TEMPLE UNIVERSITY

Department of Mathematics

Analysis Seminar

Room 617 Wachman Hall

Monday, November 18, 2013, 2:40 p.m.

Density functional theory and Donsker-Varadhan

by Omar Hijab Department of Mathematics Temple University

At the basis of much of computational chemistry and physics is density functional theory, as initiated by the Hohenberg-Kohn theorem. The theorem states that, when nuclei are fixed, nuclear potentials are determined by oneelectron densities. We recast and derive this result within the context of the principal eigenvalue of Markov semigroups.