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Quantum magnets with anisotropic infinite range random interactions

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Abstract

Using exact diagonalization techniques, we study the dynamical response of the anisotropic disordered Heisenberg model for systems of S=1/2 spins with infinite range random exchange interactions at temperature T=0. The model can be considered as a generalization, to the quantum case, of the well-known Sherrington–Kirkpatrick classical spin glass model. We also compute and study the behavior of the Edwards Anderson order parameter and energy per spin as the anisotropy evolves from the Ising to the Heisenberg limits.

Keywords: Spin glasses; Quantum effects; Disorder; Frustration; Heisenberg model

Many real materials display a spin glass phase at low enough temperature. This exotic state is characterized by a frozen configuration of local magnetic moments following a random spatial pattern, in such a way that no net macroscopic magnetization is produced.

The manifestations of this state were first observed in the seventies in systems with magnetic impurities in a metallic host (examples are Cu–Mn, Ag–Mn, Au–Mn and Ag–Mn). There the magnetic moments experiment long-range RKKY interactions, but spin glass behavior was also subsequently observed in the insulating compound $Eu_xSr_{1-x}S$ with competing ferromagnetic and random antiferromagnetic exchange interactions [1]. More recently, spin glass phases have also been observed in the bi-layer kagome $SrCr_8Ga_4O_{19}$ [2], in the pyrochlore structure $Li_xZn_{1-x}V_2O_4$ [3], in the dipolar magnet $LiHo_xY_{1-x}F_4$ [4] and in the enigmatic high Tc compounds $La_{1-x}Sr_xCu_2O_4$ [5].

Competing interactions and frustration in combination with randomness have been identified as the basic ingredients to drive a system towards a glassy state. While the concept of spin is purely quantum, it is usually stated that quantum fluctuations are not important to describe the spin glass physics. However, the relevance of quantum effects is beginning to be identified and emphasized in experimental [6–9] and theoretical work [10–13].

Exact diagonalization (ED) techniques proved to be very useful and efficient to investigate the dynamical properties of strongly correlated systems in general [5]. In recent works, we showed that it is also a useful method to deal with quantum random spin systems with long-range interactions, such as the Ising model with random exchange interaction in the presence of a transverse and longitudinal magnetic fields [10] and the random Heisenberg model [11]. Most of the analytical and numerical methods to study this kind of systems rely on the so-called replica-trick. Unfortunately, this clever technique becomes usually impractical within the glassy phase, where replica symmetry breaking occurs. As ED does not use replicas, this technical difficulty is not encountered, and the paramagnetic and glassy phases can be studied in the same way. Another appealing feature of ED is that it allows for the direct calculation of the dynamical response on the real frequency axis. In this way, it circumvents the uncertainties related to the analytical continuation procedures which are usually needed in quantum Monte Carlo simulations [14]. Finally, another

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important advantage of ED is the possibility of gaining insight on the nature of the low energy excitations. The price to pay is that only small systems are amenable to be treated within the available computer power. However, at least for the case of models with infinite range interactions, in most of the cases, the relevant physical quantities were found to extrapolate smoothly to the thermodynamic limit and a consistent description of the different phases has been possible [10,11].

In this work, we present results on the behavior of the anisotropic Heisenberg model for a system of N spins with S=1/2 and random infinite-range exchange interactions. The Hamiltonian reads,

$$H = \frac{1}{\sqrt{N}} \sum_{i,j=1}^{N} J_{ij} \left[S_i^z S_j^z + \frac{\alpha}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) \right], \qquad (1)$$

where i, j label the sites of the fully connected lattice and the interactions $J_{i,j}$ are normally distributed with variance J^2 that we set to unity. The parameter α labels the degree of anisotropy interpolating between the classical Sherrington–Kirpatrick (SK) model for α=0 and the Heisenberg model for α=1. This model has a rather close experimental realization in the above mentioned $LiHo_xY_{1-x}F_4$ [4] compound in the limit of small magnetic ion concentration x, which is dominated by random exchange interactions. The magnetic interaction in this system is strongly anisotropic [8]. We calculate the different components of the local dynamical susceptibility, defined as

$$\chi_\mu^{\mathrm{loc}}(\omega) = \frac{1}{M} \sum_{M=1}^{m} \frac{1}{N} \sum_{i=1}^{N} \left\langle \Phi_0^{(m)} \middle| S_i^\mu \frac{1}{\omega - H^{(m)}} S_i^\mu \middle| \Phi_0^{(m)} \right\rangle, \qquad (2)$$

where m denotes the number of realizations of disorder and μ=x, y, z. The state $|\Phi_0^{(m)}\rangle$ is the ground state of the Hamiltonian $H^{(m)}$, defined for the mth realization of J_{ij} and it is calculated by recourse to Lanczos algorithm. The evaluation of the spectral functions $\chi''_\mu(\omega)$=$-2\mathrm{Im}[\chi_\mu^{\mathrm{loc}}(\omega)]$ is achieved by using a continuous fraction representation of the dynamical response functions [5]. We perform averages over a number of realizations of disorder between M=3000 for the largest systems (N=15 spins) to M=100,000 for the smallest ones (N=8 spins).

