Understanding the emergence of CDW order in KCP via a 2D XY model

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Charge density wave (CDW) systems are of fundamental and enduring importance because of the competition between incipient CDW formation and superconductivity, and the possible application of CDW ground states in driving low thermal conductivity for efficient thermoelectric processes. A CDW is a periodic modulation of the carrier density coupled to the crystal lattice. The electronic modulation normally coexists with a periodic lattice distortion (PLD).

An interesting CDW compound is the Krogmann's salt, $K_2Pt(CN)_4Br_{0.3} \cdot xH_2O$ [1], which was thoroughly studied in the '70. The CDW phase can be found thanks to the sub- structure made of columnar stacks of $[Pt(CN_4)]^{1.7-}$ ions, where the distance between Pt is of 2.9 Å, similar to the metallic distance. At the same time, the distance between Pt-chains is of ~10 Å, leading to highly anisotropy behaviour associated with a partially-filled d_z^2 band. The phase transition happens in two steps, with a first CDW formation at ~600K and the final 3D structure ordering at ~77K [2]. The phase transition can be considered "sluggish" and a useful model to describe it is the 2D XY model, where the phase of the charge density wave is described as a 'pseudo-spin'. A total neutron scattering technique was chosen in order to detect and separate the inelastic and elastic contribution and follow the diffuse scattering evolution through the phase transition.

References

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