**CoE EQUITANT Seminar**

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# Spin model of volborthite $Cu_3V_2O_7(OH)_2{\cdot}2H_2O$ revisited: coupled trimers instead of zigzag chains

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Motivated by recent experiments on volborthite single crystals showing a wide 1/3-magnetization plateau, we adopt the structural data and perform microscopic modeling using density functional theory (DFT). By combining a tight-binding analysis based on Wannier projections with DFT+$U$ total energy calculations, we find four leading exchanges: antiferromagnetic $J$ and $J_2$, as well as ferromagnetic $J'$ and $J_1$, comprising a model of coupled magnetic trimers [1]. This model is different from the coupled frustrated chain model [2] proposed in our earlier study.

Simulations of the spin Hamiltonian show good agreement with the experimental susceptibility and magnetization curves for $J$:$J'$:$J_1$:$J_2$ = 1:–0.2:–0.5:0.2 with $J \simeq$ 252 K [1]. The dominance of $J$ implies that the 1/3-plateau is a product state of nearly independent polarized trimers (Fig. 1, right). Effective models around the $J \rightarrow \infty$ limit show a tendency towards condensation of bound magnons preceding the plateau. This picture was recently supported by an NMR study [3].

A peculiarity of volborthite is the pronounced difference between the magnetization data measured on single crystals and powder samples. I will show how this bewildering behavior can be rationalized in terms of partial structural disorder and the orientation of magnetic trimers.

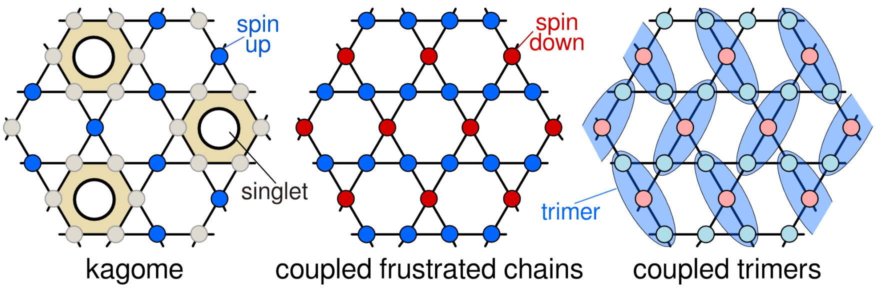


Fig. 1. The structure of the 1/3-magnetization plateau in the kagome model, coupled frustrated chains model from Ref. [2], and the $J$:$J'$:$J_1$:$J_2$ model.

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[1] O. Janson, S. Furukawa, T. Momoi, P. Sindzingre, J. Richter, and K. Held, PRL **117**, 037206 (2016).

[2] O. Janson, J. Richter, P. Sindzingre, and H. Rosner, PRB **82**, 104434 (2010).

[3] M. Yoshida, K. Nawa, H. Ishikawa, M. Takigawa, M. Jeong, S. Kramer, M. Horvatic, C. Berthier, K. Matsui, T. Goto, S. Kimura, T. Sasaki, J. Yamaura, H. Yoshida, Y.

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