Cyrill Muratov (New Jersey Institute of Technology)

A Non-local Variational Problem Arising from Studies of Nonlinear Charge Screening in Graphene Monolayers

Abstract

This talk is concerned with energy minimizers in an orbital-free density functional theory that models the response of massless fermions in a graphene monolayer to an out-of-plane external charge. The considered energy functional generalizes the Thomas-Fermi energy for the charge carriers in graphene layers by incorporating a von-Weizsaecker-like term that penalizes gradients of the charge density. Contrary to the conventional theory, however, the presence of the Dirac cone in the energy spectrum implies that this term should involve a fractional Sobolev norm of the square root of the charge density. We formulate a variational setting in which the proposed energy functional admits minimizers in the presence of an out-of-plane point charge. The associated Euler-Lagrange equation for the charge density is also obtained, and uniqueness, regularity and decay of the minimizers are proved under general conditions. In addition, a bifurcation from zero to non-zero response at a finite threshold value of the external charge is proved. This is joint work with J. Lu (Duke University) and V. Moroz (Swansea University).