Mott transition in the Hubbard model on anisotropic honeycomb lattice with implications for strained graphene

Adam Rycerz,[1] Grzegorz Rut,[1,2] Maciej Fidrysiak,[1] and Danuta Goc-Jagło[1]

[1] *Institute for Theoretical Physics, Jagiellonian University, Łojasiewicza 11, PL-30348 Kraków, Poland*

[2] *Verisk Analytics Sp. z o.o., Rakowicka 7, PL–31511 Kraków, Poland*

Modification of interatomic distances due to high pressure leads to exotic phenomena, including metallicity, superconductivity and magnetism, observed in materials not showing such properties in normal conditions. In two-dimensional crystals, such as graphene, atomic bond lengths can be modified by more that 10 percent by applying in-plane strain, i.e., without generating high pressure in the bulk. In this work, we study the strain-induced Mott transition on a honeycomb lattice by using computationally inexpensive techniques, including Gutzwiller Wave Function (GWF) and different variants of Gutzwiller Approximation (GA), obtaining the lower and upper bounds for critical Hubbard repulsion (U) of electrons. For uniaxial strain in the armchair direction the band gap is absent, and electron correlations play a dominant role. A significant reduction of the critical Hubbard U is predicted. Model considerations are mapped onto tight-binding Hamiltonian for monolayer graphene by the auxiliary Su-Schrieffer-Heeger model [1,2] for acoustic phonons, assuming zero stress in the direction perpendicular to the strain applied. Our results suggest that graphene, although staying in semimetallic phase even for extremely high uniaxial strains, may show some measurable signatures of electron correlations.

References:

[1] G.Rut, M.Fidrysiak, D.Goc-Jagło, and A.Rycerz, Int. J. Mol. Sci. 24, 1509 (2023).

[2] D.Suszalski and A.Rycerz, Phys. Rev. B 102, 165408 (2020).

The work was supported by the National Science Centre of Poland (NCN) via Grant No. 2014/14/E/ST3/00256. Computations were partly performed using the PL-Grid infrastructure.