}.(\mathbf{R}_i - \mathbf{R}_j)} \frac{1}{\beta} \sum_{\mathbf{k}} \frac{n(\mathbf{k}+\mathbf{q}) - n(\mathbf{k})}{\epsilon(\mathbf{k}+\mathbf{q}) - \epsilon(\mathbf{k})} \tag{A.15}$$

$$W_{ij}(0) = \frac{|\Delta|}{\beta} \sum_{\mathbf{q}} e^{i\mathbf{q}.(\mathbf{R}_i - \mathbf{R}_j)} \sum_{\mathbf{k}} \frac{B(\mathbf{k}) - B(\mathbf{k}+\mathbf{q})}{E^2(\mathbf{k}+\mathbf{q}) - E^2(\mathbf{k})} \tag{A.16}$$

where

$$n(\mathbf{q}) = [1 + e^{\beta(\epsilon(\mathbf{q}) - \mu)}]^{-1}$$
$$B(\mathbf{k}) = \frac{|\Delta|}{2E(\mathbf{k})} \tanh\left(\frac{\beta E(\mathbf{k})}{2}\right)$$
$$E(\mathbf{k}) = [(\epsilon(\mathbf{k}) - \mu)^2 + |\Delta|^2]^{\frac{1}{2}}. \tag{A.17}$$

The effective interaction V_{ij} in equation (A.15) was calculated to lowest order in $|\Delta|$ and it represents the familiar RKKY interaction [24] that is responsible for spin glass ordering. The interaction W_{ij} is of a different character and it represents the coupling induced by the exchange of superconducting electrons. The function $B(\mathbf{k})$ is the matrix element [25] of the pairing operator $c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger$, and since pairing interactions smooth out the jump in the single particle occupation number $n(\mathbf{k})$ we can approximate $B(\mathbf{k}) = \frac{|\Delta|}{2E(\mathbf{k})}$ at low temperatures, what gives in equation (A.16)

$$W_{ij}(0) \approx \frac{1}{2\beta} \sum_{\mathbf{q}} e^{i\mathbf{q}.(\mathbf{R}_i - \mathbf{R}_j)} \sum_{\mathbf{k}} \frac{|\Delta|^2}{E(\mathbf{k}+\mathbf{q}) E(\mathbf{k})} \times \left[\frac{1}{E(\mathbf{k}+\mathbf{q}) + E(\mathbf{k})}\right]. \tag{A.18}$$

As the last sum in equation (A.18) is very weakly dependent on $\mathbf{q}$ it can be approximated by its value when $q = 0$, what gives

$$W_{ij}(0) \approx \frac{1}{4\beta} \sum_{\mathbf{k}} \frac{|\Delta|^2}{E^3(\mathbf{k})} \delta_{ij}. \tag{A.19}$$

Introducing equations (A.15, A.19) in equation (A.14) we obtain for the static part of the interaction

$$A^{st}_{eff}(\phi^*_{is}, \phi_{is}) \approx -\sum_{ij} J_{ij}(RKKY)\mathbf{S}_i(0).\mathbf{S}_j(0) - g\sum_i S^+_i(0)S^-_i(0). \tag{A.20}$$

We argue that the last term in equation (A.20) is the static part of the action corresponding to the Hamiltonian $H_I = g\sum_i c^\dagger_{i\uparrow}c_{i\downarrow}c^\dagger_{i\downarrow}c_{i\uparrow}$ that within Gorkov's formalism would give rise to terms $-g[\Delta^\dagger_l \sum_i c_{i\downarrow}c_{i\uparrow} + \Delta_l \sum_i c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}]$, what ultimately justifies our choice of Hamiltonian in equation (1).

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