« Atelier sur les méthodes mathématiques et informatiques pour les systèmes quantiques » 11 au 14 décembre 2018

> "Workshop on Mathematical and Computational Methods for Quantum Systems" December 11-14, 2018

Strong-field induced vibronic coupling

Michael Spanner*

michael.spanner@nrc-cnrc.gc.ca

Strong laser fields can significantly distort the electronic wave functions of atoms and molecules. When the field-free molecule possesses symmetries, the laser-induced spatial distortion of the electronic wave functions couples field-free electronic states of different symmetries. It is shown in this talk that this symmetry mixing gives rise to strong-field-induced vibronic couplings (i.e. derivative and scalar non-Born-Oppenheimer couplings) that would have been zero by symmetry in the field-free case. Formally, these couplings are the non-Born-Oppenheimer components of the polarizability interaction. A new field-dependent coupling term, similar in origin to the Stark-shift term, is derived that allows one to include the field-induced vibronic effects into time-dependent Schrödinger equation (TDSE) simulations. These ideas are explored using N2+ in a strong laser field as a test-case.

^{*}Quantum Theory Group, National Research Council of Canada, 100 Sussex, Ottawa, ON K1A 0R6, CANADA