Quantum critical effects in mean-field glassy systems

Felix Ritort

Institute of Theoretical Physics
University of Amsterdam
Valckenierstraat 65
1018 XE Amsterdam (The Netherlands).
E-Mail: ritort@phys.uva.nl
(March 23, 2022)

Abstract

We consider the effects of quantum fluctuations in mean-field quantum spin-glass models with pairwise interactions. We examine the nature of the quantum glass transition at zero temperature in a transverse field. In models (such as the random orthogonal model) where the classical phase transition is discontinuous an analysis using the static approximation reveals that the transition becomes continuous at zero temperature.

64.70.Nr, 64.60.Cn
Spin glasses are models which deserve considerable interest [1]. In these systems the presence of randomness and frustration can yield very rich behaviour. In particular, there is much current interest in the behaviour of glassy systems in the presence of quantum fluctuations where the nature of the zero-temperature phase transition is driven by the competition between randomness and quantum effects rather than thermal fluctuations [2]. This makes the order-disorder transition in quantum glasses belong to a new universality class.

Much work has been devoted to the study of mean-field quantum spin glass models. In particular, attention has been paid to models with a continuous transition in the Edwards-Anderson order parameter. The simplest example in these class of models is the Sherrington-Kirkpatrick (SK) model [3] in a transverse field. In this system the critical temperature is depressed when the transverse field is switched on and vanishes for a critical value of the field [4–7]. Analytical work in the quantum SK model reveals that replica symmetry is broken in the quantum glass phase at zero temperature [8]. This is an indication that quantum fluctuations do not destroy one of the most interesting features in glassy systems, that is the coexistence of a large number of phases or states.

There has been also much recent interest in the study of classical spin-glass models with a discontinuous transition in the order parameter. These models are characterised by the existence of a dynamical singularity at a temperature above the static transition [9]. Concerning the statical and dynamical behaviour these models are very good candidates for describing real glasses [10]. On the one hand, the statics gives a natural explanation for the existence of a thermodynamic ideal glass transition driven by an entropy collapse. On the other hand, the dynamics of these mean-field models are described by the mode coupling equations introduced to describe relaxational phenomena in glasses [9–11]. In mean-field models metastable states have an infinite lifetime, hence dynamics is frozen at the dynamical singularity well above the static transition temperature. Below the dynamical transition temperature the system gets trapped in states with have larger energy than the equilibrium one [12]. All these features are absent in models with a continuous transition.
The purpose of this letter is the study of models with a discontinuous transition in the presence of quantum fluctuations at zero temperature. The motivation is twofold. Concerning the statics we note that the transition cannot be driven in the quantum case by an entropy collapse. The reason is that the entropy vanishes everywhere at zero temperature. Concerning the dynamics we can also expect a quite different behaviour from the classical case. In macroscopic quantum systems at $T = 0$ the dynamics is governed by the Schröedinger equation and there is no room for any kind of thermal activated processes. It could well be that trapping dynamics in the metastable glassy phase are considerably modified or even suppressed in the presence of quantum fluctuation effects.

The main conclusion of this work is that the glassy scenario presented before is indeed suppressed by quantum fluctuations in a certain class of spin-glass models. We will provide a general proof for this statement within the static approximation [4]. In models where the classical transition is continuous it remains continuous at zero temperature.

The family of models we are interested in are quantum Ising spin glasses with pairwise interactions in the presence of transverse field. These are described by the Hamiltonian,

$$\mathcal{H} = - \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$$

where $\sigma_i^z, \sigma_i^x$ are the Pauli spin matrices and $\Gamma$ is the the transverse field. The indices $i, j$ run from 1 to $N$ where $N$ is the number of sites. The $J_{ij}$ are the couplings taken from an ensemble of random symmetric matrices. In the case that the $J_{ij}$ are independent Gaussian variables this Hamiltonian reduces to the quantum $SK$ model [2] in a transverse field. If the $J_{ij}$ are orthogonal matrices then eq.(1) reduces to the random orthogonal model ($ROM$) [13] in a transverse field. At zero transverse field the models become classical and display quite different behaviour. The $SK$ model has a continuous finite temperature transition without jump in the Edwards-Anderson order parameter [1] while the $ROM$ presents a strong discontinuous transition where the Edwards-Anderson order parameter jumps to a value close to 1 at the transition temperature [13].

