J. Phys. A: Math. Gen. **29** (1996) 7355–7366. Printed in the UK

Quantum Monte Carlo study of the infinite-range Ising spin glass in a transverse field

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Received 11 March 1996, in final form 2 July 1996

Abstract. We study the zero-temperature behaviour of the infinite-ranged Ising spin glass in a transverse field. Using spin summation and Monte Carlo methods we characterize the zero-temperature quantum transition. Our results are well compatible with a value $\nu = \frac{1}{4}$ for the correlation length exponent, $z = 4$ for the dynamical exponent and an algebraic decay t^{-1} for the imaginary-time correlation function. The zero-temperature Monte Carlo relaxation of the energy in the presence of the transverse field shows that the system monotonically reaches the ground-state energy due to quantum fluctuations and displays glassy effects due to the strong anisotropy in the effective Hamiltonian.

1. Introduction

The purpose of this work is to present some results concerning the zero-temperature critical behaviour of the Ising spin glass in the presence of a transverse magnetic field. While classical spin glasses have been extensively studied during the recent years, the role of the quantum fluctuations in the low-temperature regime are not so well understood. Most work has been devoted to the study of the one-dimensional case [1] and the mean-field theory [2–4]. These two limit cases seem to capture one of the most relevant features associated with the quantum fluctuations, i.e. the presence of tunnelling effects at zero-temperature. The effect of the transverse field is to allow the system to jump over the free-energy barriers even at zero temperature. In this work we will focus our attention on the study of the zero-temperature critical behaviour and some features concerning the Monte Carlo relaxation. We have considered the infinite-range model where some analytical results can be obtained. The infinite-range model has been studied in several works. In particular, the phase diagram of the model has been computed within the static approximation [5], by doing perturbation expansions [4] and by spin summation calculations [3]. Miller and Huse [6] and Read *et al* [7] have obtained the imaginary-time correlation function at the zero-temperature quantum critical point using a perturbative approach and a Landau expansion respectively. On the other hand, recent numerical work [8, 9] in two- and three-dimensional quantum spin glasses reveals that the Monte Carlo method can yield precise estimates of the critical temperature and reasonable estimates of the critical exponents associated with the quantum transition by using finite-size scaling techniques.

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0305-4470/96/237355+12$19.50

The body of the results we present in this work can be divided into three sections (3, 4 and 5) and the purpose of the work is two-fold. First we want to show how the Monte Carlo technique used in [8, 9] can be used for determining the critical point and the critical exponents in the infinite-range case. This will be done comparing the results obtained using numerical spin summation (section 3) and Monte Carlo finite-size scaling calculations (section 4). The results obtained from both sections 3 and 4 are complementary even though they have been obtained with different techniques. Once the critical point is obtained we will obtain the main critical exponents z and ν and we will study the decay of the imaginary-time correlation function at the critical point. Unfortunately, our results concerning the value of the dynamical exponent z are in disagreement with theoretical expectations [6, 7]. Second, we will consider the role of quantum fluctuations on the zero-temperature Monte Carlo relaxation of the model. While these last results concern the infinite-range model we argue how our main conclusions are valid also in the short-range case.

2. The model

The model we are interested in is defined by the Hamiltonian

$$\mathcal{H} = -\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x \tag{1}$$

where the $\{\sigma_i; i = 1, N\}$ are the Pauli spin matrices and Γ is the transverse field. The J_{ij} are Gaussian distributed variables with zero mean and variance $1/N$. For $\Gamma = 0$ the model reduces to the classical Sherrington–Kirkpatrick spin-glass model [10]. It is well known [11, 12] that the ground-state energy of the above Hamiltonian can be written as the free energy of a classical model with a new imaginary-time dimension,

$$E_g(\Gamma) = -\lim_{\beta\to\infty}\lim_{M\to\infty}\frac{\log(Z_{\text{eff}})}{N\beta} \tag{2}$$

where

$$\begin{aligned} Z_{\text{eff}} &= \text{Tr}_{\sigma_i}\exp(-\beta H_{\text{eff}}(\Gamma, M, \beta)) \\ &= \sum_{\sigma_i=\pm 1}\exp\left(A\sum_{i<j}\sum_{t=1}^{M} J_{ij}\sigma_i^t\sigma_j^t + B\sum_{i=1}^{N}\sum_{t=1}^{M}\sigma_i^t\sigma_i^{t+1} + C\right) \end{aligned} \tag{3}$$

and the spins σ_i are now classical variables which take the values ± 1. The parameters A, B and C are given by,

$$A = \frac{\beta}{M} \qquad B = \tfrac{1}{2}\log\left(\coth\left(\frac{\beta\Gamma}{M}\right)\right) \qquad C = \frac{MN}{2}\log\left(\tfrac{1}{2}\sinh\left(\frac{2\beta\Gamma}{M}\right)\right). \tag{4}$$

