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Spin-wave theory analytic solution of a Heisenberg model with RKKY interactions on a Bethe lattice ☆

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Abstract

An analytic solution for the Heisenberg Hamiltonian with long-range RKKY interactions on a Bethe lattice is obtained in the semi-classical approximation ($S \to \infty$). The main difficulty that has to be overcome is the exponential growth of the number of neighbors in a Bethe lattice. We suggest a way of handling this problem and derive physically meaningful results.

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1. Introduction

The Heisenberg Hamiltonian [1,2] has been a powerful tool in the description and understanding of a large variety of magnetic systems [3,4], ever since it was independently put forward, three quarters of a century ago, by Heisenberg [1,2] and Dirac [5,6]. However, and in spite of numerous and significant efforts, few analytic results have been achieved [7]. This is in sharp contrast with the wealth of approximate and numerical results that have been obtained during this time span.

A significant feature of most of the treatments implemented so far is that they are limited to nearest-neighbor interactions. At least three reasons explain this state of affairs: (i) generally the magnetic exchange interaction originates in the direct overlap of orbitals on neighboring ions and thus decays rapidly with distance; (ii) the considerable additional complications the inclusion of longer-range interactions implies; and (iii) the fact that the magnitude of the longer-range interactions was not well established until very recently. However, the powerful development of the ab initio computational machinery has allowed extraction of precise values of exchange integrals, even beyond the ten first neighbors. An example of the latter is the computation by Zhou et al. [8] of the J_k's, for $1 \leq k \leq 11$, of antiferromagnetic fcc Fe and Mn. These results are quite surprising: not only does the sign of the J_k's display an oscillating behavior, but also a much slower decay with k than expected. In fact, the values of $|J_{11}/J_1| \sim 0.06$ for Fe and 0.014 for Mn were obtained. Even more remarkable is the fact that, for this fcc structure, the absolute value of the computed next-nearest-neighbor exchange parameter $|J_2|$ for Fe is larger in magnitude than $J_1 \approx -0.134$ mRy, yielding $|J_2/J_1| \approx 1.42$. The same happens with the sixth-neighbor for which $|J_6/J_1| \approx 1.10$.

The above situation is not at all limited to particular elementary metals. In fact, in FeF_2 and MnF_2, both materials of interest for the manufacture of spin-valve devices [9], also the first-neighbor exchange is slightly ferromagnetic, while the second-neighbor one is antiferro and significantly larger in magnitude [10].

In addition, there are several systems, such as the rare earths and their alloys, where the exchange interaction is well known to be long-ranged. The magnetic order of these materials is adequately described by the RKKY interaction, initially introduced by Ruderman and Kittel [11] to describe the indirect interaction of two nuclei via their

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hyperfine coupling with the conduction electron sea. Later on, the mechanism was extended, and widely applied, to the indirect exchange interaction of the f-shells of rare-earth ions [12,13]. The experimental evidence, obtained by neutron diffraction [14,15], shows that many of the rare earths order magnetically, principally in ferromagnetic and helical structures.

In a recent paper, we presented an analytic solution of the Heisenberg Hamiltonian with long-range interactions on a Bethe lattice, in the spin-wave approximation [16]. The latter approximation corresponds to the semi-classical limit in which the spin component in a given direction is quasi-continuous [17,18] or, equivalently, the spin S is assumed $S \to \infty$. In spite of its semi-classical nature, it has contributed to the understanding of magnetism and provided many surprisingly accurate results [16,19,20], even in the extreme quantum limit $S = 1/2$.

As far as the topology is concerned, the Bethe lattice allows one to treat problems, which are too difficult to handle on a regular (Bravais) lattice, while keeping constant the number of nearest neighbors. In other words, each lattice point maintains the same coordination, but the closed loops that are present in a Bravais lattice disappear. This simplified topology has been widely used, for example in the treatment of the anisotropic next-nearest-neighbor Ising model (ANNNI) [21–23].

In 1983, Trias and Yndurain [24] obtained an analytic solution of the Heisenberg Hamiltonian with long-range interactions on a Bethe lattice. In our recent work [16], we removed the restriction of using a ferromagnetic ground state as the initial configuration and, thus, we were able to obtain analytically the one-magnon excitation spectrum for an arbitrary helical structure, including the classical ferro- and antiferromagnetic initial configurations.

