

Nickel(II) cyanide as a physical realisation of the anisotropic 1D quaternion chain

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One-dimensional statistical mechanical models continue to assume a particular importance in contemporary condensed-matter physics. Common themes amongst one-dimensional systems are (i) the absence of long-range order and (ii) the emergence of collective behaviour (e.g. in the form of quasiparticles with their own continuous excitation profile).^{1,2}

Much of the focus within the field thus far has been on systems with one-dimensional electronic or magnetic behaviour, yet, it has long been known that the one-dimensional Ising model is also relevant to the structural behaviour of some bulk phase. This mapping can be used to interpret otherwise unexpected physical properties of these fundamentally important systems.

In our work we consider the problem of structural disorder in the layered inorganic material nickel(II) cyanide and demonstrate its relevance to a simple one-dimensional model of interacting anisotropic quaternions. The continuous degrees of freedom in the model are related to those of the $S=1/2$ particle. Our more general interest is in establishing meaningful correspondences between complex structural states and exotic magnetic and/or electronic phases in order to develop physical realisations of the latter for detailed study or exploitation.

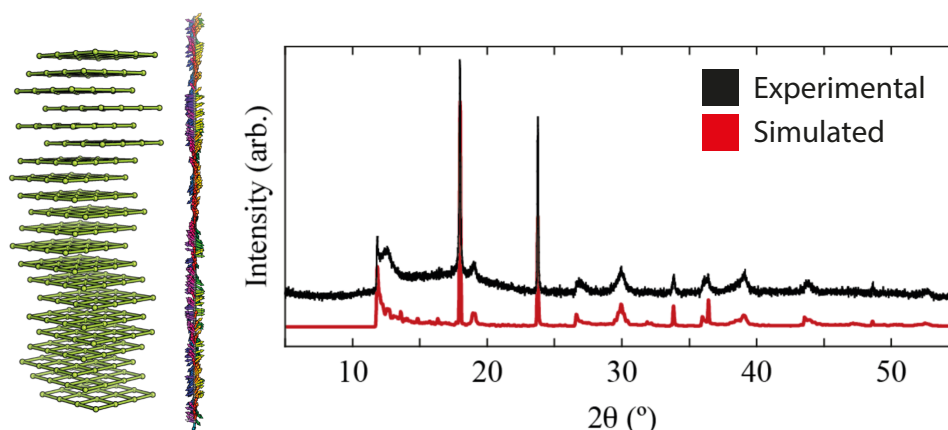


Figure 1. Mapping of nickel cyanide displacements such that the positions of the layers to be represented as quaternions projecting in four-dimensional space. Experimental (black) and simulated (red) X-ray diffraction patterns of nickel cyanide.

We show that the sheet position (x,y) can be mapped onto the unit quaternion \mathbf{p} torus (Fig. 1) where as x,y vary between 0 and 1, \mathbf{p} traces a surface on the hyper sphere known as a Clifford torus. X-ray and neutron diffraction patterns therefore exhibit the mixture of sharp (Bragg) and diffuse features, characteristic of correlated disordered states.³ Carrying out Monte Carlo simulations of the one-dimensional chain and mapping this back onto the structure of nickel

cyanide displacements we have calculated the X-ray diffraction pattern which reproduces the features of the experimental pattern remarkably well (Fig. 1).

1. M. Steiner, J. Villain, and C. G. Windsor, *Adv. Phys.* **25**, (1976), 87-209.
2. H.-J. Mikeska and A.K. Kolezhuk, *Lect. Notes Phys.*, **645**, (2004), 1–83
3. A. L. Goodwin *et al.*, *Phys. Rev. B*, **80**, (2009), 054101