# The low-energy models of Mott insulators with a finite spin-orbit coupling

Dorota Gotfryd, Faculty of Physics at the University of Warsaw


## *Abstract*

This dissertation deals with the low-energy physics of the Mott-insulating systems with a finite spin-orbit coupling. In general, for the Mott-insulating materials one sees a finite charge gap in experiments, while the conventional density functional theory predicts them to be metals. If the materials in question belong to the class of the $3d$ transition metal compounds, the on-site Coulomb repulsion $U$ is large enough to open the charge gap. In contrast, for some of the $4d$ and $5d$ transition metal compounds the realistic $U$ value is too weak to open the gap and simulating the insulating behaviour is possible only after taking into account the on-site spin-orbit coupling, significant for these materials.

Recently it has been shown that the low energy models for two materials belonging to the latter class—$Na_2IrO_3$ and $\alpha$-$RuCl_3$, contain the celebrated Kitaev term, whose ground state is exactly solvable Kitaev spin liquid—a highly quantum entangled state. This drove immense interest to the field due to the topologically protected excitations possible for the gapped versions of the state, giving hope for the stable qubits. Despite the materials turning out to be magnetically ordered instead, the hope for realising Kitaev physics is not completely gone, and the continuous effort to estimate the "distance" of the above materials coupling parameters to the Kitaev spin liquid regions on the phase diagrams of the so-called Kitaev-like models is starting to bring fruits.

In this dissertation we consider the physics of the Mott insulators with a large spin-orbit coupling in two contexts:

*Firstly*, we consider which ground state properties of the Kitaev-like models can be measured experimentally and whether they can help with localizing $Na_2IrO_3$ and $\alpha$-$RuCl_3$ in the parameter space of the models. To this end we calculate the dependence of the ordered moment on the parameters of the Kitaev-like models, and compare it to the experimentally obtained magnetic moment of $Na_2IrO_3$ and $\alpha$-$RuCl_3$. We thoroughly discuss the relevance of our predictions in narrowing down the range of Hamiltonian parameters for the materials in question and suggest further steps how to improve the computations.

*Secondly*, we explore how one can induce quantum entanglement (which is one of the defining features of the Kitaev spin liquid) by finite spin-orbit coupling. Thus, we investigate the spin-orbital entanglement evolution with increasing spin-orbit coupling on the example of the minimal 1D model for a Mott insulator with a finite spin-orbit interaction, consisting of the $SU(2)\otimes SU(2)$ symmetric (Kugel-Khomskii) term and the on-site spin-orbit coupling term of the Ising type. In particular, we examine the relation between the quantum entanglement in the effective degrees of freedom enforced by the large spin-orbit coupling and the spin-orbital entanglement in the full spin-orbital model. As a result, we find that even the classical spin-orbit coupling can both enhance and suppress the spin-orbital entanglement and we discuss the universality of this result.