The aim of this paper is to focus our attention on the RKKY interaction and tackle the difficulties that the use of the Bethe lattice topology brings about. These difficulties are due to the exponential growth of the results as a function of the coordination number and we suggest a way to properly treat this problem. In addition, we study the commensurability effects between the exchange field and the lattice periodicity.

This paper is organized as follows: after Section 1, we present the model and its solution in Section 2. Next, in Section 3, we apply the model to the RKKY interaction and discuss its implications for the physical properties of these systems, in particular for the magnetic ordering of the rare earths. The paper is closed in Section 4 with a summary and the drawing of conclusions.

2. Model and formalism

Our system consists of an arrangement of atoms located on the nodes of a Bethe lattice. Each atom has a single degree of freedom: its spin component along a spatial axis is subject to an arbitrarily long-ranged interaction. That is, the spin $\vec{S}_j$ (at site j) interacts, with a coupling constant J_{jk} with spin $\vec{S}_k$ (at site k) located at a distance L. This distance L is measured in units of the Bethe lattice parameter a, which we adopt as our unit of length.

The Heisenberg Hamiltonian for our system thus reads

$$H = -\frac{1}{2}\sum_{j,k} J_{j,k}\vec{S}_j\vec{S}_k, \tag{1}$$

where the sum extends over all pairs (j,k) so that $j \neq k$. The factor 1/2 compensates for the double counting.

Our treatment of the system dynamics is carried out using Zubarev-type [25] Green functions. The initial configuration is assumed to be helical and the constant angle between adjacent spins is denoted by θ. Obviously, making $\theta = 0$ leads to the re-derivation of the results obtained by Trias and Yndurain [24]. $\theta = \pi$, on the other hand, implies the adoption of the Néel antiferromagnetic ground state as the starting configuration. Without repeating the analysis of Ref. [16], to which we refer the interested reader for details, we write down the one magnon dispersion relation $\omega(k)$, for the case of a Bethe lattice of coordination c and lattice parameter a. It reads

$$\omega_\theta(\phi) = \sqrt{W_1(\phi,\theta)W_2(\phi,\theta)}, \tag{2}$$

where $\phi = ka$, and W_1 and W_2 are given by

$$W_1(\phi,\theta) = \sum_{n=1}^{\infty} V_n \cos(n\theta)\Bigg[c(c-1)^{n-1} - (c-1)^{n/2} \times\left(2\cos(n\phi) + \frac{c-2}{c-1}\frac{\sin[(n-1)\phi}{\sin(\phi)}\right)\Bigg], \tag{3}$$

$$W_2(\phi,\theta) = \sum_{n=1}^{\infty} V_n\Bigg[\cos(n\theta)c(c-1)^{n-1} - (c-1)^{n/2} \times\left(2\cos(n\phi) + \frac{c-2}{c-1}\frac{\sin[(n-1)\phi]}{\sin(\phi)}\right)\Bigg]. \tag{4}$$

Above $V_n = SJ_n$ corresponds to the interaction of two spins S which are separated by n lattice parameters. This yields, for the local density of states at the lattice origin $D_0(\omega)$

$$D_0(\omega) = \frac{2c(c-1)}{\pi}\frac{\sin^2[\phi(\omega)]}{c^2 - 4(c-1)\cos^2[\phi(\omega)]}\frac{d\phi}{d\omega}, \tag{5}$$

where ϕ is obtained solving the implicit Eq. (2). Finally, the angle θ is obtained by minimization of the per site energy $E(\theta,k)$, given by the $N \gg 1$ limit of

$$E(\theta,k) = -\frac{S}{2}\sum_{n=1}^{\infty} V_n c(c-1)^{n-1}\cos(n\theta) + \frac{\omega_\theta(k)}{N}. \tag{6}$$

