

Biophysical Chemistry 115 (2005) 135-138

Biophysical Chemistry

http://www.elsevier.com/locate/biophyschem

Quantum magnets with anisotropic infinite range random interactions

Liliana Arrachea^{a,b,*}, Marcelo J. Rozenberg^{a,c}

^aDepartamento de Física, FCEN, Universidad de Buenos Aires, Ciudad Universitaria Pab.1, 1428 Buenos Aires, Argentina ^bInstituto de Biocomputación y Física de Sistemas Complejos (BIFI), Corona de Aragón 42, Zaragoza 50009, Spain ^cLaboratoire de Physique des Solides, Université de Paris-Sud, Orsay 91405, France

Received 25 June 2004; received in revised form 22 November 2004; accepted 10 December 2004 Available online 24 December 2004

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. © 2004 Elsevier B.V. All rights reserved.

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

E-mail address: lili@df.uba.ar (L. Arrachea).

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

^{*} Corresponding author. Departamento de Física, FCEN, Universidad de Buenos Aires, Ciudad Universitaria Pab.1, 1428 Buenos Aires, Argentina. Tel.: +54 11 4576 3353; fax: +54 11 4576 3357.

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.

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

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 $_x$ Y $_{1-x}$ 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

$$\chi_{\mu}^{\text{loc}}(\omega) = \frac{1}{M} \sum_{M=1}^{m} \frac{1}{N} \sum_{i=1}^{N} \left\langle \Phi_{0}^{(m)} \middle| S_{i}^{\mu} \frac{1}{\omega - H^{(m)}} S_{i}^{\mu} \middle| \Phi_{0}^{(m)} \right\rangle, (2)$$

where m denotes the number of realizations of disorder and $\mu=x,\ y,\ z$. 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:

$$\chi_{z}''(\omega) = K\delta(\omega) + \chi_{low}''(\omega) + \chi_{high}''(\omega) + \chi_{reg}''(\omega)$$
 (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 $S\neq 0$ which have 2S+1 fold degenerate ground states. A close analysis of the finite size

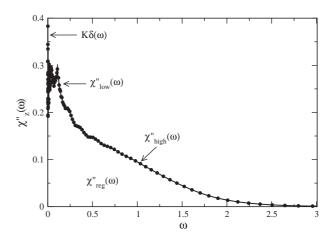


Fig. 1. The spectral function $\chi_z''(\omega)$ for the Heisenberg model (α =1) in a system of N=14 spins. The arrows indicate contributions from different kind of excitations (see text).

effects on the average magnetization per site indicates that $\langle S \rangle / N \rightarrow 0$ 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 $\chi''_{low}(\omega)$ as N grows reveals that this contribution of the spectral function gets sharper, evolving towards a function $\sim \delta(\omega)$. Its origin has been associated to slow coherent excitations of manyspin 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_{ii} 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 $\chi''_{low}(\omega)$ 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 $\chi''_{high}(\omega)$ 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 $\chi''_{reg}(\omega)$ that remains almost unaffected as the size of the system increases. This piece of the response has been identified as due to incoherent excitations.

Download English Version:

https://daneshyari.com/en/article/9573561

Download Persian Version:

https://daneshyari.com/article/9573561

Daneshyari.com