In order to solve model (1) we apply the Trotter-Suzuki decomposition [14] and rewrite
the Hamiltonian in terms of classical spins with an extra imaginary time dimension,

\[ H_{\text{eff}} = A \sum_{i<j} J_{ij} \sum_{t} \sigma_{i}^{t} \sigma_{j}^{t} + B \sum_{it} \sigma_{i}^{t} \sigma_{i+1}^{t} + C \]  

(2)

where the time index \( t \) runs from 1 to \( M \) and the spins \( \sigma_{i}^{t} \) take the values \( \pm 1 \). The constants \( A, B \) and \( C \) are given by

\[ A = \beta M; \quad B = \frac{1}{2} \log(\coth(\frac{\beta \Gamma}{M})); \quad C = \frac{MN}{2} \log(\frac{1}{2} \sinh(\frac{2\beta \Gamma}{M})). \]

Now we apply the replica trick and compute the average over the disorder of the replicated partition function,

\[ \mathcal{Z}_{J}^{n} = \int [dJ] \sum_{\{\sigma_{i}^{t}\}} \exp(\sum_{a=1}^{n} H_{a}^{\text{eff}}) \]  

(3)

where \( \int [dJ] \) means integration over the random ensemble of matrices. This integral can be done using known methods in matrix theory [13,13]. The final result of eq. (3) can be written in terms of a generating function \( G(x) \) which depends on the particular ensemble of \( J_{ij} \) couplings via its spectrum of eigenvalues. For the two examples we will consider in this paper we have \( G_{SK}(x) = \frac{2x^{2}}{2} \) (SK model) and \( G_{ROM}(x) = \frac{1}{2} \log(\frac{1+4x^{2}}{2x^{2}} - \frac{1}{2}) \) (ROM model). From (3) we get,

\[ \mathcal{Z}_{J}^{n} = \int dQ d\Lambda \exp(-NF(Q, \Lambda)) \]  

(4)

where

\[ F(Q, \Lambda) = -\frac{nC}{N} + \frac{1}{M^{2}} \text{Tr}(QA) - \frac{1}{2} \text{Tr}G(AQ) - \log(H(\Lambda)) \]  

(5)

with \( Q_{ab}^{tt'}, \Lambda_{ab}^{tt'} \) being the order parameter and the trace \( \text{Tr} \) is done over the replica and time indices. The term \( H(\Lambda) \) is given by,

\[ H(\Lambda) = \sum_{\sigma} \exp(\sum_{ab} \frac{1}{M^{2}} \sum_{tt'} \Lambda_{ab}^{tt'} \sigma_{a}^{t} \sigma_{b}^{t'} + B \sum_{a} \sigma_{a}^{t} \sigma_{a}^{t+1}) \]  

(6)

and the free energy is obtained by making the analytic continuation \( \beta f = \lim_{n \to 0} \frac{F(Q^{*}, \Lambda^{*})}{n} \)

