Properties of the antiferromagnetic Cr8 ring calculated from a multi-band Hubbard Hamiltonian

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Molecular magnets are clusters composed of finite numbers of magnetic centers surrounded by organic ligands. In these materials magnetic phases are formed mostly due to strong intra-cluster interactions. Theoretical tools most often used to describe molecular magnets consist of spin Hamiltonian approach [1] or density functional theory calculations [2]. Recently, it has been proposed to study these systems by applying a perturbation theory to the multi-band Hubbard like Hamiltonian [3]. We elaborate this approach by performing exact numeric calculations on a version of the multi-band Hubbard Hamiltonian. It allows us to calculate an approximate energetic spectrum and thermodynamic properties. We then compare our results with available experimental data and with oucomes obtained by other, aforementioned theoretical methods. In particular, we focus our attention on $Cr_8F_8(O_2CH)_{16}$ molecule ($Cr8$ in short), which is a ring-like shaped antiferromagnetic molecular magnet.

References:

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