Let us first summarize the main properties of the spectral function in the limit α=1 (usual Heisenberg model) where the three components of the susceptibilities coincide [10,11]. This is shown in Fig. 1. Four different contributions to the dynamical response can be distinguished:

$$\chi''_z(\omega) = K\delta(\omega) + \chi''_{\mathrm{low}}(\omega) + \chi''_{\mathrm{high}}(\omega) + \chi''_{\mathrm{reg}}(\omega) \qquad (3)$$

The pure delta-function of the first term is a consequence of the SU(2) rotational invariance of the Hamiltonian in this limit. This response is due to a “soft mode” present in disorder realizations with total S≠0 which have 2S+1 fold degenerate ground states. A close analysis of the finite size

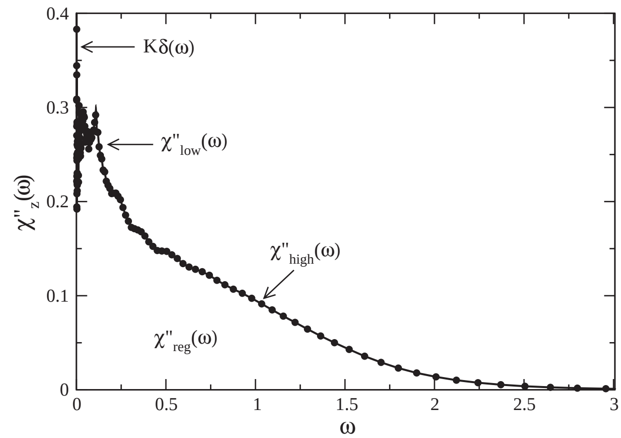

Fig. 1. The spectral function $\chi''_z(\omega)$ for the Heisenberg model (α=1) in a system of N=14 spins. The arrows indicate contributions from different kind of excitations (see text).

effects on the average magnetization per site indicates that <S>/N→0 as the size of the system evolves to the thermodynamic limit. Hence, this contribution to the spin response is expected to vanish as N increases.

The analysis of the low frequency feature $\chi''_{\mathrm{low}}(\omega)$ as N grows reveals that this contribution of the spectral function gets sharper, evolving towards a function ~$\delta(\omega)$. Its origin has been associated to slow coherent excitations of many-spin states which eventually become frozen. These states bear some resemblance to the magnons of the model without disorder. In fact, by examination of the structure of the ground-state in typical realizations of disorder, one finds that these excitations are built-up on a ground state whose wave function has large amplitudes on just a few configurations (out of the 2^N states) corresponding to unfrustrated sub-clusters, i.e., a sub-set of spins that are in a configuration that is compatible with the sign of the random J_{ij} bonds. Such configurations appear in pairs together with their time-reversal counterparts, having the same weight in the ground-state wave function and some relative sign that depends on the total S of the ground state. The wave functions of excited states that contribute to $\chi''_{\mathrm{low}}(\omega)$ also have a large weight on the unfrustrated clusters where the pairs of configurations appear with the opposite relative sign with respect to the ground state. The typical energy scale for these lowest energy excitations is $O(J{=}N)$. The high-energy part $\chi''_{\mathrm{high}}(\omega)$ is a small contribution with the form of a mild hump which is produced by excitations generated from the unbinding of single spins out of the unfrustrated clusters, the classical picture being a precession of individual spins around the effective quasistatic local field of the remaining frozen ones (of the unfrustrated sub-cluster). It is remarkable that the three abovementioned features, which are the consequence of some kind of magnetic order, are mounted on a broad and large background $\chi''_{\mathrm{reg}}(\omega)$ that remains almost unaffected as the size of the system increases. This piece of the response has been identified as due to incoherent excitations.