In the limit $M \to \infty$ the parameters A and B are highly anisotropic (the coefficient A goes to zero while B goes to infinity). This makes it extremely difficult to perform Monte Carlo simulations of the quantum model. It has been recently shown [8, 9] that it is enough to consider an isotropic Hamiltonian which nevertheless lies in the same universality class. We generalize the type of model considered in [8, 9] and we consider the family of models with parameters $A = \beta_{\text{cl}}$, $B = \beta_{\text{cl}}^p$, $C = 0$. The case $p = 1$ was already considered in [8, 9]. It is natural to expect that all the models within this family belong to the same universality class. The reason being that all these models have the same effective Hamiltonian and the same type of spin-glass transition as we will see in the next section. We expect the critical exponents to be independent of the particular model considered. Within this family of models the parameter β_{cl} plays the role of the inverse of a classical temperature (not to be confused with the real temperature) which controls the intensity of the quantum fluctuations. In other words, this effective classical temperature $1/\beta_{\rm cl}$ plays the role of a transverse field in the *true* model (4). Concerning the critical behaviour, we have concentrated our attention in the previous models with $p = 1$ (model (a)), and $p = 2$ (model (b)) and we have studied them using direct spin summation of the mean-field equations and the Monte Carlo method. While our Monte Carlo numerical results are consistent with the universality hypothesis we have discovered that model (a) is still hampered by strong Monte Carlo sampling problems while model (b) gives more confident results.

3. Spin summation results

We have analytically solved the previous model (3) using the replica trick with general coefficients A and B. The analytical solution of the infinite-range model has been already considered in the literature [2, 4, 5] and here we will only sketch the results. Applying the replica trick and performing the usual technical steps in the theory of spin glasses (introducing the order parameters and decoupling the different sites) one gets the effective free energy,

$$F_{\rm cl} = -\frac{\overline{\log(Z_{\rm eff})}}{N\beta_{\rm cl}} = \lim_{n\to 0} \frac{\overline{Z^n_{\rm eff}}}{Nn\beta_{\rm cl}} = \lim_{n\to 0} \frac{A[Q, R]}{n\beta_{\rm cl}} \tag{5}$$

where $\overline{(\ldots)}$ stands for average over the disorder and n is an integer which denotes the number of replicas. The saddle-point free energy $A[Q, R]$ reads,

$$A[Q, R] = \frac{A^2}{4}\left(\sum_{\alpha\neq\beta}\sum_{t,t'}(Q^{tt'}_{\alpha\beta})^2 + \sum_{\alpha}\sum_{t\neq t'}(R^{tt'}_{\alpha})^2\right) - \log F[Q, R] \tag{6}$$

with

$$F[Q, R] = \sum_{\sigma^t_\alpha} \exp\left[B\sum_{t,\alpha}\sigma^t_\alpha\sigma^{t+1}_\alpha + \frac{A^2}{2}\left(\sum_{\alpha\neq\beta}\sum_{t,t'} Q^{tt'}_{\alpha\beta}\sigma^t_\alpha\sigma^{t'}_\beta + \sum_{\alpha}\sum_{t\neq t'} R^{tt'}_\alpha\sigma^t_\alpha\sigma^{t'}_\alpha\right)\right]. \tag{7}$$

The indices $\alpha, \beta = 1, \ldots, n$ stand for replica indices while the indices $t, t' = 1, \ldots, M$ run over the imaginary-time direction with periodic boundary conditions (i.e. $\sigma^{M+1}_\alpha = \sigma^1_\alpha$). The saddle-point equations yield the order parameters Q and R,

$$Q^{tt'}_{\alpha\beta} = \langle\sigma^t_\alpha\sigma^{t'}_\beta\rangle \qquad R^{tt'}_\alpha = \langle\sigma^t_\alpha\sigma^{t'}_\alpha\rangle \tag{8}$$

where the thermal averages $\langle\ldots\rangle$ are done over the effective partition function defined in (7). To solve the previous equation we impose the static condition (i.e. no dependence on the imaginary-time variables t, t') in the set of parameters Q while the Rs are assumed to be not static but translationally time invariant, i.e. depend only on the difference of times $t - t'$. The form of this condition is a direct consequence of the time-translation invariance of the effective Hamiltonian (10) (see below). In order to determine the critical value of $\beta_{\rm cl}$ it is enough to consider replica symmetry. In this case the order parameters assume the form $Q^{tt'}_{\alpha\beta} = q$, $R^{tt'}_\alpha = R(t - t')$ and the free energy reads,