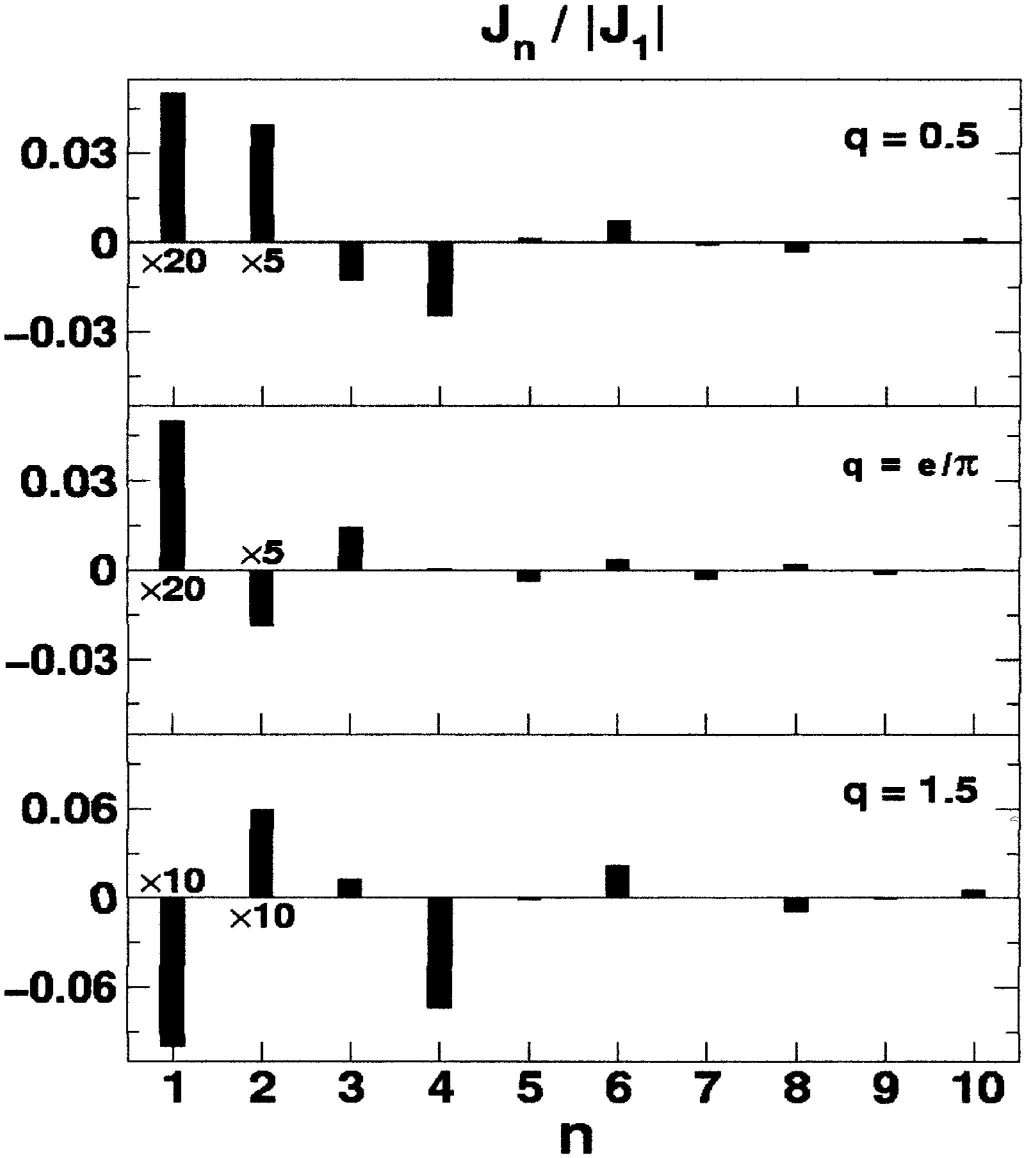

Fig. 1. Exchange coupling constant J_n, normalized to the module of the nearest-neighbor interaction. In order to make visible the values of J_n for $n > 2$, the magnitudes of J_1 and J_2 have been rescaled by the factor indicated in the graph.

