EIPAM Exchange Grant - Final Report

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Purpose of the Visit

The aim of the visit was to familiarize with the Bonn implementation of the R-matrix method for calculation of electron-molecule scattering cross section and to test new modules for MRCI correlation treatment.

Description of the Work

Recently the R-matrix code developed by Dr. Bernd Nestmann has been installed on computers at the Heyrovsky Institute of Czech Academy of Sciences. I have been testing this installation by comparing the results obtained by using these programs with previous calculations. Another part of the work was to introduce higher correlation treatment. The new codes provide much more balanced correlation than the previous version and I have studied the effect of correlation on the scattering of electrons off F_2 molecule as well as resonance-background separation of the scattering phase shifts and cross sections.

Main Results Obtained

It has been showed that the new codes are suitable for scattering calculations of electrons off small molecules. In the case of $e - F_2$ scattering has been showed that the correlation influences the resonant scattering much more than the background scattering. In addition, the module for estimation of the correct R-matrix sphere radius has been developed and successfully tested.

Future collaboration

I will continue with collaboration with the institute as the PhD student. Main direction of my collaboration is the development of the implementation of the R-matrix code, the next development of the FFR method as well as introduction of calculations where the relativistic corrections take place.

Projected publications

The publication of discussion of the correlation effect in the $e - F_2$ and $e - Cl_2$ scattering is prepared.