$$\beta f = \frac{A^2}{4}\sum_{t\neq t'}(R(t-t'))^2 + \frac{A^2 M}{4}(1-q^2) - \frac{A^2 M}{2}(1-q) - \int_{-\infty}^{\infty}\frac{{\rm d}x}{(2\pi)^{\frac{1}{2}}}\,{\rm e}^{-(x^2/2)}\log\Theta(x) \tag{9}$$

where the function $\Theta(x)$ is given by

$$\Theta(x) = \sum_{\sigma^t} \exp(\Xi(x,\sigma))$$
$$= \sum_{\sigma^t} \exp\left(B \sum_t \sigma^t \sigma^{t+1} + (A^2 q)^{\frac{1}{2}} x \sum_t \sigma^t + \frac{A^2}{2} \sum_{t \neq t'} (R(t-t') - q) \sigma^t \sigma^{t'} \right) \tag{10}$$

and the order parameters q and $R(t-t')$ can be obtained solving the equations,

$$q = \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{(2\pi)^{\frac{1}{2}}} \mathrm{e}^{-(x^2/2)} \left(\frac{\sum_\sigma \sigma^t \exp(\Xi(x,\sigma))}{\Theta(x)} \right)^2 \tag{11}$$

$$R(t-t') = \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{(2\pi)^{\frac{1}{2}}} \mathrm{e}^{-(x^2/2)} \left(\frac{\sum_\sigma \sigma^t \sigma^{t'} \exp(\Xi(x,\sigma))}{\Theta(x)} \right). \tag{12}$$

We have numerically solved the previous nonlinear equations for the models (a) and (b) at different values of M ranging from 2 to 15. In the same way as in [3] we have extrapolated the different parameters q and $R(t-t')$ to the $M \to \infty$ limit. We have found that a second-degree polynomial in $1/M$ yields very stable and good results. Our calculations show that there is a continuous spin-glass transition from a paramagnetic phase ($q = 0$) to a spin-glass phase where q is finite. The $R(t-t')$ are non-zero at any finite temperature and have a non-trivial time dependence. Within the spin-glass phase we computed the value of q which vanishes linearly with the temperature at the critical temperature. This is in agreement with the expected quantum critical exponent $\beta = 1$ [7]. Extrapolating q to 0 we extract the value of T_{cl}. For the model (b) we are very interested to find that $T_{\mathrm{cl}}^{(\mathrm{b})} = 2.11 \pm 0.01$ (a less accurate determination for model (a) yields $T_{\mathrm{cl}}^{(\mathrm{a})} \simeq 2.81$). The spin summation method yields the thermodynamic quantities with good precision but is not very accurate in yielding the quantum critical exponents z and ν at the transition point.

4. Monte Carlo results

In order to characterize the quantum critical point we have done Monte Carlo numerical simulations of both models (a) and (b). In our preliminary study of both models we noted that model (a) presented strong Monte Carlo sampling problems. In fact, we observed that some observables displayed strong temperature-dependent fluctuations. These bad sampling effects are absent in model (b) which yields the critical behaviour with modest computational effort. Note that model (a) corresponds to the case considered in [8, 9]. In what follows, and otherwise stated, we will present the numerical results for model (b). In order to simulate the system described by (3) we consider M coupled systems along the time direction with the same realization of disorder. To increase the speed of the computations we have considered the case of discrete couplings $J_{ij} = \pm \frac{1}{\sqrt{(N)}}$ which yields the same behaviour in the large N limit as in the case of a Gaussian distribution of couplings. We have simulated two different replicas $\{\sigma_i^t, \tau_i^t; i = 1, \ldots, N; t = 1, \ldots, M\}$ of the system (6) with the same realization of the disorder. The main quantity we are interested in is the spin–spin overlap

$$q = \frac{1}{nM} \sum_{i=1}^{N} \sum_{t=1}^{M} \sigma_i^t \tau_i^t \tag{13}$$

which yields the spin-glass susceptibility,

$$\chi_{\mathrm{SG}} = NM \left(\overline{\langle q^2 \rangle_J} - \overline{\langle q \rangle_J}^2 \right). \tag{14}$$

Following [8, 9] we consider the Binder parameter for different values of N and M. This adimensional parameter measures the Gaussianity of the statistical fluctuations and is defined by,

$$g = \overline{g_J} = \frac{1}{2}\left[3 - \overline{\left(\frac{\langle q^4\rangle_J}{\langle q^2\rangle_J^2}\right)}\right]. \tag{15}$$

Note that the Binder parameter is averaged over different realizations of samples. This is in contrast with usual calculations in classical spin glasses where one averages the moments $\langle q^2\rangle$, $\langle q^4\rangle$ before computing g.