With this picture in mind, let us now carry out a similar analysis on the model with anisotropy. For $\alpha \neq 0$, SU(2) rotational invariance is broken and only the rotational invariance with respect to the z axis is preserved, so that $\chi''_x(\omega) = \chi''_y(\omega) \neq \chi''_z(\omega)$. The behavior of these spectral functions for different values of the parameter α is shown in Fig. 2. Both spectral functions contain a piece of the form $K\delta(\omega)$. Its origin is the degeneracy of ground states with large S_z (or $S_x = S_y$ components). In the case of $\chi''_x(\omega)$, this piece carries a very low spectral weight and, in both cases, it is observed to decrease as the size of the system grows. Therefore, as in the pure Heisenberg case, this contribution is expected to vanish in the thermodynamic limit. Save from this feature, $\chi''_x(\omega)$ does not show any clear indication of glassy order along this direction. The remaining part of the spectral function behaves as produced by an incoherent continuum, experimenting negligible changes when N is modified, without developing low-energy features. We identify it with the regular part $\chi''_{x,\mathrm{reg}}(\omega)$. The spectral function corresponding to the response along the z direction also contains some portion of its weight distributed on a wide range of frequencies that is interpreted as caused by incoherent excitations. Interestingly, at least for strong enough anisotropy, $\chi''_{x,\mathrm{reg}}(\omega)$ and $\chi''_{z,\mathrm{reg}}(\omega)$ seem to behave linearly in ω at low frequency, as predicted by a mean-field description which is exact for the SU(M) extension of the Heisenberg model in the limit of $M \rightarrow \infty 1$ [13]. A more detailed study of the origin of this behavior is left for future investigations.

We now turn to analyze the contribution $\chi''_{\mathrm{low}}(\omega)$ which is clearly distinguished within the low-frequency region of $\chi''_z(\omega)$. In an analogous way to what happens in the case of the isotropic Heisenberg model, the typical width of this

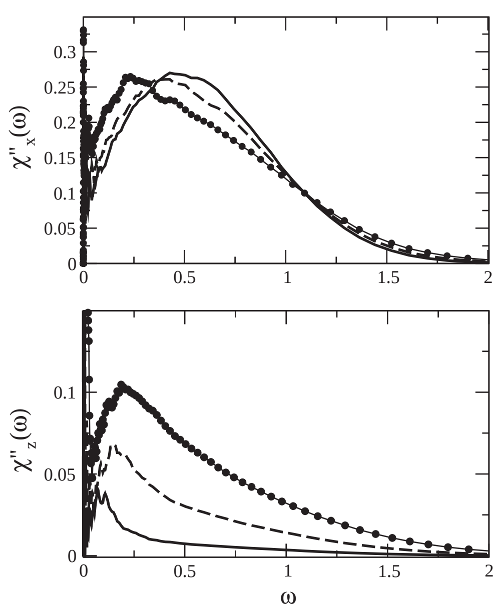

Fig. 2. The spectral function $\chi''_x(\omega)$ (upper panel) and $\chi''_z(\omega)$ (lower panel) for α=0.2, 0.4, 0.6 (bold line, dashed line, circles) in a system of N=14 spins.

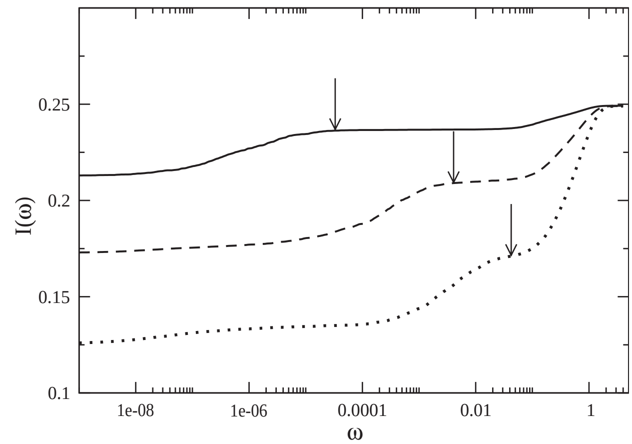

Fig. 3. The integrated spectral weight corresponding to $\chi''_z(\omega)$ for α=0.2, 0.4, 0.6 (bold, dashed and dotted line) in a system of N=14 spins. The arrows indicate the weight accumulated in the low-frequency piece $\chi_{\mathrm{low}}(\omega)$.

feature is $O(\alpha J = N)$ and evolves towards $a \sim \delta(\omega)$ as the system approaches the thermodynamic limit. Its origin is also due to excitations where the spin configurations conforming unfrustrated clusters, which in the ground state are frozen along the z direction, become canted with a finite component on the xy plane in a coherent fashion. Assuming that the functional form of the spectral function in the thermodynamic limit is $\chi''_z(\omega) = q\delta(\omega) + \chi''_{z,\mathrm{reg}}(\omega)$, the extrapolations for the weight accumulated in $\chi''_{\mathrm{low}}(\omega)$ as $N \rightarrow \infty$ provide an estimate of the Edwards Anderson parameter q.

