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DYNAMICS OF RANDOMLY DILUTED ANTIFERROMAGNETS

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Abstract. – The fracton scaling model, and the effective-medium-approximation are used to describe the excitation spectrum of randomly diluted antiferromagnets. The calculated scattering structure factor exhibits a crossover from extended magnons to localized fractons. These calculations are in agreement with experimental data of inelastic-neutron-scattering off spin-waves in Mn$_x$Zn$_{1-x}$F$_2$.

1. Introduction

Randomly diluted antiferromagnets (AF) are a subject of considerable interest. They form systems in which phenomena related to disordered effects can be studied (see Ref. [1] and references therein). In particular, one can study magnetic excitation dynamics of such systems as measured, for example, by inelastic neutron scattering.

When short-range exchange interactions are dominant, the magnetic ions in diluted AF form a percolating system [1]. The excitation spectrum of percolating structures were first discussed by Alexander and Orbach [2]. They proposed a scaling picture, which is called the fracton model. The model is based upon the notion of a crossover behaviour: a percolation system appears to be homogeneous on length scales $L$ longer than the percolation connectivity length $\xi$, and has fractal features on length scales smaller than $\xi$. Consequently, excitations of length scales longer than $\xi$ are basically those of an homogeneous system, here, spin waves (magnons) of an AF. The excitations typical at short length scales can be much different. Over these length scales the system is irregular, (with self-similar geometry for site dilution) and the modes are expected to be localized with localization length smaller than $\xi$. These modes are referred to as fractons. Thus, the structural crossover is reflected in the dynamics. This has been observed experimentally in neutron scattering studies [1] of Mn$_x$Zn$_{1-x}$F$_2$ and in light scattering off silica aerogels [3], in which the vibrational modes of small length scales are fractons.

In the fracton model, the characteristic length $\xi$ specifies a characteristic frequency $\omega_c$, which separates the spectrum into two portions: modes of frequencies $\omega$ less than $\omega_c$ are similar to the magnons of an homogeneous AF; the localized modes belonging to frequencies higher than $\omega_c$ are fractons. The latter are characterized by a single length, their frequency-dependent localization length. This fact has implications upon the density of states and upon the scattering width, both of which are reflected in the dynamic structure factor – the quantity measured in neutron and light scattering experiments.

In the present problem it is found, however, that the EMA fails to generate the correct scaling exponents, and exhibits exaggerated structure in the vicinity of the crossover frequency. This is discussed in section 4, together with some general conclusions.

2. The fracton model

The fracton model is based upon crossover from homogeneous behaviour at length scales $L > \xi$ to anomalous behaviour at $L < \xi$. The connectivity length $\xi$ is related to the crossover frequency $\omega_c$, by

$$\omega_c \sim \xi^{-\left(1+\frac{\theta}{2}\right)}.$$  (1)

The exponent $\theta$ was first introduced in the context of anomalous diffusion [4]. In the present problem it describes the dependence of the magnon stiffness coefficient upon the connectivity length $\xi$. As the percolation threshold is approached, $\xi$ diverges and the stiffness coefficient $c$ tends to zero,

$$c \approx \xi^{-\theta/2}.$$  (2)

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The magnon modes of frequency $\omega$ less than $\omega_c$ have wave lengths larger than $\xi$. They are the modes of the homogeneous regime, and consequently one expects their dispersion law to be that of ordinary spin modes of AF, i.e., linear in the wave vector $k$,

$$\omega = ck \approx \xi^{-\delta/2} k, \quad \omega < \omega_c$$

(3)

which implies $k\xi \ll 1$ by equation (1). Thus modes of $\omega < \omega_c$ are characterized by two length scales, $\xi$ and $k^{-1}$. The fracton modes, belonging to the higher frequency part of the spectrum ($\omega > \omega_c$) are characterized by a single length scale, $\lambda_{fr}$, through the "dispersion law"

$$\chi^{-\left(1+\delta\right)} \approx \omega, \quad \omega > \omega_c$$

(4)

This is the fracton localization length, which decreases rather sharply with frequency and is smaller than $\xi$. Thus modes of $\omega > \omega_c$ are characterized by a single length scale, $\lambda_{fr}$, and do not (cannot) depend upon $\xi$.

The crossover in the dispersion law (Eqs. (3, 4)) is seen explicitly in the neutron scattering data, through the observed dynamic structure factor, $S(k,\omega)$. One expects a plot of $S(k,\omega)$ for fixed $k$ as a function of $\omega$ to be sharply peaked at $\omega = ck$, just as for ordinary magnons. The contribution of the fractons, for $k\xi \ll 1$, however, will appear as a small shoulder around $\omega \sim \omega_c$. This is caused by the localized character of fracton excitations. As the neutron momentum transfer $k$ is increased, excitations of smaller and smaller length scales are probed. Around $k\xi \sim 1$, the scaling model predicts a crossover in the dynamic structure factor, from a sharp peak, typical of extended excitations, to a much broader structure, arising from the localized fracton modes. This is the general behaviour of the experimental data of reference [1]. The width of the peak in the dynamic structure factor can also be deduced from the scaling model [5]. The width is related to the inverse excitation lifetime $1/\tau$, resulting from the fact that the modes are probed by plane-wave neutrons, whereas they, by themselves, are not plane-waves. The scaling argument for $1/\tau$ states that it is given by

