Study of Kane-Mele-Hubbard ladders with DMRG-MPS

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Topological insulators are materials which behave as insulators in the bulk, but present topologically protected metallic states on the edges, therefore differing from usual insulators. Despite the extensive recent research on these materials, there are still many unanswered questions regarding the effects of electronic interaction on the properties of such systems. The goal of this project is to study these effects by applying the Kane-Mele-Hubbard (KMH) model to a hexagonal chain.

Following the tight-binding approach, the KMH Hamiltonian can be written as

$$\hat{H}_{\text{KMH}} = -t \sum_{\langle i,j \rangle, s} c_{i,s}^\dagger c_{j,s} + i\lambda_{\text{SO}} \sum_{\langle\langle i,k \rangle\rangle, s} c_{i,s}^\dagger \hat{e}_{ik} \cdot \sigma_{s,s'} c_{k,s'} + U \sum_{i,s} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

where $c_{i,s}^\dagger$ ($c_{i,s}$) creates (destroys) an electron with spin $s$ in the site $i$, $\hat{n}$ is the number operator, $\sigma$ is a vector of the Pauli matrices and the notation $\langle...\rangle$ and $\langle\langle...angle\rangle$ refers to sums over first and second neighbours on the hexagonal chain.

The first term corresponds to the kinetic energy of electrons, obtained through the tight-binding approximation, while the second term is given by the spin-orbit coupling and the third term is the Hubbard interaction on each site of the chain.

In the absence of electronic interaction, the KMH model includes a topological phase with edge states, which can be studied analytically. However, when electronic interactions are considered, it becomes necessary to take use of a computational approach, namely the density matrix renormalization group (DMRG) written in the matrix product states (MPS) representation. In this work, we study the KMH model in two-leg hexagonal ladders. As a preliminary step, we calculate the energy states for the non-interacting ($U=0$) ladder with both hard-wall and periodic boundary conditions in the ladder direction. We then move to the $U>0$ case, using the Itensor package to obtain the ground-state of the system with DMRG-MPS.

The DMRG calculations performed focus on the interesting regime in which spin-orbit interactions and Coulombic repulsion have the same order of magnitude, where the expected behaviour is a phase transition between the topological insulator regime and an usual Mott insulator phase.