3. RKKY interaction

The 15 elements with atomic number $57 \leq z \leq 71$ are denominated lanthanides or rare earths. They have very strongly localized 4f states, which make the lanthanide atom magnetic, unless all states are either empty or completely full. In a solid, the 4f states on different ions interact, via the long-range RKKY indirect exchange coupling, and their magnetic behavior can properly be described by the Heisenberg Hamiltonian. The explicit form of the indirect interaction is given by

$$V_n = Jq^4 \frac{\sin(\pi qn) - \pi qn \cos(\pi qn)}{(\pi qn)^4} = \frac{Jq^2}{(\pi n)^2} j_1(\pi qn), \quad (7)$$

where J is a positive constant introduced to scale the magnitude of the exchange coupling, while q is defined as

$$q = \frac{2k_F}{k_B^{\max}} = \frac{2k_F a}{\pi}, \quad (8)$$

and j_1 is the index 1 spherical Bessel function.

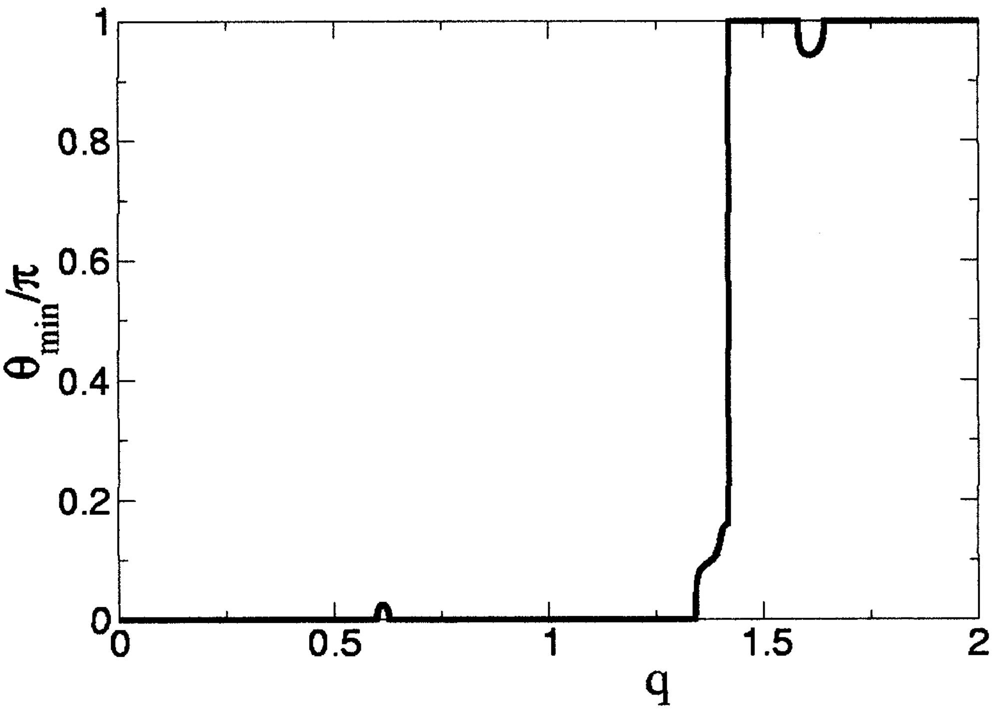

Fig. 2. Angle between neighboring spins along the Bethe lattice, as a function of the commensurability parameter q, calculated on the basis of replacing the number of neighbors by the fcc Bravais lattice value.

Above, in Eq. (7), it is usual to include an exponential decay factor to incorporate mean free path effects, which limit the range of the interaction. Since we are considering a perfect lattice at zero temperature, we will ignore this decay factor. However, if one does incorporate a weakening of the interaction with distance its only consequence is to reinforce the effect of the first-neighbor interaction. It is noticed that V_n is a spatially decaying oscillatory function of distance $\propto n$. On the other hand, q characterizes the commensurability of the interaction with the lattice periodicity; integer and half-integer values of q correspond to commensurate interactions. The following are several examples of commensurate q values, except for the second row ($q = e/\pi$), which is incommensurate:

The analytic properties of the spherical Bessel function allow one to develop an understanding of the strongly oscillating interactions V_n of Eq. (7). For small nq values $V_n > 0$, i.e. it is always ferromagnetic; this is the case while $nq < 1.43$, value that corresponds to the first zero of j_1. It is important to stress that, due to the fact that the RKKY interaction decreases rather rapidly with distance (actually as $r_{i,j}^{-3}$), the dominant term is always V_1, and $V_1 > 0$ as long as $q < 1.43$. Thus, in spite of the fact that the RKKY interaction is long-ranged, its strong decrease with interatomic separation, in the case of a lattice, limits its effects to a few neighbors. We illustrate this behavior in Fig. 1.