In the vicinity of the critical point the spin-glass susceptibility (14) and the Binder parameter (15) are expected to scale with the size of the system N and the temporal dimension M in the following way,

$$\chi_{\rm SG} = N^p \hat{\chi}(N(T - T_c)^q, N/M^r) \tag{16}$$

$$g = \hat{g}(N(T - T_c)^q, N/M^r) \tag{17}$$

where $\hat{\chi}$, $\hat{g}$ are scaling functions and p, q, r are mean-field exponents related to the exponent ν and the dynamical exponent†.

Now we face the problem that the finite-size scaling depends on two variables N and M. As noted in [8, 9] the phase transition is signalled by the behaviour of the parameter g as a function of N and M. For large values of M the system behaves as a one-dimensional system and for small values of M the system behaves as the classical Sherrington–Kirkpatrick model [10]. So the Binder parameter (15) is expected to go to zero for large and small values of M. At intermediate values of M a maximum for g is expected. Above the critical temperature the system becomes disordered and the value of g associated to that maximum decreases with N. Below T_c it increases with N since the system tends to order. At the critical point $T = T_c$ the maximum value of g is constant with N. According to (16) the scaling with N of the value of M corresponding to the position of maximum determines the mean-field exponent r. The previous criteria yields the critical temperature with very good precision. We find $T = 2.11 \pm 0.01$ in agreement with the results that we obtained in the previous section. Our results for the spin-glass susceptibility $\chi_{\rm SG}$ and the Binder parameter g are shown in figures 1 and 2 at $T = 2.11$. The values of N we studied cover the range $N = 32$–160 with 5000 samples in each case. Note that in figure 1 data for the smallest size $N = 64$ tend to be slightly out of the region where data collapse. The situation is even worse with data for smaller sizes. In fact we have observed that small values of N (less than $N \simeq 50$) are affected by strong subdominant corrections to the critical behaviour. It is not too difficult to explain this result. Since the scaling behaviour is expected to occur in the limit $M \to \infty$ the corrections can be very large if the considered values of M are too small. In fact, in our case the maximum of g is located at quite small values of M (for instance, at $N = 32$ the value of M where the g has its maximum is less than 2 which is certainly very small). This is in contrast to what is found in two- and three-dimensional quantum-spin glasses [8, 9].

Larger values of N allow the values of the critical exponents to be extracted. The exponents p, q, r can be derived as a function of ν and the dynamical exponent z. These are given by, $\nu = pq/2$, $z\nu = q/r$ which yield $\gamma = 2\nu$. The numerical results for g show that the exponent $r = 2$ fits well the scaling of the function g at the critical point. The fit of the spin-glass susceptibility as a function of the temperature in the region of scaling (where

† The quantum exponent z is different from the classical dynamical exponent associated with the critical-time dynamics.

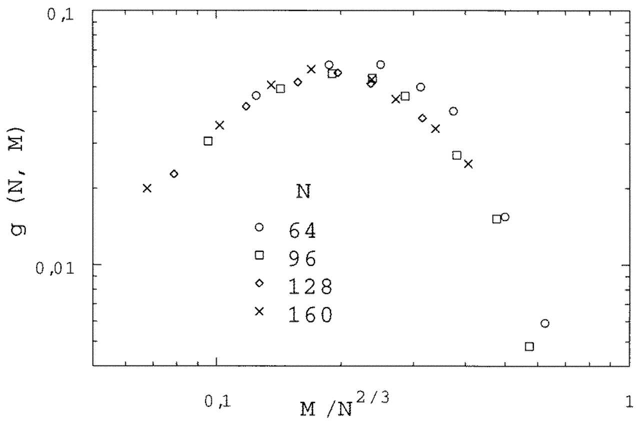

Figure 1. Binder parameter $g(N, M)$ in model (b) at $T = T_c = 2.11$ for different sizes $N = 64$, 96, 128, 160 as a function of $M/N^{\frac{2}{3}}$.

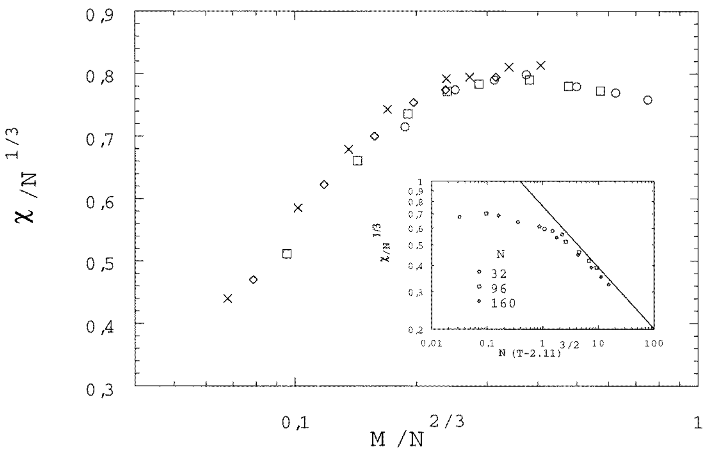

Figure 2. Spin-glass susceptibility $\chi(N, M)/N^{\frac{1}{3}}$ in model (b) at $T = T_c = 2.11$ for different sizes $N = 64$, 96, 128, 160 as a function of $M/N^{\frac{2}{3}}$. The inset shows the $\chi(N, M)/N^{\frac{1}{3}}$ as a function of the temperature for $N = 32$, 96, 160 for values of N, M where the g takes its maximum value. The straight line in the inset is the asymptotic behaviour $x^{-\frac{1}{2}}$ of the scaling function.

