Finite temperature cluster mean-field calculation of spin-orbital state of LaMnO$_3$ crystal

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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: