UNIVERSITY OF TORONTO
FACULTY OF ARTS & SCIENCE | Department of Mathematics

Departmental PhD Thesis Exam

Monday, August 12th, 2024 at 2:00 p.m. (sharp)
via Zoom / BA6183

PhD Candidate : Sebastian Tudor Gherghe

Supervisor : Professor Israel Michael Sigal

Thesis title : On Adiabatic Quantum Molecular Dynamics

Abstract

In this thesis, we consider the time-dependent Born-Oppenheimer approximation of a non-relativistic quantum molecule involving a possibly large number of nuclei and electrons described by the Schrödinger equation. The full molecular equation is difficult to solve and compute approximations for, due to the highly oscillatory nature of the solutions in space and time and due to the high dimensionality of the state space. In the spirit of Born and Oppenheimer, we study quantitatively the approximation of the molecular evolution. We obtain an iterable approximation of the molecular evolution to arbitrary order and we derive an effective equation for the reduced dynamics involving the nuclei, equivalent to the original Schrödinger equation and containing no electron variables (thus reducing the large state space of the full evolution). For example, a molecule of ozone O_3 contains 3 nuclei and 24 electrons. The state space for the full molecular evolution is the symmetry subspace of $L^2(\mathbb{R}^{81})$, while the reduced dynamics involving only the nuclei occurs on the smaller state space $L^2(\mathbb{R}^9)$. We estimate the coefficients of the new equation and find tractable approximations for it.