the g takes its maximum value) is shown in the inset of figure 2 and is quite consistent with $q = \frac{3}{2}$, $p = \frac{1}{3}$ which yields $\nu = \frac{1}{4}$ and $\gamma = \frac{1}{2}$ as predicted within the Gaussian approximation [7]. Unfortunately, it is difficult for us to conclude, from the numerical data, on the exact value of the exponent z. Our best fit reveals $r = 2$, $z = 3$ which yields $\beta = \frac{7}{8}$. But we cannot discard a slightly smaller value like $r = \frac{3}{2}$ for instance, which is also good within our numerical precision. This is also a plausible result if one considers the presence in the numerical results of the aforementioned finite M corrections. What we definitely discard from our numerical data of the Binder parameter and the susceptibility is the value $r = 3$ which would yield $z = 2$ and $\beta = \frac{3}{4}$ (using the quite consistent values of $q = \frac{3}{2}$, $p = \frac{1}{3}$). Then we find that $z = 3$ or $z = 4$ (we consider the simplest possibility of integer values of z for the dynamical exponent in mean-field theory) our data fits quite well while

$z = 2$ does not. Because $z = 4$ also yields the natural exponent $\beta = 1$ (unlike $z = 3$ which yield $\beta = \frac{7}{8}$) we conclude that the *canonical* exponents $r = \frac{2}{3}$, $z = 4$ are the ones which fit the numerical data reasonably well. These are the values of the exponents used to scale data in figures 1 and 2. To definitely conclude on the value of z we should explore larger sizes. But this is a very difficult task due to the long-range nature of the model we are studying which makes simulations very time consuming. It is interesting to note that the critical value of $g(g_c = \max_M\{g(N, M, T_c)\})$ is close to 0.056 and smaller than the value obtained in two and three dimensions [8, 9] as expected. As previously said, we have also performed numerical simulations of model (a) which shows a critical value of g of order 0.07 slightly higher than that of model (b). But in this case we have not been able to make the data for g collapse in a single universal curve. As said previously, we are suspicious that strong Monte Carlo sampling problems are the reason for such bad results. This is presumably related to the value of B in the critical point which is higher in model (a) than in model (b). This implies stronger anisotropic interactions in the first case which makes Monte Carlo relaxations slower (see section 5).

Finally, to give further numerical support to the previous reported value $z = 4$, we have considered the imaginary-time correlation function. Recently Miller and Huse [6] and Sachdev *et al* [7] have obtained the imaginary-time correlation function at the critical point using a perturbative approach. Our dynamical mean-field exponent z is in disagreement with their results. At the critical point they obtain,

$$C(t) = \langle \sigma_i^0 \sigma_i^t \rangle \sim t^{-\alpha} \tag{18}$$

with the value $\alpha = 2$. Figure 3 is a check of the theoretical expectation for the imaginary-time correlation function at the critical temperature $T = 2.11$. Simulations have been done for a large system $N = 2272$, $M = 20$ such that it is in the scaling region where we expect the $g(N, M, T_c)$ takes its maximum value. We have carefully checked that the system is in thermal equilibrium and data has been averaged over eight samples. The results for the decay of the correlation function (7) yields an exponent $\alpha \simeq 1.2$ consistent with the exponent $\alpha = \beta/\nu z$ which ranges from 1 to $\frac{7}{6}$ depending whether $z = 3$ or $z = 4$. Note that the decay of the imaginary-time correlation function (18) is quite sensitive to how close we are to the critical region. Obviously, if we are not precisely in the critical region we expect the system to be slightly more disordered and the correlation function to decay faster. Then, in the general case one finds the dynamical exponent z to be larger than expected [15] while in our case we find the opposite result. Consequently the fitted value 1.2 is an upper limit to the true exponent α which we naturally find to be 1 and then $z = 4$. Again, it is not clear to us how the predicted dynamical exponent $\alpha = 2$ (and $z = 2$) can fit our numerical data.