We now turn our attention to the per site energy as given by Eq. (6). For the RKKY interaction, it adopts the form

…	n	=	1	2	3	4	5	6	7	8	9	10
$q = 1/2$ |	sgn(V_n)	=	+	+	−	−	+	+	−	−	+	+
$q = e/\pi$ |	sgn(V_n)	=	+	−	+	+	−	+	−	+	−	+
$q = 1$ |	sgn(V_n)	=	+	−	+	−	+	−	+	−	+	−
$q = 3/2$ |	sgn(V_n)	=	−	+	+	−	−	+	+	−	−	+
$q \to 2$ |	sgn(V_n)	=	−	−	−	−	−	−	−	−	−	−

Since it is our interest to study both commensurate and incommensurate systems, we allow q to vary in the interval]0, 2[. The value $q = 0$ implies $k_F = 0$, and $q = 2$ corresponds to a full band; both these limits are physically uninteresting.

$$E(\theta, k = 0) = \frac{1}{2} J S q^4 \sum_{n=1}^{\infty} \left(\frac{\sin(\pi q n) - \pi q n \cos(\pi q n)}{(\pi q n)^4} \right) \times Z_c(n) \cos(n\theta), \tag{9}$$

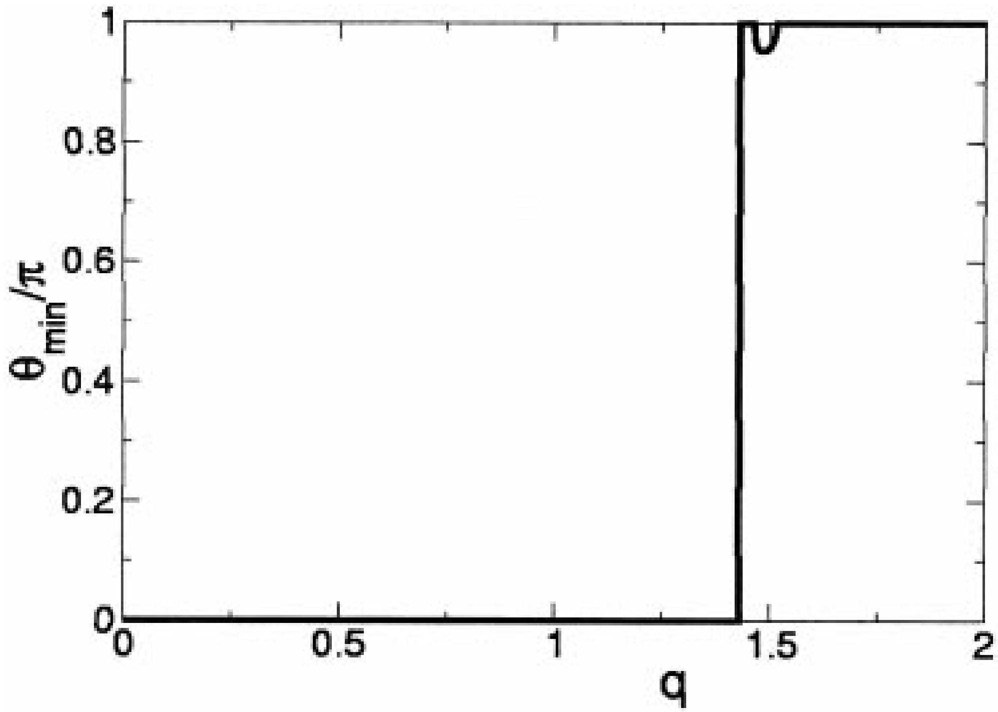

Fig. 3. Angle between neighboring spins along the Bethe lattice, as a function of the commensurability parameter q, calculated on the basis of replacing the number of neighbors by the hcp Bravais lattice value.

where $Z_c(n) = c(c-1)^{n-1}$ is the number of n-nearest neighbors on a Bethe lattice of coordination c. The angle between consecutive spins is obtained minimizing E with respect to θ. However, the sum in Eq. (9) only converges for the trivial linear chain ($c = 2$) case. This constitutes an undesired consequence of choosing the Bethe lattice topology and we now focus our attention on surmounting this shortcoming.

