Variational approach to spin-orbital polarons in $KCuF_3$

K. Bieniasz,[1,2] M. Berciu,[2] and A.M. Oleś[1,3]

[1] *Institute of Physics, Jagiellonian University, Kraków, Poland*

[2] *Department of Physics, University of British Columbia, Vancouver, Canada*

[3] *Max Planck Institute for Solid State Research, Stuttgart, Germany*

Copper-fluoride perovskite, $KCuF_3$, is a quintessential spin-orbital system that exhibits long range order in both spin $S = 1/2$ and orbital e_g degrees of freedom. Its ground state has alternating-orbital order in the *ab* planes (C-AO) and antiferromagnetic chains along the *c* direction (A-AF). An electron injected into the system can move freely within the ferromagnetic *ab* planes, or couple to either of the polaronic degrees of freedom by generating excitations in the system. Coupling to orbital excitations produces quasiparticle states with a well developed band in the whole Brillouin zone and an increased effective mass [1], whereas magnetic excitations seem to primarily scatter the electron. We develop a spin-orbital, t-J-like model, whose full treatment has never been attempted before, and solve it using the variational approximation, which is an exact, primarily analytical method for solving Green's functions by means of equations of motion. We present a number of spectral results and analyse the nature and properties of the quasiparticles arising in the system.

References:

[1] K. Bieniasz, M. Berciu, M. Daghofer, and A.M. Oleś, Phys. Rev. B **94**, 085117 (2016)