where \( Q^{*}, \Lambda^{*} \) are solutions of the saddle point equations, \( \Lambda_{ab}^{tt'} = \frac{AM^{2}}{2} \left(G^{t'}(AQ)\right)_{ab}^{tt'} \) and \( Q_{ab}^{tt'} = \langle \sigma_{a}^{t} \sigma_{b}^{t'} \rangle \). The average \( \langle (\cdot) \rangle \) is done over the effective Hamiltonian in (6). We assume that the order parameters \( Q_{ab}^{tt'}, \Lambda_{ab}^{tt'} \) are independent of the time indices when \( a \neq b \) but they are only
translational time invariant if \( a = b \). To study the high-temperature phase and the phase boundary of the model we consider a general one step replica symmetry breaking solution. We divide the \( n \) replicas into \( n/m \) boxes \( K \) of size \( m \) such that \( m \) divides \( n \). The saddle point solution when \( a \neq b \) takes the form \( Q_{ab}^{\mu'} = q; \Lambda_{ab}^{\mu'} = \lambda \) if \( a, b \in K \) and \( Q_{ab}^{\mu'} = \Lambda_{ab}^{\mu'} = 0 \) otherwise. For \( a = b \) we take \( Q_{aa}^{\mu'} = R_{|t-t'|}, \Lambda_{aa}^{\mu'} = \Lambda_{|t-t'|} \). Going to the frequency space we define \( \hat{R}_p = M^{-1} \sum_{l=0}^{M-1} e^{i\omega_p l} R_l, \hat{\Lambda}_p = M^{-1} \sum_{l=0}^{M-1} e^{i\omega_p l} \Lambda_l \) and \( \hat{\sigma}_p = M^{-1} \sum_{l=0}^{M-1} e^{i\omega_p l} \sigma_{t+1} \) where \( \omega_p = \frac{2\pi p}{M} \). The free energy (f) is given by,

\[
\beta f = -\frac{C}{N} + \sum_{p=0}^{M-1} \hat{R}_p \hat{\Lambda}_p^* + (m-1)q\lambda - \frac{1}{2} \sum_{p=0}^{M-1} G(\beta \hat{R}_p) - \frac{1}{2m} G\left(\beta(\hat{R}_0 + (m-1)q)\right) - \frac{m-1}{2m} G\left(\beta(\hat{R}_0 - q)\right) + \frac{1}{2} G\left(\beta \hat{R}_0\right) - \frac{1}{m} \log \int_{-\infty}^{\infty} dp(x) \Xi^m(x) \tag{7}
\]

where \( dp(x) = (2\pi)^{-\frac{d}{2}} e^{-\frac{x^2}{2}} dx \) is the Gaussian measure and \( \Xi(x) = \sum_{\sigma_p} \exp(\Theta(\hat{\sigma}_p, x)) \) with

\[
\Theta(\hat{\sigma}_p, x) = \sum_{p=0}^{M-1} \left(\hat{\Lambda}_p + MB e^{-i\omega_p}\right)|\hat{\sigma}_p|^2 + (2\lambda)^\frac{1}{2} x \hat{\sigma}_0 - \lambda \hat{\sigma}_0^2 . \tag{8}
\]

In order to investigate the glassy scenario we compute the static and dynamical transition temperatures. Following [16] we expand the free energy (f) around \( m = 1, f = f_0 + (m-1)f_1 + O((m-1)^2) \) and determine the paramagnetic free energy \( f_0 \) and the correction \( f_1 \). We get,

\[
\beta f_0 = -\frac{C}{N} + \sum_p \hat{R}_p \hat{\Lambda}_p^* - \frac{1}{2} \sum_p G(\beta \hat{R}_p) - I(\hat{\Lambda}) \tag{9}
\]

\[
\beta f_1 = q\lambda - \frac{\beta q}{2} G'(\beta \hat{R}_0) + \frac{1}{2} G(\beta \hat{R}_0) - \frac{1}{2} G\left(\beta(\hat{R}_0 - q)\right) + I(\hat{\Lambda}) - \exp\left(-I(\hat{\Lambda})\right) \int dp(x) \Xi(x) \log(\Xi(x)) \tag{10}
\]

