Magnetism and Correlations of Fractionally Filled Zero-energy States in Graphene Quantum Dots

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Graphene quantum dots are atomically thick nanometer-scale islands etched out of a single graphene sheet. In this work, we focus on electronic and magnetic properties of triangular dots with zig-zag edges. Strikingly, such structures were suggested [1,2] to lead to a band of degenerate zero-energy states at the Fermi level (Dirac point). Therefore, electrons in the zero energy band (shell) can be expected to form a strongly correlated electronic system, in analogy with the fractional quantum Hall effect. The degeneracy is proportional to the edge size and can be made macroscopic. This opens up a possibility of designing strongly correlated systems as a function of the fractional filling of the shell at the zero energy, in analogy with the quasi-two-dimensional electrons exhibiting the fractional quantum Hall effect, but without the need for magnetic field. Furthermore, it was shown [1,2] that within Hubbard approximation the edges of the dot are spin polarized and the ground state can be treated as a solid ferromagnet.

In this work, we present new results demonstrating the important role of electronic correlations, beyond the Hubbard and mean-field models [1,2]. The interactions are treated by a combination of density functional theory (DFT), tight-binding, Hartree-Fock and configuration interaction methods (tb-HF-CI). In addition to the on-site interaction term, all scattering and exchange terms within second nearest neighbors, and all direct interaction terms are included in the calculations. Our model also includes the effect of next nearest neighbor hopping term, positive background charge, and charge induced on the gate. We show that the magnetic properties of the ground and excited states of triangular graphene quantum dots are strongly dependent on the filling fraction of the band of zero-energy states and on the dot size, in contrast with the Hubbard model that favorizes fully magnetized zero-energy states.

[1] J. Fernandez-Rossier and J.J. Palacios, *Phys. Rev. Lett.* **99** 177204 (2007).
[2] M. Ezawa, *Phys. Rev.* **B 77**, 155411 (2008).