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How spin-orbital entanglement depends on spin-orbit coupling in a Mott insulator

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Strong relativistic spin–orbit coupling (SOC) in 4d and 5d materials leads to novel phenomena such as the complex phase behaviour observed in the extended Kitaev-Heisenberg model [1]. In this context we investigate spin–orbital entanglement (SOE) which plays a crucial role in the understanding of strongly correlated electrons in transition metal oxides. We study a transparent example of the intimate relation between quantum entanglement and SOC. To this end we numerically diagonalize one-dimensional spin–orbital model with the SU(2) ⊗ SU(2) 'Kugel – Khomskii' exchange supplemented by SOC of the Ising type for chains up to L = 20 sites [2].

We observe a substantial difference in the entanglement for small versus large SOC. While most of the features of the ground state with small SOC resemble the vanishing SOC limit, the phase diagram for large SOC regime is divided between the classical fluctuation—free region and surprisingly vast region where quantum fluctuations persist, including highly quantum 'stripe'—like area with maximal SOE. From a broader perspective, these results provide a basis to infer the generic properties of entanglement in transition metal oxides with finite SOC at higher dimension.

[1] J. Rusnacko, D. Gotfryd, and J. Chaloupka, Phys. Rev. B 99, 064425 (2019)
[2] D. Gotfryd, E. M. Paerschke, J. Chaloupka, A. M. Oles, and K. Wohlfeld, Phys. Rev. Research 2, 013353 (2020), Condens. Matter 5, 53 (2020)

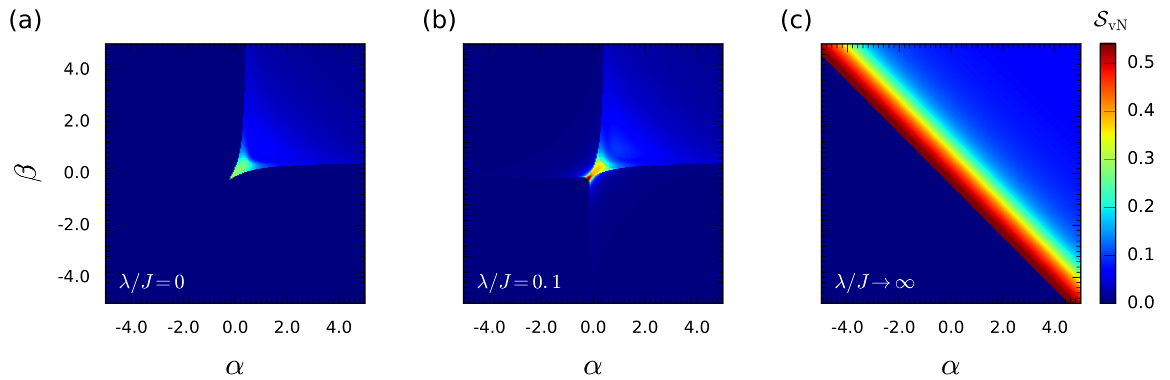

Figure 1 : Evolution of the spin-orbital entanglement entropy SvN in the on-site spin-orbit coupling parameter λ . Figure has been published in [2].