where \( I(\hat{\Lambda}) = \log(\Xi(\lambda = 0)) \). Note that \( f_0 \) does not depend on \( q \) and \( \lambda \) as expected for the paramagnetic part of the free energy. The static and dynamical transition are obtained by solving the saddle point equations \( \frac{\partial f_1}{\partial q} = \frac{\partial f_1}{\partial \lambda} = 0 \). The static transition appears when the free energy \( f \) coincides with the paramagnetic free energy \( f_0 \), i.e. \( f_1 = 0 \). The dynamical transition is given by the presence of a soft mode above the static transition and is obtained by solving the equation \( \left(\frac{\partial^2 f_1}{\partial q^2}\right)\left(\frac{\partial^2 f_1}{\partial \lambda^2}\right) - \left(\frac{\partial^2 f_1}{\partial q \partial \lambda}\right)^2 = 0 \).
The solution to these equations yields the critical temperature and the value of the jump of the order parameter \( q \) at the transition. In case the dynamical and the static transition coincide it can be shown that \( q = \lambda = 0 \) and the transition is continuous in the order parameter. These three equations are complemented by the saddle point equations for the parameters \( \hat{R}_p, \hat{\Lambda}_p \) i.e. \( \frac{\partial f_0}{\partial \hat{R}_p} = \frac{\partial f_0}{\partial \hat{\Lambda}_p} = 0 \).

We now derive a simple expression for the dynamical transition temperature. The equation for the soft mode can be worked out and one finds,

\[
\beta^2 e^{-I(\Lambda)} G'' \left( \beta (\hat{R}_0 - q) \right) \int_{-\infty}^{\infty} dp(x) \left( \langle \hat{s}_0^2 \rangle - \langle \hat{s}_0 \rangle^2 \right)^2 \Xi(x) = 1 \tag{11}
\]

where the average \( \langle \langle \cdot \rangle \rangle \) is taken over the effective Hamiltonian eq.(8). For a continuous transition \( (q = \lambda = 0) \) eq.(11) can be written in the simple form

\[
\chi_0^2 G''(\chi_0) = 1 \tag{12}
\]

where \( \chi_0 = \beta \langle \langle \hat{s}_0^2 \rangle - \langle \hat{s}_0 \rangle^2 \rangle = \beta \hat{R}_0 \) is the longitudinal magnetic susceptibility. This equation can be solved (for a given \( G(x) \)) and yields the critical \( \chi_0 \). In particular, for the SK model \( G''_{SK}(x) = 1 \) which yields the result \( \chi_0 = 1 \) in agreement with known results \([4]\). In the ROM the only solution to that equation is \( \chi_0 = \infty \). For a continuous transition this implies a divergent susceptibility at the critical field. Using a perturbative expansion in powers of \( 1/\Gamma \) it is possible to use eq.(12) to obtain \( \Gamma_c \) with reasonable accuracy \([5]\).

Now we come to the main result of this paper, namely that at zero temperature the quantum transition becomes continuous. Then, the static and the dynamical transition temperature coincide. We first consider the static approximation where \( \hat{R}_p = \hat{\Lambda}_p = 0 \) for \( p > 0 \). Putting \( R = \hat{R}_0, \Lambda = \hat{\Lambda}_0 \) we find the following saddle point equations for \( R, \Lambda, q, \lambda, \)

\[
\Lambda = \frac{\beta}{2} G'(\beta R) ; \quad R = \langle\langle \frac{\sinh(\Xi_0(x))}{\Xi_0(x)} \rangle\rangle_0
\]

\[
\lambda = \frac{\beta}{2} \left( G'(\beta R) - G'(\beta (R - q)) \right) ; \quad q = \langle\langle \frac{\int_{-\infty}^{\infty} dp(z) \sinh(T) (\frac{z}{T})^2}{\int_{-\infty}^{\infty} dp(z) \cosh(T)} \rangle\rangle_0 \tag{13}
\]

where
\[
\langle (\cdot) \rangle_0 = \frac{\int_{-\infty}^{\infty} dp(x)(\cdot)}{\int_{-\infty}^{\infty} dp(x)cosh(\Xi_0(x))}
\]
with \( \Xi_0(x) = (2\Lambda x^2 + \beta^2 \Gamma^2)^{1/2} \), \( T = (b^2 + \beta^2 \Gamma^2)^{1/2} \) and \( b = (2(\Lambda - \lambda))^{1/2} x + (2\lambda)^{1/2} x \).