$$1/\tau = \omega f(\omega/\omega_c),$$

(5)

where $f(x)$ is a scaling function, characterized by the single scaling variable $\omega_c$ of the theory, and the $\omega$-prefactor sets up the correct dimensionality of $1/\tau$. In the low frequency regime, $\omega < \omega_c$, $f(x) \sim x^d$, where $d$ is the Euclidean dimensionality of the system. This form reproduces Rayleigh's law for the scattering width

$$1/\tau \approx \omega^{d+1}/\omega_c^d, \quad \omega < \omega_c$$

(6)

as is the case for magnons of an homogeneous AF. At frequencies higher than $\omega_c$, scaling requires that $f$ be independent of $\omega_c$. As a result, $f(x) \sim \text{const. for } x > 1$

and

$$1/\tau \approx \omega, \quad \omega > \omega_c$$

(7)

consistent with fracton localization according to the Ioffe-Regel criterion. A detailed analysis of light scattering data [3] reveals that the Ioffe-Regel limit (7) is attained for vibrational fracton modes in aerogels.

We now review the behaviour of the mode density of states. In the magnon regime, $\omega < \omega_c$, we expect the usual Debye law, characterizing homogeneous systems,

$$N(\omega) \approx \omega_c^{d-1} \omega^{d-1}, \quad \omega < \omega_c.$$ 

(8)

Here, as in the dispersion law (3), the prefactor is a consequence of the tenuous nature of the system. The exponent $d$ is the fracton dimensionality,

$$d = 2D / (2 + \theta),$$

(9)

where $D$ is the Hausdorff dimensionality, and is less than $d$, the Euclidean or embedding dimension. In essence, $D$ denotes the dependence of the number of magnetic ions upon the length scale: $n \sim L^D$. Because $D < d$, the density of magnetic ions in the fractal network $n$, diminishes with increasing $L$.

In the fracton regime the scaling model predicts

$$N(\omega) \approx \omega_c^{d-1} \omega^{d-1}, \quad \omega < \omega_c.$$ 

(10)

One sees that fracton dimension $d$ places $d$, the Euclidean dimension appearing in the Debye law. In all systems studied so far, $d < 2$. This, according to the localization criterion [6], implies that fracton modes are localized.

The arguments above (Eqs. (8-10)) pertain to the infinite cluster of the percolation system. When the finite clusters are included as well [7], $d$ equals $2d / (2 + \theta)$. In the next section we present a microscopic model for the dynamics of a percolation system which allows us to examine the predictions of the scaling model, and to carry out a detailed comparison with experiment.

In this article, we concentrate upon the dynamic aspects of the fracton model. However, one may also use it to study thermodynamic properties related to the spin waves of a percolating system, much in the same way that has been done for ferromagnets by Shender [8].

3. Effective medium approximation

In the effective medium approximation (EMA), the random system under consideration is replaced by an effective homogeneous medium, which one is able to solve for its dynamics. The parameters of the effective medium depend, in a self-consistent way, upon the pa-
rameters of the random system. The EMA can be used to treat various problems. Here we present its application to a dilute AF, in which the couplings obey a bond-percolation distribution [9, 10].

Our aim is to present results based on EMA and to compare them with inelastic-neutron-scattering experiments [1]. The scattering intensity is proportional to the (imaginary part of the) double Fourier transform of the spin-deviation Green’s function, defined by [11],

\[ g^{ab}(q, \omega) = \langle T a^+_n (t) a^+_{n'} (0) \rangle_{q, \omega}. \]  

Here \( T \) is the time-ordering operator; \( \omega \) and \( q \) denote time and spatial Fourier transforms; and \( a^+_n \) creates a spin-deviation on site \( n \) of sublattice \( \alpha \) (up – or down – spin sublattice).

The dynamics is governed by the Hamiltonian

\[ H = \sum_{(n,n')} J_{nn'} S_n S_{n'}, \]  

where the sum is taken only over nearest-neighbours. The couplings \( J_{nn'} \) obey a probability distribution of the bond percolation type

\[ P(J_{nn'}) = p \delta (J_{nn'} - J) + (1 - p) \delta (J_{nn'}). \] 

The results should not be significantly different for a site-dilution problem [12], which is appropriate to the experimental system studied in reference [1].

As stated above, within the EMA, the random system is replaced by a periodic one, with frequency-dependent complex coupling \( W(\omega) \). Practically this is done as follows. Imagine all couplings to be replaced by the effective coupling \( W(\omega) \), except for one bond, which is allowed to fluctuate with the percolation, equation (13). The equation for the Green’s function, \( g \), of this simplified problem, is [11],

\[ g = G + GTG. \]  

Here, \( G \) is the Green’s function of the uniform effective medium, with all couplings having the value \( W(\omega) \), and \( T \) describes the scattering from the single fluctuating bond. The \( W(\omega) \) are determined self-consistently by requiring the scattering matrix, \( T \), to vanish upon averaging with the given distribution, equation (13). The equation for the Green’s function, \( G \), of this simplified problem, is

\[ \frac{G(q, \omega)}{\omega^2 - W^2 q^2} = W^2(q^2). \] 

Here \( \omega \) and \( W \) are in units of \( J \).