It is a known fact that the number of neighbors on a Bethe lattice grows exponentially with n, while the interaction strength only decreases as n^{-3}. To visualize this trend, it is sufficient to realize that, in an N-atom 3D Bravais lattice, the number of surface atoms is $N^{2/3}$. For a quantitative illustration, we mention that, for the fcc and hcp lattices of coordination $c = 12$ we are interested in, the number of 10th nearest neighbors is of the order 10^2, while for a Bethe lattice, it is of order 10^{10}. The way we treat this overestimate is to substitute the number of neighbors, given by $Z_c(n) = c(c-1)^{n-1}$, with the actual number of neighbors on the particular Bravais lattice of interest.

The results of implementing this procedure are given in Figs. 2 and 3, where the angle θ as a function of q for both the fcc and hcp lattices is plotted. It is observed that, in both cases, the formalism yields ferromagnetism for $q < 1.3$, while for $q > 1.5$, the ground state is antiferromagnetic, in agreement with previous authors [7]. Moreover, it is also apparent that the transition between the two magnetic phases is quite abrupt and coincides with $q \approx 1.4$, which corresponds to the first change of sign of the nearest-neighbor interaction V_1. However, the fcc structure exhibits two narrow regions of helical order; one around $q = 0.6$, in the ferromagnetic region, with a rather long pitch compared to the lattice parameter. Another helically ordered region appears in the antiferromagnetic domain, around $q = 1.6$, with a pitch of around two lattice parameters, and which is slightly wider than the $q = 0.6$ region.

On the contrary, the hcp case of Fig. 3 exhibits a featureless ferromagnetic region, with an abrupt transition to antiferromagnetism. In the antiferromagnetic regime, a helically ordered region, also with a pitch of around two lattice parameters, is observed around $q = 1.6$.

The results for the angle between contiguous spins $\theta(q)$ only exhibit an abrupt transition, from ferromagnetism to antiferromagnetism, at $q \approx 1.43$, the first zero of V_1. It should be kept in mind that our model makes several approximations, like spherical Fermi surfaces and forcing the angles between nearest-neighbor spins to be constant, which preclude the possibility of a detailed comparison with experiment.

4. Summary and conclusions

For many years, the RKKY interaction has been extensively used [14,15] to describe the magnetic properties of the rare earths. In this paper, an analytic treatment of the Heisenberg Hamiltonian with RKKY long-range interactions on a Bethe lattice topology was developed, on the basis of a formalism we presented previously [16].

While the Bethe lattice topology allows one to derive an analytic solution, there is a price that has to be paid: for coordination $c > 2$, the number of neighbors is grossly overestimated in relation to a Bravais lattice of the same coordination. We tackled this problem by substituting the Bethe lattice $Z_c(n)$ value with the actual number of neighbors of the particular Bravais lattice we chose to study. Once this substitution is implemented, we obtain results in satisfactory qualitative agreement with the literature [7].

We found that for the RKKY interaction, the magnetic ordering is dominated by the nearest-neighbor exchange coupling, which is significantly larger than the rest, as long as $q < 1.4$, for the fcc and hcp structures. In both cases, for small q values, the system is ferromagnetically ordered and undergoes a rather sharp transition to antiferromagnetism around $q = 1.4$. The transition is slightly smoother in the fcc structure, which displays a narrow intermediate helically ordered region.

Another feature worth mentioning is the fact that the commensurability of q with the lattice symmetry is irrelevant as far as the magnetic ordering is concerned. Actually, it is the change of sign of the first-neighbor interaction, as q varies, which is the key element to trigger the ordering transition.

In summary, we have developed an analytic treatment for the Heisenberg Hamiltonian with long-range RKKY interactions on a Bethe lattice and suggested a way to handle the exponential growth in the number of neighbors this topology implies.

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