Exact expressions are also obtained for the free energies \( f_0, f_1 \) and for equation (11). This set of equations can be always numerically solved but explicit results can be analytically obtained in the zero temperature limit. Plugging the solution \( \Lambda = u\beta, \lambda = v\beta \) into (13) and performing the integrals with the saddle point method we find after some lengthy computations that \( u, v \) and the critical field \( \Gamma_c \) satisfy the equations

\[
u = \frac{1}{2} G'\left( \frac{1}{\Gamma_c - 2u} \right)
\]

\[
v = \frac{1}{2} \left( G'\left( \frac{1}{\Gamma_c - 2u} \right) - G'\left( \frac{1}{\Gamma_c - 2(u - v)} \right) \right)
\]

It is easy to check that equations (15),(16) only admit the trivial solution \( v = 0 \). It is also possible to show that in case \( v = 0 \) also \( f_1 = 0 \). Because \( q \) and \( R \) vanish with \( T \) and the free energy of this solution coincides with the paramagnetic free energy \( f_0 \) we conclude that the transition becomes continuous at zero temperature. In order to determine the critical field \( \Gamma_c \) we solve eq.(11) in the \( \beta \to \infty \) limit which yields

\[
(\Gamma_c - 2u)^{-2} G''\left( \frac{1}{\Gamma_c - 2u} \right) = 1
\]

with \( \chi_0 = (\Gamma_c - 2u)^{-1} \). Equation (17) together with (15) determine the value of \( u \) and \( \Gamma_c \). At the quantum transition point the internal energy is given by \( U = -\Gamma_c \) while the entropy is given by \( S = \frac{1}{2} G\left( \frac{1}{\Gamma_c - 2u} \right) - \frac{G(u)}{2(\Gamma_c - 2u)} + \frac{1}{2} \log(\frac{\Gamma_c}{\Gamma_c - 2u}) \). In case of the \( SK \) model we obtain \( u = \frac{1}{2}, \Gamma_c = 2 \) reproducing known results \([3,17]\). In the case of the \( ROM \) we obtain \( u = \frac{1}{2}, \Gamma_c = 1 \). Note that in both models the value of the critical field is given by the maximum eigenvalue of the coupling matrix \( J_{ij} \). For the \( ROM \), one finds that the entropy at zero temperature diverges. This is a consequence of the general failure of the static approximation at low temperatures. In figure 1 we show the phase boundaries for the dynamical and static transitions in the \( ROM \) as a function of the transverse field obtained numerically solving equations (13). Both transition temperatures decrease quadratically as
a function of the transverse field merging into the same point at zero temperature. In figure
2 we show the Edwards-Anderson order parameter $q = \langle \sigma^2 \rangle^2$ in the ROM as a function
of $\Gamma$ as we move along the static ($q_S$) and dynamical ($q_D$) phase boundaries.

The static approximation yields inaccurate quantitative results for the thermodynamic
properties at zero temperature. Nevertheless we expect the order of the transition to be
correctly predicted. To go beyond the static approximation we should consider all the
Fourier modes $\hat{R}_p, \hat{\Lambda}_p$ in the saddle point equations. This is a non trivial task which remains
open.

We stress that the main results of this work are restricted to pairwise interaction models.
In case of $p$-spin interaction spin-glass models \[18\] the scenario presented here does not apply
anymore. For $p$ larger than 2 we have obtained different results indicating that the transition
does not become continuous at zero temperature. This implies that the quantum transition
in $p$-spin interaction models with $p$ larger than 2 belong to a different universality class.
This is in agreement with known results in case of $p$-spin models in the limit $p \to \infty \[19\]$ as
well as in $1/p$ analytical expansions \[20\].

