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Magnetic excitations in the longitudinally amplitude modulated magnetic structure of PrNi₂Si₂

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Abstract. Interest in PrNi₂Si₂ has been renewed recently because the magnetic structure remains longitudinally amplitude modulated down to low temperatures as inferred from single-crystal neutron diffraction. Based on a dynamical matrix diagonalisation (DMD) formalism considering exchange and crystal field interactions, we have calculated the dispersion of the magnetic excitations of PrNi₂Si₂ below the Néel temperature. The prediction of a low-energy soft-mode excitations around the scattering vector (0, 0, Q_z) within the first Brillouin zone, where $Q_z \equiv k_z = 0.875$ is the value of the propagation vector of the magnetic structure, is in good agreement with the experimental results obtained from inelastic neutron scattering.

1. Introduction

Nature shows different examples of spatially modulated systems, where the periodic phase is a lattice distortion, a charge-density wave, or an ordered magnetic structure. In particular, in rare-earth intermetallic compounds the oscillatory and long-range character of the indirect exchange interactions (Ruderman-Kittel-Kasuya-Yosida type) mediated from one site to another through the conduction-band electrons, leads naturally to the existence of modulated magnetic structures [1, 2, 3, 4, 5]. If also the system has a strong easy-axis anisotropy (due to crystal effects) the resulting magnetic structure may be amplitude modulated (AM), i.e., the size of ordered magnetic moments changes from one site to other. These magnetic structures are characterized by their propagation vector \vec{k} which is incommensurate with the lattice periodicity. For many materials, amplitude-modulated structures are often stable only just below the magnetic transition temperature, T_N .

One of such representative cases for a longitudinally AM magnetic structure is Er metal [2], in which the ordered magnetic moments are parallel to the c-axis of the hexagonal close packed crystal structure between $T_N = 84$ K and 52 K. In this temperature region, the transverse magnetic excitations show a quite broad energy distribution owing to the fact that both exchange and anisotropy energies are changing from site to site, while the longitudinal fluctuations gives rise to rather sharp peaks showing a linear dispersion [6]. These experimental results can be accounted for by a random-phase-approximation (RPA) formalism that uses a N-site diagonalization of the molecular-field Hamiltonian, although some aspects have no clear explanation: above T_N , some of the calculated dispersion branches are not observed; below T_N , the RPA does not explain the appearance of a quasielastic signal found for both polarizations.

The fact that in Er metal the AM structure is only stable at relative high-temperatures makes the analysis much more difficult.

The body-centered tetragonal rare-earth intermetallic compound PrNi_2Si_2 is of particular interest in this context, as it represents one of the few examples in nature of an AM magnetic structure that is stable down to zero temperature, as was recently inferred from single-crystal neutron diffraction [7]. The existence of a singlet crystal-field ground state in PrNi_2Si_2 that is coupled to the excited levels is responsible for the AM ordered magnetic moment, which is confined to be along the c -axis due to single-ion anisotropy. The magnetic structure at low temperature (4 K) is well described by a single wave vector $\vec{k} = (0, 0, k_z)$ with $k_z = 0.87$ (in rlu) such that the magnetic moment at the site l is given by $\langle M_l^z \rangle = \cos(2\pi z k_z)$, where z is the coordinate of the Pr^{3+} ions. The magnetic excitations of the amplitude-modulated phase of PrNi_2Si_2 have been studied by inelastic neutron scattering [8, 9]. They reveal the existence of a low-energy longitudinal excitation whose energy strongly decreases close to \vec{k} , where its intensity is considerably enhanced. These features motivated us to develop a magnetic model aiming to get a better insight in the nature of the magnetic excitations in an AM structure, based on recent progress in the diagonalisation of the dynamical matrix [10]. In this work, we apply the DMD formalism to calculate the dispersion of the magnetic excitations and the related inelastic neutron scattering cross section of PrNi_2Si_2 .

2. Direct matrix diagonalization method

The quantitative analysis of the inelastic neutron scattering is based on the dynamical susceptibility formalism [11]. The Hamiltonian includes both crystal field and exchange interactions. The calculations were performed with the McPhase program [12, 13]. For the case of PrNi_2Si_2 , the five crystal field parameters and two parameters characterizing the Fourier transform $J(\vec{q})$ of the exchange interactions, namely, $J(\vec{q} = 0) = -0.211$ K and $J(\vec{q} = \vec{k}) = 2.27$ K, were obtained from a joint analysis of the specific heat, magnetic susceptibility and magnetization and inelastic neutron scattering measurements on a single crystal of PrNi_2Si_2 [8, 9, 14, 15, 16]. The magnitude of the ordered moments of the Pr^{3+} ions within a magnetic period have been obtained from a N-site self-consistent periodic-field model within the mean field approximation, using $N=16$ and an effective propagation vector $\vec{k}_{eff} = (0, 0, 0.87/2) \sim (0, 0, 7/16)$ (in rlu). The use of a rational value for the modulation of the magnetic structure is required for the numerical calculations.

