Finite temperature cluster mean-field calculation of spin-orbital state of $LaMnO_3$ crystal

Mateusz Snamina[1] and Andrzej M. Oleś[2]

[1] *Faculty of Chemistry, Jagiellonian University, Kraków, Poland*

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

$LaMnO_3$ crystal is a textbook example of interplay between spin and orbital degrees of freedom. In this crystal there is one e_g electron per each manganese ion which together with three t_{2g} electrons gives a total spin $S = 2$. In this case Kugel-Khomskii-like superexchange model is supplemented by the Jahn-Teller orbital interactions between Mn ions [1]. Commonly disentanglement of spin-orbital terms and on-site mean field approximation are used to estimate the transition temperatures. In our work [2] we went beyond these approximations and performed cluster calculations at finite temperature to verify them and to determine bond correlations. We have found opposite trends: $(i) \sim 10\%$ increase of the Néel temperature (T_{N}) due to on-site, and $(ii) \sim 10\%$ decrease of T_{N} due to on-bond spin-orbital entanglement. Altogether our results confirm that the spin-orbital interactions are indeed disentangled in $LaMnO_3$.

References:

[1] A. M. Oleś, G. Khaliullin, P. Horsch, and L. F. Feiner, Phys. Rev. B **72**, 214431 (2005).
[2] M. Snamina and A. M. Oleś, Phys. Rev. B **94**, 214426 (2016).