5. Zero-temperature Monte Carlo relaxation

Now that we have characterized the zero-temperature quantum transition we want to present some results concerning the quantum Monte Carlo relaxation of the model at zero temperature. In the classical case (zero transverse field) we already know that the relaxation at zero temperature of the system stops whenever it finds a metastable state [16]. Because the dynamics is non-ergodic in the classical case (the system cannot jump over energy barriers) then the system cannot reach the ground-state energy. When a transverse field is applied the system can tunnel through energy barriers allowing for a new type of relaxation. In order to avoid misunderstandings we want to clearly stress that our purpose in this section is the study of the relaxational features associated with the Monte Carlo dynamics in the presence of anisotropy effects. We are not aware of this kind of study in the literature (see

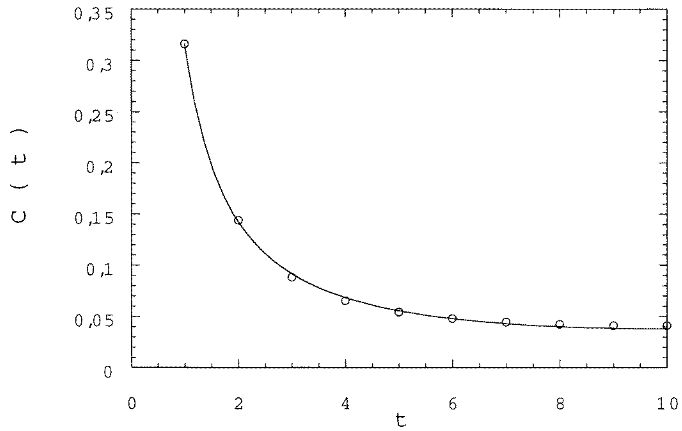

Figure 3. Imaginary-time correlation function in model (b) for $N = 2272$, $M = 20$ in the scaling region averaged over eight samples. The fit is of the form $C(t) = A/T^{\alpha} + A/(20-t)^{\alpha}$ with the best-fit parameters $\alpha = 1.2$, $A = 0.3$.

[13]). In principle this is different from the real-time dynamics in a macroscopic system in the presence of quantum fluctuations. Hopefully our studies could shed light on the features of the relaxational processes involved in real-time dynamics in a quantum system. This is a very interesting point which is outside of the scope of the present work and we will not address it here. In real systems the quantum tunnelling effects are a consequence of the coupling of many degrees of freedom while in our simple model these effects are mimicked by the ferromagnetic coupling in the imaginary-time direction. This coupling prevents the system (at zero temperature and in the presence of a small transverse field) from persisting forever in a metastable state.

In order to investigate the Monte Carlo relaxation we have considered the *true* anisotropic quantum model of (3) with the coefficients A, B, C given in (4) at very low temperatures as a function of the transverse field. One could also study the Monte Carlo relaxation of the effective models (a) and (b) used to study the critical properties throughout this work. Because our main purpose is to study the Monte Carlo relaxation in the presence of a strong anisotropy in the coefficients A and B, in what follows we will focus on the study of the effective model (3, 4). Specifically we are interested in the behaviour of the model for large β in the limit $M \to \infty$ with β/M as small as possible†. In this limit the Hamiltonian (3) is strongly anisotropic, the coefficient A resembles $1/M$ while B is much larger and resembles $\log(M)$. The total energy in (3) can be decomposed in two parts E_J, E_F plus a configuration-independent constant $C : E = AE_J + BE_F + C$ where E_J is the sum of all interaction energies in the different imaginary-time slices and E_F is a nearest-neighbour ferromagnetic interaction between spins in the different imaginary-time slices.

The interaction energy E_J can be analytically computed in the infinite-range model. This quantity is given by

$$E_J = -\frac{1}{MN}\overline{\sum_{t=1}^{M}\sum_{i<j} J_{ij}\langle\sigma_i^t\sigma_j^t\rangle} \tag{19}$$

where $\langle\ldots\rangle$ stands for the thermal average and $\overline{(\ldots)}$ stands for the average over the disorder.

† Note that in (2) the limit $\beta \to \infty$ is performed after the limit $M \to \infty$.

Applying the results of section 3 and standard analytical methods (see [17] for a review) we get (in the replica symmetric approximation),

$$E_J = -\frac{AM}{2}\left(1 + \sum_{t\neq 0} R(t)^2 - Mq^2\right). \tag{20}$$

Note that when $M = 1$, $A = \beta$, and we get the expression for the internal energy in the Sherrington–Kirkpatrick model in the replica symmetric approximation $E_J = -\frac{\beta}{2}(1 - q^2)$ [10].

