

数学与系统科学研究院

计算数学所学术报告

报告人: Dr. Faizan Qadeer NAZAR

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报告题目:

Locality of the TFW equations

邀请人: 戴小英 副研究员

报告时间: 2018年3月26日(周一)

上午 10:00--11:00

报告地点: 数学院南楼N902 教室

报告摘要:

In this talk, I will discuss the properties of solutions to the Thomas-Fermi-von Weizsäcker 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.

欢迎大家参加！