Vienna School of Mathematics

PhD Colloquium

Lorenzo Pigozzi

Mathematical Insights into Density Functional Theory

Abstract: Density Functional Theory (DFT) is one of the most widely used methods in computational chemistry and physics, providing an efficient framework for studying the electronic structure of atoms, molecules, and solids. This talk focuses on the mathematical foundations of DFT, in particular Lieb's framework, which rigorously defines the universal functional using convex analysis and variational principles. Key properties of , such as convexity and lower semicontinuity, will be discussed along with their practical implications. The talk will also explore the Local Density Approximation (LDA) as a practical realization of, highlighting its strengths, limitations, and connection to Lieb's approach. By linking theory and application, the talk provides some key ideas for the foundations of DFT and outlines challenges for future research.

January 13 2024, 16:50-17:50

Seminarraum 13, Universität Wien
(Oskar-Morgenstern-Platz 1)