Model Hamiltonian for three-centered spin-electric systems

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The field of quantum computing has many advantages over classical computing including secure communication and data driven search for materials and drugs discovery. Over the last two decades enormous effort has been focused on discovery, synthesis, and technology of materials suitable for this purpose. Among many studied and proposed candidates, single-molecule magnets show promising behaviors, such as slow relaxation of magnetism, for being considered as qubits. The control of these systems, when possible, with an external electric field, rather than magnetic field, provides a faster and more space-confined strategy for manipulating the spin states in these materials. A novel class of these molecules are the three-center molecules with antiferromagnetic coupling between spin-carrying centers. The appearance of an electric dipole moment in these molecules makes the control of their spin-spin interaction via direct coupling to an electric field even more feasible. A theoretical framework in which the interactions between the charge cloud on the centers with external stimuli is correctly described is necessary for understanding how the spin-spin interactions and/or spin-orbit couplings change as a function of applied electric field. Using a formalism proposed by Khomskii [1], we have developed a computational framework to estimate charge, dipole moment and spin-electric coupling in three-center molecules. In this talk I will discuss the generalized Hamiltonian used in our method, compare it to other existing methods which use other parametrizations, and will show our results on a group of three center molecules with centers of Fe, Mn, Co, and Ni to demonstrate the effect of electric field on the properties of these molecules. I will further show how this framework can be applied to understanding as well as predicting of spin-electric effects in single-molecule magnets.

[1] D. Khomskii, *Nat Commun* **3,** 904 (2012).