Summarising, we have investigated the glassy behaviour in Ising spin glass models with
pairwise interactions in the presence of a transverse field. In models with a discontinuous
finite temperature transition we have shown, within the static approximation, that the
transition becomes continuous at $T = 0$ and there is no room for a metastable glassy phase.
This implies that at $T = 0$ all spin-glass models with pairwise interactions belong to the
same universality class.

**Acknowledgements.** I thank D. Lancaster, Th. M. Nieuwenhuizen and F. G. Padilla
for discussions and D. Lancaster for a careful reading of the manuscript. This work has been
supported by FOM (The Netherlands).
REFERENCES

[1] M. Mézard, G. Parisi and M. A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore 1987); K. H. Fischer and J. A. Hertz, *Spin Glasses* (Cambridge University Press 1991);

[2] H. Rieger and A. P. Young, Preprint cond-mat/9707005.

[3] D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35** (1975) 1792.

[4] A. J. Bray and M. A. Moore, J. Phys C. **13** (1980) L655.

[5] K. D. Usadel, Solid State Commun. **58** (1986) 629.

[6] H. Ishii and Y. Yamamoto, J. Phys. C **18** (1985) 6225; J. Phys. C **20** (1987) 6053;

[7] J. Miller and D. Huse, Phys. Rev. Lett. **70** (1993) 3147.

[8] G. Büttner and K. D. Usadel, Phys. Rev. B **41** (1990) 428; Y. Y. Goldsmichdt and P.Y. Lai, Phys. Rev. Lett. **64** (1990) 2467.

[9] T. R. Kirkpatrick and D. Thirumalai, Phys. Rev. B **36** (1987) 5388; T. R. Kirkpatrick and P. G. Wolyness, Phys. Rev. B **36** (1987) 8552.

[10] C. A. Angell, Science **267** (1995) 1924; W. Götze, *Liquid, freezing and the Glass transition*, Les Houches (1989). J. P. Hansen, D. Levesque, J. Zinn-Justin editors, North-Holland.

[11] S. Franz and J. Hertz, Phys. Rev. Lett **74** (1995) 2114.

[12] L. F. Cugliandolo and J. Kurchan, Phys. Rev. Lett, **71** 173.

[13] E. Marinari, G. Parisi and F. Ritort, J. Phys. A **27** 7647.

[14] H. F. Trotter, Proc. Am. Math. Soc. **10** (1959) 545; M. Suzuki, Prog. Theor. Phys. **56** (1976) 1554.

[15] C. Itzykson and J-B Zuber, J. Math. Phys. **21** 411.
[16] G. Cwilich and T. R. Kirkpatrick, J. Phys A 22 (1989) 4971; E. De Santis, G. Parisi and F. Ritort, J. Phys A 28 (1995) 3025.

[17] D. Thirumalai, Q. Li, T. R. Kirkpatrick, J. Phys. A. 22 (1989) 3339

[18] E. Gardner, Nucl. Phys. B 257 747.

[19] Y. Y. Goldsmichdt, Phys. Rev. B 41 (1990) 4858.

[20] V. Dobrosavljevic and D. Thirumalai, J. Phys. A 22 (1990) L767; L. De Cesare, K. Lubierska, I. Rabuffo and K. Walasek, J. Phys. A 29 (1996) 1605.
Figure Captions

Fig.1 Phase boundaries $T_s(\Gamma)$ (lower line) and $T_D(\Gamma)$ (upper line) in the $ROM$ in the static approximation. At zero transverse field $T_s \simeq 0.0646, T_D \simeq 0.1336$.

Fig.2 Edwards-Anderson parameter $q_s$ (upper line) and $q_D$ (lower line) in the $ROM$ on the static and dynamical phase boundaries as a function of the transverse field. At zero transverse field $q_s \simeq 0.99983, q_D \simeq 0.961$. $q_s$ and $q_D$ vanish linearly with $T^{\frac{1}{2}}$ at zero temperature.
