Title: Excitation of molecules by cold electrons

Author: Miroslav Šulc

Department / Institute: Institute of Theoretical Physics, Charles University in Prague

Supervisor of the doctoral thesis: prof. RNDr. Jiří Horáček, DrSc.,
Institute of Theoretical Physics, Charles University

Abstract: Several methods for low energy collisional processes are investigated. In the first part, attention is especially devoted to examination of applicability of the R-matrix method combined with the Schwinger-Lanczos (SL) variational principle for potential scattering with long-range forces. Next sections deal with the development of the interaction correlation-polarization (CP) potential in the framework of the Discrete Momentum Representation (DMR) method on the grounds of the Local Density Approximation in the Density Functional Theory (DFT) context. Obtained results are then utilized in body-frame (BF), static exchange + polarization (SEP), calculations within an analysis of experimental data for $e^-$–$N_2$ scattering comprising a part of a larger project addressing theoretical examination of rotational excitations of small molecules in the gas phase induced by electron impact. For $N_2$, a new phenomenon consisting in suppression of backward cross-section below 95 meV is observed and consequently attributed to destructive interference in the angular $l \leq 1$ space. Treatment for polar molecules introduces generalized dipole phase shifts determined by fitting to the experimental data. Their knowledge enables then to determine the differential as well as individual stat-to-state cross-sections. This approach is demonstrated on experimental data for $CH_3Cl$ and $SO_2$.

Keywords: R-matrix, Discrete Momentum Representation (DMR), low energy electron-molecule collisions, dipole interaction, Volterra integral propagator