The measured and calculated dispersion curves of the magnetic excitations along the ΓZ direction of the first Brillouin zone are shown in Figure 1.

The theoretical dependence accounts for the principal features observed experimentally, namely: i) the strong Q -dependence of both the energy and intensity of the lowest longitudinal mode ($E \sim 1.5$ meV) is clearly reproduced; ii) the higher longitudinal and transverse modes appear much more fragmented and the maximum intensity of the magnetic excitations is not necessary found to be close to $(1, 1, 2 - k_z)$; iii) the high energy excitations ($E \sim 6.5$ meV) are weak with almost no dispersion. Presumably the existence of a broad band of excitations (longitudinal and transverse) between 3.5 meV and 5.5 meV is related to the presence of singlet and doublet crystal field excited levels around 40–60 K. In this way, the experimental dispersion curves show that a long-range longitudinal amplitude modulated magnetic structure removes all the spin waves excitations and the energy spectrum is essentially dispersionless, in contrast to the case of a simple ferromagnet, where the spin waves are strongly dispersive. The magnetic and charge distributions can be calculated within our model for the soft mode at $\vec{Q} = \vec{K} + \vec{k}$ with $K = (1, 1, 2)$. The results are shown in Figure 2.

Clearly, PrNi_2Si_2 has important charge density fluctuations associated with the purely magnetic excitations, and the former needs to be taken into account in order to obtain a complete picture of the dynamics of the system.

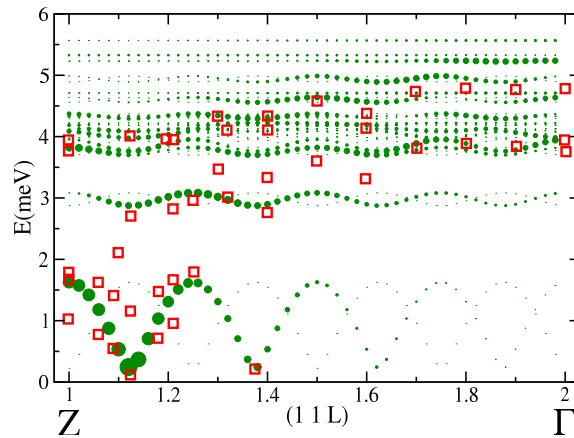


Figure 1. Experimental (open squares) and calculated (solid circles) dispersion curves for PrNi_2Si_2 at 4 K along the ΓZ of the Brillouin zone direction with neutron scattering vectors $(1, 1, L)$. The size of the solid circles is proportional to the intensity of the excitations.

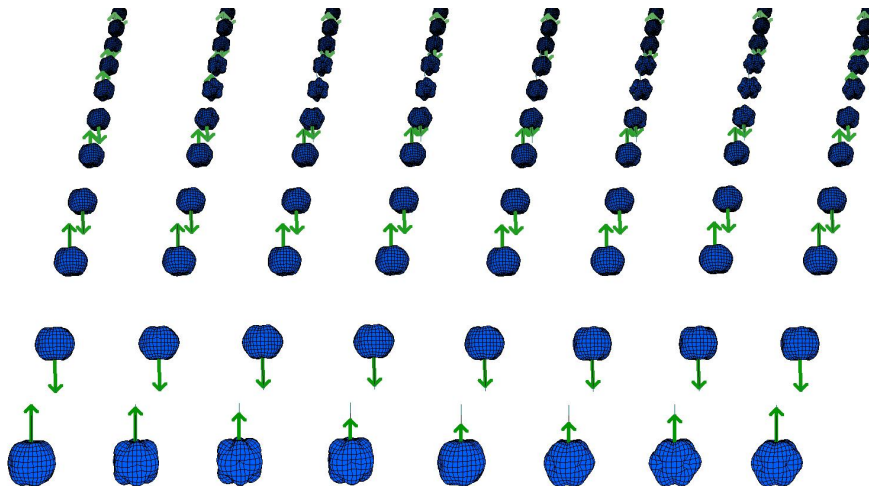


Figure 2. Magnetic and charge oscillations for the soft magnetic mode at the neutron scattering vector $\vec{Q} = (1, 1, 2 - k_z)$ in PrNi_2Si_2 measured at 4 K. The magnetic moments are represented by arrows, constant charge density surfaces are shown in blue. A line of Pr^{3+} ions along $[111]$ is shown for different times of the oscillation.

3. Conclusions

In conclusion, the combination of a strong uniaxial anisotropy and competing exchange interactions in PrNi_2Si_2 is responsible for the existence of an amplitude modulated structure. This magnetic ordering is stable down to zero temperature, and displays the presence of soft magnetic modes whose intensity is enhanced when the scattering vector is close to the propagation vector of the magnetic structure. Further inelastic neutron scattering experiments with high resolution are needed to elucidate the nature of the lowest longitudinal excitations.

Acknowledgments

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