Magnetic properties of graphene nanoflakes with Kane-Mele spin-orbit coupling

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Graphene nanoflakes have unique magnetic properties. Their so-called zigzag edges are spin-polarized. The reason is that this kind of edge introduce edge states, which can form a degenerate shell at the Fermi level. The degeneracy of this shell, and, in consequence, the magnetic properties of the flake are determined by its size and shape. Also, the magnetic ordering is geometry-dependent: it can be ferromagnetic, antiferromagnetic or ferrimagnetic [1].

Here we study magnetism in triangular zigzag nanoflakes, where the edges have ferromagnetic polarization. We investigate the behaviour of this polarization under the influence of spin-orbit coupling. In systems with large degeneracy, the correlations become important. Indeed, in the graphene nanoflakes they lead e.g. to spin depolarization after adding one electron [2]. To describe the correlations we use the exact diagonalization technique. As a starting point we use the tight-binding model with spin-orbit coupling described by Kane-Mele model [3]. We describe the electron-electron interaction with Hubbard model and extended Hubbard model. The comparison of these two allows us to investigate the role of long-range interaction. We study the electronic and magnetic properties of the flake in function of spin-orbit coupling strength. We find that increasing the spin-orbit coupling strength splits the degenerate shell and, in consequence, leads to spin depolarization of the flake.

References

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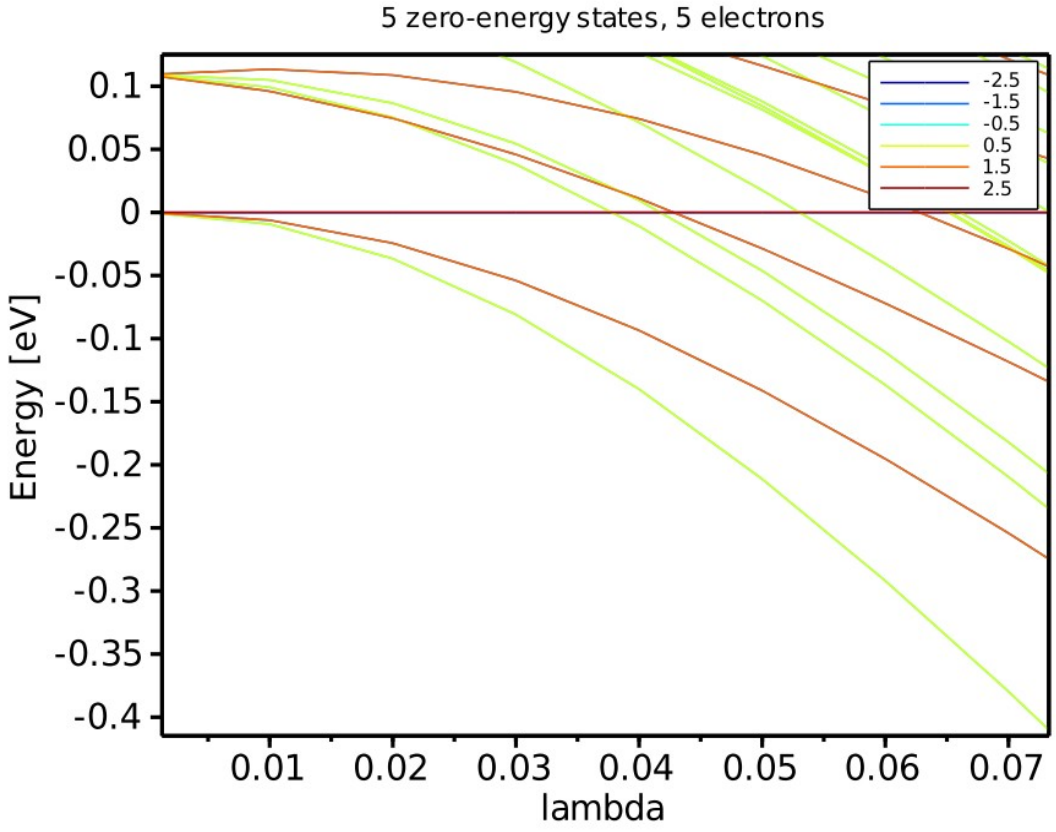
Figures



Energy spectrum of a charge-neutral 61-atom graphene nanoflake as a function of spin-orbit coupling strength λ. The calculation was done within the Hubbard model. Colours denote the S_z spin projection of the eigenstate.