Our main interest is the relaxational behaviour of the interaction part E_J as a function of time. Note that in the limit $M \to \infty$ the relaxation of the energy E_J is extremely slow with time (because the main contribution to the full energy in the Hamiltonian (3) is due to the ferromagnetic term E_F). Now we want to show that the Monte Carlo relaxation of the energy E_J is the same if the Monte Carlo time is rescaled by the factor $(\beta/M)^2$. This is a natural result since the parameters A and B in (4) are only a function of that ratio. The proof is quite simple. For small values of β/M the ferromagnetic part of the energy E_F is very large. Then one gets an acceptance rate completely dominated by the energetic term BE_F. Because the ferromagnetic coupling is one dimensional, the main change of energy when one spin is flipped is $4B$, and the probability to accept this change is $\exp(-4B) \simeq (\beta/M)^2$ for small values of β/M and a fixed value of Γ which yields the desired result. This is quite general and also applies to short-range systems.

We performed two kinds of experiment. We have studied zero-temperature Monte Carlo relaxations at a fixed transverse field and we have considered the model at different low temperatures and different values of M. In figure 4 we show the relaxation of the energy E_J as a function of Monte Carlo time for different values of M and β such that the ratio β/M is small. The simulations were performed for two different sizes, $N = 320$, 640, finding the same qualitative results. We studied several different ratios of β/M ranging from 0.2 to 0.001. The explored temperatures were $T = 0.1$, 0.02, 0.01, deep in the low-temperature region, and the following values of $M = 50$, 100, 500, 1000. Relaxations were studied with a small transverse field $\Gamma = 0.1$ (the critical value of the transverse field is close to 1.5 [3, 4]). In order to make the relaxation curves collapse in a single curve we have rescaled the time by the factor $(\beta/M)^2$. It is interesting to observe that the energy E_J decreases to a value close to -0.76 which is the expected value in the classical Sherrington–Kirkpatrick

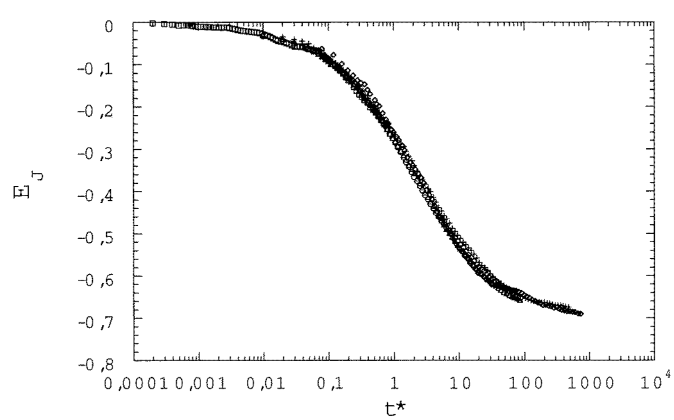

Figure 4. Relaxation of the interaction energy E_J with $\Gamma = 0.1$ for different ratios β/M as a function of the rescaled Monte Carlo time $t^* = t(\beta/M)^2$.

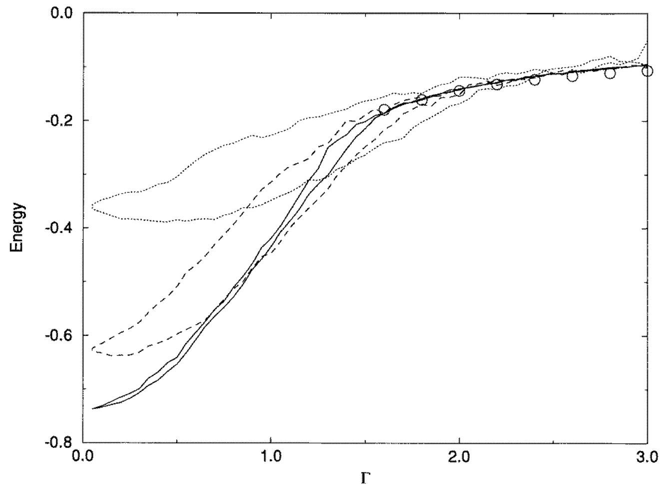

Figure 5. Hysteresis cycles of the interaction energy E_J at three different cooling rates r (dotted curve $r = 100$, broken curve $r = 10$, full curve $r = 1$). The circles are the analytical result in the quantum paramagnetic phase above $\Gamma_c \simeq 1.5$ [3, 4].

model at zero temperature at first order of replica symmetry breaking [14]. Note also that the energy E_J decreases with time but it can fluctuate and sometimes increase due to the presence of the transverse field. We have clearly seen this effect especially in the large time regime. The origin of these fluctuations is not thermal but purely quantum and are mimicked by the ferromagnetic coupling which allows the system to jump over the energy barriers.

