Faizan Nazar (Ceremade)

Locality of the TFW equations

Abstract

In this talk, I will discuss the properties of solutions to the Thomas-Fermi-von Weizscker equations. This is a system of coupled PDEs, arising from Density Functional Theory, that models the ground state electron density corresponding to a given nuclear arrangement. In addition to the known existence and uniqueness results, I will introduce a locality property for solutions. This is a pointwise stability estimate that demonstrates the exponential response of the electron density to a perturbation of the nuclei.

As the main application, I will also introduce the lattice relaxation problem, which considers the rearrangement of a crystal lattice after the introduction of a defects as a variational problem. Using the locality estimates, we can formulate the relaxation problem and establish far-field decay properties for minimising displacements.

This talk is based on joint work with Huajie Chen and Christoph Ortner.