Strongly anisotropic S=1 (pseudo)spin systems: from mean field to quantum Monte-Carlo

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The S=1 pseudospin formalism was suggested to describe the charge degree of freedom in a model high-T_c cuprate [1] with the on-site Hilbert space reduced to the three effective valence centers, nominally $Cu^{1+;2+;3+}$. With small corrections the model becomes equivalent to a strongly anisotropic S=1 quantum magnet in an external magnetic field. We have applied several techniques from a generalized mean-field approach, special algorithm for CUDA architecture for NVIDIA graphics cards and classical Monte-Carlo technique [2], to two different quantum Monte-Carlo methods to find the ground state with its evolution under deviation from half-filling and T-n phase diagrams for the model S=1 system. Special attention is given to the role played by on-site correlation (single-ion anisotropy) and emergent topological structures.

References:

[1] A.S. Moskvin, JETP 121, 477 (2015); Journal of Physics: Conference Series 592 012076 (2015).
[2] A.S. Moskvin, Yu.D. Panov, F.N. Rybakov, A.B. Borisov, J. Supercond. Nov. Magn. 30, 43 (2017).