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Pair correlations and structure factor of the J_1-J_2 square lattice Ising model in an external field

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HIGHLIGHTS

- Compute pair correlation functions of the J_1-J_2 model in an external field.
- Analyze local maxima in the structure factor and its relation with phase transitions.
- Identify the disorder variety of the model.

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ABSTRACT

We compute the structure factor of the J_1-J_2 Ising model in an external field on the square lattice within the Cluster Variation Method. We use a four point plaquette approximation, which is the minimal one able to capture phases with broken orientational order in real space, like the recently reported Ising-nematic phase in the model. The analysis of different local maxima in the structure factor allows us to track the different phases and phase transitions against temperature and external field. Although the nematic susceptibility is not directly related to the structure factor, we show that because of the close relationship between the nematic order parameter and the structure factor, the latter shows unambiguous signatures of the presence of a nematic phase, in agreement with results from direct minimization of a variational free energy. The disorder variety of the model is identified and the possibility that the CVM four point approximation be exact on the disorder variety is discussed.

1. Introduction

The structure factor, being a quantity of direct experimental access by neutron scattering and many other spectroscopic techniques, is a central quantity in condensed matter physics [1,2]. Mathematically, it is the Fourier transform of the connected pair correlation function, and as such its knowledge gives direct access to fluctuations and phase transitions associated to them. Computing the structure factor then amounts to compute correlation functions, which is known to be a hard task in statistical mechanics models. In order to characterize a phase transition it is often possible to look at simpler one-point quantities, typically order parameters, like the magnetization or the density. A qualitative understanding of a phase transition can be obtained by simple mean field approximations. If one wants to compute universal quantities, like

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critical exponents, then it is necessary to go beyond mean field approximations, for example through a Renormalization Group analysis. But there are special kinds of order which are essentially associated with fluctuations and then, even if one is interested in a qualitative description, simple mean field theory does not work. This is the case, e.g. of broken orientational phases in systems with competing interactions [3,4]. When a competing attraction and repulsion or ferromagnetic and anti-ferromagnetic interactions are simultaneously present, the system can develop modulated structures in the form of stripes or bubbles [3]. These structures break rotational symmetry of space but may not break translational symmetry, giving rise to phases with intermediate (in temperature or external field), purely orientational or nematic-like order, in analogy with the nematic phases of liquid crystals [5,2]. Anisotropic phases with nematic-like order are relevant, e.g. in low dimensional systems like electronic liquid-crystals [6–9] and ultrathin ferromagnetic films [10–13].

In order to characterize these nematic-like phases from microscopic models it is necessary to go beyond naive mean field approximations. In particular, the orientational or nematic order parameter in two dimensional modulated systems is proportional to the difference between correlation functions in two orthogonal space directions [4,14]. As will be better described below, a nematic order parameter can be defined as a weighted integral of the structure factor. Then, computing the structure factor gives direct access to the nematic-like order in systems with competing interactions and orientational order.

In a lattice, a systematic way of obtaining better approximations for the thermodynamics of a system is to consider clusters of increasing size exactly. The Cluster Variation Method (CVM) is one of a family of cluster techniques [15–18]. Although of mean field character, it allows to improve considerably the locus of phase transition lines, specially for systems with competing interactions where naive mean field usually gives a very poor approximation to the phase diagram. It is also suitable for computing approximations to multipoint correlation functions in a systematic way. The CVM has been applied previously to compute the structure factor of a few models as the ferromagnetic Ising model [19] and the two dimensional ANNNI model [20]. In Ref. [21] the authors introduced a general approach for the computation of the structure factor within the Cluster Variation Method, and applied it to the Ising model with nearest neighbors (NN), next-nearest neighbors (NNN) and plaquette interactions in two and three dimensions. For the case of NN and NNN interactions in the square lattice, the so called $J_1 - J_2$ Ising model, they computed the structure factor at zero external field in the paramagnetic phase. The phase transition lines between paramagnetic, ferromagnetic and collinear (stripe) phases where characterized and the presence of a disorder line in the paramagnetic phase was obtained within the approximation and discussed in relation to the exactly known result [22]. Interestingly, in Ref. [22], the four point CVM approximation was proved to render the exact solution of the model at zero external field. In a recent work, we applied the CVM to the $J_1 - J_2$ Ising model in an external field [23] and found a nematic phase of the kind discussed above, which had not been identified previously. Because of the close relation between the nematic order parameter and the structure factor, we decided to extend the method of Ref. [21] to compute the structure factor of the model in an external field in the whole phase diagram, i.e. also in the relevant ordered phases.

Results on the $J_1 - J_2$ Ising model may be relevant to understand part of the phenomenology of high temperature superconductors, specially the iron pnictides. For these compounds, a much studied model is the quantum Heisenberg $J_1 - J_2$ [24,25,8]. This model was shown to have a Ising-nematic phase driven by spin fluctuations, which break the Z_4 symmetry of the square lattice, without the development of anti-ferromagnetic order [24]. Strong spin fluctuations in this 2D system induce a biquadratic or quadrupolar interaction leading to Ising-like behavior in spin space and eventually to the presence of an Ising-nematic phase. Nevertheless, it is not clear if the quadrupolar coupling is strong enough to apply to the experimental compounds which show $J_1 - J_2$ behavior. Another route to nematic order in the pnictides seems to be related with doping. Recent results of Monte Carlo simulations on a model with magnetic, electronic and orbital degrees of freedom imply that the nematic phase is enhanced through Fe substitution by impurities, i.e. by introducing quenched disorder and magnetic dilution in the parent compound [26]. Very recently, Kitada et al. [27] reported on an extensive series of experiments on the layered perovskite $RbLaNb_2O_7$ transformed by substitution of the Rb on the oxyhalides $(MCl)LaNb_2O_7$ (M=Mn, Cr, Co), which are two dimensional antiferromagnets. Neutron diffraction measurements show the presence of magnetic modulations with wave vectors $(0,\pi)$ for the samples with Mn and Co. The samples with Cr showed instead a (π, π) Néel antiferromagnetic structure. Interestingly, hysteresis measurements on the $(CoCl)LaNb_2O_7$ compound indicate a way to saturation in two steps, as the field is raised. This is interpreted as Ising-like behavior, in which the striped ground stated is destabilized by a ferromagnetic component by first flipping half of the antiferromagnetic stripes and at a higher field value the other half is flipped, leading to the completely saturated state. If confirmed, this is the first compound to show a phenomenology typical of the Ising $J_1 - J_2$ model studied in the present work.

In the following, we make a brief discussion of known results on the $J_1 - J_2$ Ising model, the CVM approach, and compute the structure factor of the model in presence of an external field in the whole parameter range. We interpret the results in connection with the recently published phase diagram [23]. We also identify the disorder variety of the model in an external field and discuss the possible exactness of the four point CVM approximation on this variety.

2. $J_1 - J_2$ Ising model and the CVM approximation

The $J_1 - J_2$ Ising model on the square lattice is defined by the Hamiltonian:

$$\mathcal{H} = J_1 \sum_{\langle xy \rangle} S_x S_y + J_2 \sum_{\langle\langle xy \rangle\rangle} S_x S_y - h \sum_x S_x, \tag{1}$$