

Atomistic modelling of amorphous magnets

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Amorphous magnetism was a popular topic of study in the 1970s. Nevertheless, amorphous magnets are still commonly used in experiments and applications, such as GdFeCo for magneto-optics and CoFeB for spintronics. Modelling of these materials is often done using random lattice models or homogeneous systems, ignoring the true local disorder. Here, I will present methods and results from our studies where we attempt to include the true atomic disorder.

We use reverse Monte Carlo methods to generate realistic amorphous structures based on experimental X-ray and neutron diffraction data. We then use a Heisenberg Hamiltonian with distance-dependent exchange interactions and solve the Landau-Lifshitz-Gilbert equation to study the dynamics and thermodynamics of these systems. In particular, we studied CoP [1], a material where past experiments suggested the possible existence of roton-like magnon excitations [2].

We calculated the inelastic neutron scattering cross-section from our non-lattice model and found a feature at the same location as the supposed roton dip (Fig. 1). Our conclusion, however, is that this feature is a remnant of short-range local order, rather than an exotic magnon excitation.

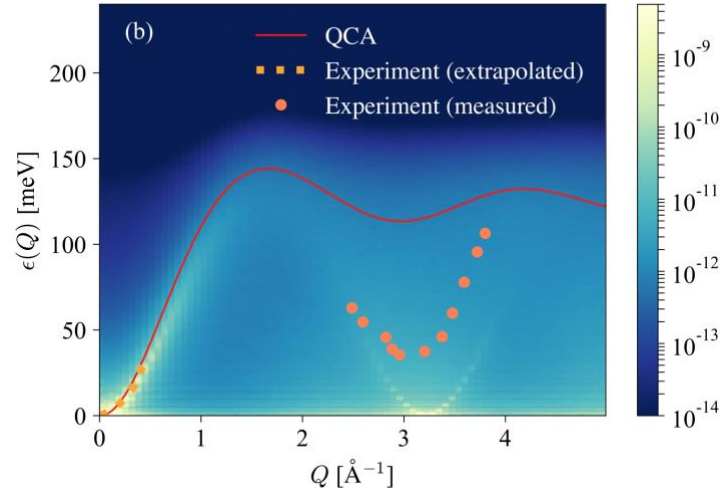


Fig.1: Calculated inelastic neutron scattering cross section of Co_4P compared with red: quasi-crystalline approximation (QCA) and orange: experimental inelastic neutron measurements of the ‘roton-like’ excitations.

[1] M. Kameda *et al.*, Magnon spectrum of the amorphous ferromagnet Co_4P from atomistic spin dynamics, *Phys. Rev. B* **106**, L060403 (2022)

[2] H.A. Mook *et al.*, Magnetic Excitations in the Amorphous Ferromagnet Co_4P , *Phys. Rev. Lett.* **34**, 1029 (1975)