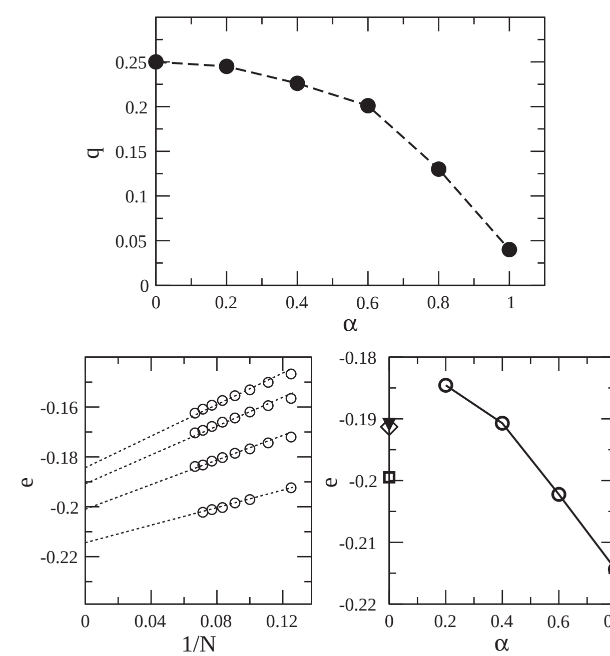

Fig. 4. Upper panel—the extrapolated values for the Edwards Anderson order parameter as a function of the strength of anisotropy. Lower left panel—energy PER site as a function of the inverse of the lattice size. Lower right panel—extrapolated energy per site as a function of α. The square, diamond and triangle correspond to the replica symmetric [16], one- and two-step replica symmetry breaking [17] solutions.

Recalling that the sum rule for the spectral functions is

$$\int_{-\infty}^{+\infty} d\omega\chi''_{\mu}(\omega) = \frac{1}{4}, \quad (4)$$

it is clear in Fig. 2 that an important transfer of spectral weight takes place from $\chi''_{z,\mathrm{reg}}(\omega)$ to q as α approaches the classical limit α=0. A more quantitative picture of this effect is shown in the logarithmic plot of the integrated weight $I(\omega)=\int_{-\infty}^{\omega} d\omega'\chi''_z(\omega')$ shown in Fig. 3. The weight accumulated in the low-frequency peaks defines plateaus in $I(\omega)$ that are indicated with arrows in the figure. Extrapolations of the ordinates of these plateaus as the size of the system increases provide us a reliable estimate of the Edwards Anderson parameter q in the thermodynamic limit. Results are shown in the upper panel of Fig. 4. This plot can be reasonably fitted with the function $q = 1/4\sqrt{1-(\alpha/\alpha_c)^2}$, with α_c~1.02. Interestingly enough, this functional form suggests that, starting from the SK model, the fluctuations introduced via the interaction between the x, y components of the spins behave in a similar way to those driven by the temperature T in the pure classical model. In the latter case, it has been found $q-1/4 \propto T^2$ [1], for T~0. Instead, it seems that the effect of quantum fluctuations in the anisotropic Heisenberg model is different from those caused by adding a transverse field Γ to the classical SK model, where q=1/4(1$-\Gamma/\Gamma_c$) [15]. This kind of behavior should be relevant in the analysis of quantum vs. classical annealing recently studied experimentally in the $LiHo_xY_{1-x}F_4$ compound [7,8]. The energy per site as a function of the inverse of the system size is shown in the lower left panel of Fig. 4. The result of the extrapolations to the limit $N\to\infty$ is shown in the lower right panel. For comparison, we also show the estimates provided by the replica symmetric solution [16] and the one- and two-step replica symmetry breaking solutions [17] for the classical model, corresponding to e=$-$0.1995; $-$0.1913; $-$0.1909, respectively [18]. It is worth to stress that, within that approximation, improving the level of symmetry breaking leads to higher values of the ground state energy per site. We have not explicitly investigated the limit α=0. However, it is clear from Fig. 4 that a simple monotonic continuation of the curve depicted by our numerical results leads at this limit to e~$-$0.183, i.e., to a value even larger than that predicted by the two-step replica symmetry breaking solution. As it is likely that higher levels of symmetry breaking give higher energies, we can say that our estimate provides an upper bound to the exact ground-state energy of the classical model.

To conclude, we have investigated a model of a quantum spin glass with long-range anisotropic interactions which is a quantum generalization of the Sherrington–Kirkpatrick model. Our results show that both $\chi''_z(\omega)$ and $\chi''_x(\omega)$ have a rich structure. We found that the z-component remains frozen for all values of the anisotropy and that the order parameter q decreases very fast for anisotropies α>0.6, being remarkably weak in the pure Heisenberg limit.

It is worth mentioning that, for large enough anisotropy, the low-frequency edge of the regular part of $\chi''_x(\omega)$ and $\chi''_z(\omega)$ seem to be consistent with linear behavior. This point is in contrast with our previous analysis for the SU(2) isotropic model [10,11], but it is in agreement with the results obtained in the large M limit [13].

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[18] There is a factor 1/4 between our results for e and q in comparison to those reported in the literature for the classical model. This is due to the fact that it is frequently assumed S_i^z=±1 for the classical model, while in our case S_i^z=1/2.