Another interesting aspect of the quantum model we are considering concerns its glassy properties in the presence of strong anisotropic effects. The transverse field controls the intensity of quantum fluctuations and we expect strong hysteresis effects as the transverse field is varied. This is shown in figure 5 where we plot the relaxation of the energy E_J at three different *cooling–heating* rates as a function of the transverse field Γ†. The cooling rate is defined by the number of Monte Carlo steps per temperature step ($\Delta\Gamma = 0.05$ in figure 5). Hysteresis curves for different values of M and β collapse to the same curve once the cooling rate is appropriately scaled by the time factor $(\beta/M)^2$. The area enclosed in the hysteresis curves decreases as the cooling–heating rate decreases in a manner similar to what happens in real glasses. We also show in the figure 5 the analytical result E_J in the quantum paramagnetic phase for different values of the transverse field. The energy was computed using expression (20) by exactly solving the saddle-point equations (12) with $q = 0$ in the quantum paramagnetic phase. This was done for different values of M ranging from 2 to 15 and extrapolating to the $M \to \infty$ limit. The agreement between the analytical prediction and the numerical Monte Carlo results is quite good. These analytical results can also be read as a check of our Monte Carlo procedure.

6. Conclusions

In this work we have studied the zero temperature behaviour of the infinite-range quantum Ising spin glass in a transverse field. In particular we have studied the critical properties at

† In our case the parameter which is varied is the transverse field and not the temperature as in real glasses.

the quantum transition point and the Monte Carlo relaxation behaviour as a function of the transverse field.

Concerning the quantum critical properties we have studied an effective model (the so-called model (b)) which is expected to be in the same universality class as the original quantum model $(3, 4)$. This effective model does not present strong Monte Carlo sampling problems and gives results we can be confident of. Even though our results show strong finite M corrections for small sizes, our data is in agreement with the mean-field quantum exponents $\nu = 1/4$, $\beta = 1$, $\gamma = 1/2$ [7]. Unfortunately we have not been able to corroborate the prediction for the dynamical exponent and the imaginary-time autocorrelation function (18) where $\alpha = 2$ [6, 7]. This result is expected for a dynamical quantum exponent $z = 2$ which we definitely rule out from the analysis of the data shown in figures 1, 2 and 3. In particular, numerical data shown in figure 3 reveals an exponent of $\alpha \simeq 1.2$ which should be a bit lower if we are not precisely within the scaling region. The values $\alpha = 1$, $z = 4$ seem to us the natural exponents compatible with our numerical results. We do not see any simple solution to avoid the conflict with the existing theory. Note that the main discrepancy with the theory is in the value of the exponent z, the other ones being in agreement with the theory. This is an interesting point which deserves further investigation. Unfortunately, from the numerical side, it is very difficult to go to larger sizes since we would need much more computational time. The reason for such discrepancy is not clear to us. Usually one expects to find a smaller dynamical exponent if the system stays slightly outside the critical region of scaling. In our case we find the opposite tendency which makes z always larger than 3. We do not attach this result to the specific model (b) we have studied since the value of the dynamical exponent should be universal as they are also the other exponents ν and γ. Further investigation (theoretical and numerical) is needed to clarify this issue.

We have also investigated the zero-temperature Monte Carlo relaxation of the model. We have found that the interaction energy E_J in the quantum model $(3, 4)$ in the zero-temperature limit $\beta \to \infty$, with $\beta/M \to 0$ shows a universal relaxation if the Monte Carlo time is rescaled by the factor $(\beta/M)^2$. This result is related to the scaling of the acceptance rate with β/M and is a consequence of the one-dimensional nature of the ferromagnetic interaction. For a low transverse field we have observed that the decay curve for the interaction energy E_J monotonically converges to a value quite close to the static value predicted in the classical Sherrington–Kirkpatrick model at first order of replica symmetry breaking. Obviously there are some small corrections to the ground-state energy due to the small (but finite) value of the transverse field. Because the effective model $(3, 4)$ mainly depends on the ratio β/M we expect that similar conclusions about the Monte Carlo relaxation of the infinite-range model are also valid in the short-range case. We have observed glassy features in the Monte Carlo relaxation by studying the hysteresis effects as a function of the *cooling–heating* rate variation of the transverse field. The results shown in figure 5 indicate a relaxation of the model quite reminiscent of that observed in real glasses. In the presence of a transverse field the system can jump over energy barriers due to tunnelling effects. Then, at zero temperature, the system is not constrained to remain forever in a metastable state. It is interesting to speculate whether this jumping of the system over the energy barriers corresponds to some kind of activated processes in classical glassy models. This point and the study of a real-time dynamics in disordered systems in the presence of quantum fluctuations are interesting issues which deserve further investigation.

Acknowledgments

We are grateful to J Gonzalez Carmona for discussions on this and related subjects. We are indebted to David Lancaster for a careful reading of the manuscript. JVA has been supported by a grant from the Universidad Carlos III de Madrid. FR has been supported by the DGICYT of Spain under grant PB92-0248 and the EC Human Capital and Mobility Programme contract ERBCHRXCT930413.

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