Electron-electron interaction in graphene quantum dots

Błażej Jaworowski[1], Paweł Potasz[1], and Devrim Güçlü[2]

[1] *Institute of Physics, Wrocław University of Technology, PL-50-370 Wrocław, Poland*
[2] *Department of Physics, Izmir Institute of Technology, IZTECH, TR35430, Izmir, Turkey*

We investigate electron-electron interaction effects in graphene quantum dots using variational and diffusion quantum Monte Carlo (QMC) tehniques. Following the recent isolation of a single graphene layer, both experimental and theoretical research on graphene structures has increased exponentially due to their unique physical properties and promising potential for technological applications, especially in nanoscale electronics [1, 2, 3]. Recent theoretical work based on tight-binding and configuration interaction approach has shown that many-body correlation effects due to electron-electron interactions can play an important role in the electronic and magnetic properties in graphene quantum dots [4, 5, 6]. In this work, we build accurate many-body trial wave functions using tight-binding and density functional theory molecular orbitals multiplied by a Jastrow factor [7, 8]. Once the trial wave function is optimized, we perform diffusion Monte Carlo calculations to obtain fixed-node solutions, which allow us to investigate electronic and magnetic structure of small graphene quantum dots of various sizes and shapes.

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