The density of states resulting from equation (17) is as follows. In the magnon regime, we find

\[ N(\omega) \sim \frac{\omega^2}{\omega_c^2}, \quad \omega \ll \omega_c, \]  

while,

\[ N(\omega) \sim \omega^{-\frac{4}{3}}, \quad \omega \gg \omega_c, \] 

for the fracton regime. Thus, within EMA, the fracton dimensionality \( d = 2/3 \), to be compared with the conjectured value of 4/3. The EMA result for the density of magnon states, clearly does not generate the correct prefactor in equation (8) as derived from scaling considerations.

The exponent is consistent with scaling because of equation (4) and \( \theta_{EMA} = 4 \).

The structure factor \( S(q, \omega) \), measured in scattering experiments, is directly proportional to the imaginary part of the Green’s function. Using equation (17), it may be cast into a quasi-Lorenzian form

\[ S(q, \omega) \propto \frac{c(\omega) q^2}{\omega} \left[ \frac{\tau^{-1}(\omega)}{(\omega - c(\omega) q^2 + \tau^{-2}(\omega))} + \frac{\tau^{-1}(\omega)}{(\omega + c(\omega) q^2 + \tau^{-2}(\omega))} \right], \] 

with a frequency dependent effective stiffness coefficient,

\[ c(\omega) \approx |W|^2 / \text{Re} W, \] 

and a life-time,

\[ \omega \tau(\omega) \approx \text{Re} W / \text{Im} W. \] 

Numerical solution of the self-consistent equation for \( W(\omega) \) (Eq. (15)), for a simple cubic lattice \( (z = 6) \),...
yields the \( c(\omega) \) and \( (\omega T(\omega))^{-1} \) curves shown in Figure 1. As expected, \( c(\omega) \) is constant in the magnon regime, obeying a linear dispersion relation, while in the fracton region it has a power-law dependence on \( \omega \). The ratio \( c(\omega)/(p-p_c) \) does not depend strongly on \( p-p_c \) over the full frequency range.

![Fig. 1. The effective stiffness coefficient \( c(\omega) \) (normalized by \( p-p_c \)) for \( p-p_c = 10^{-3} \), and the inverse life-time \( T^{-1}(\omega) \) [made dimensionless by plotting \( (\omega T(\omega))^{-1} \)] for several values of \( p-p_c \), within EMA. In the latter, note the absence of scaling in the magnon regime, \( \omega/\omega_c < 1 \). \( c(\omega)/(p-p_c) \) is hardly dependent on \( p-p_c \).](image-url)

The life-time obeys Rayleigh's law, equation (6), in the magnon regime, and crosses-over to the Ioffe-Regel limit, equation (7) in the fracton regime, just as predicted by scaling arguments. However, the EMA result for \( (\omega T(\omega))^{-1} \) does not entirely conform to scaling requirements, since the curves, plotted against \( \omega/\omega_c \), still show dependence upon \( p-p_c \).

In Figure 2, \( S(q,\omega) \) is shown as a function of \( \omega/\omega_c \), for several values of \( q\xi \). It is seen that EMA reproduces some important features of the experimental data [1]. For \( q\xi < 1 \), the magnon contribution is sharply peaked around \( \omega(q) = cq \), while a broad fracton contribution is found around \( \omega_c \), with a long tail extended to higher frequencies. For \( q\xi > 1 \), only the fracton contribution remains, and it is strongly overdamped, consistent with localization.

### 4. Conclusion

We have adapted the fracton scaling model to describe the magnetic excitations of a diluted AF on a percolation network. The crossover to a fractal structure at small length scale induces a crossover from magnon to fracton dynamics at a characteristic frequency \( \omega_c \). The fractons are strongly localized collective modes, and their localization length is the only relevant length scale to a description of the spectrum above \( \omega_c \).

More detailed description of the spectrum is provided by the EMA. We have calculated the scattering structure factor, and found it to resemble the response measured in inelastic-neutron-scattering of diluted AF [1]. A disconcerting feature of EMA is, however, that it is not entirely consistent with scaling requirements. It suggests the need for another frequency scale (or, equivalently, length scale) to describe the excitation dynamics [5]. However, Green's function perturbation calculations of Cristou and Stinchcombe find only a single length scale for AF [14]. In view of an alternative approximation for the Green's function [16], which is found to obey scaling for vibrational excitations, we believe that absence of scaling for AF is also an artifact of EMA. Indeed, numerical calculations of the structure factor \( S(q,\omega) \) for deterministic fractals confirm that \( S(q,\omega) \) is a scaling function of \( q^{(2+\epsilon)/2}/\omega \), in the fracton regime [17].

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