

This thesis uses the phenomenon of the Siegert states and the R-matrix approach to analyze quantum scattering. The main task of the work is to implement the multichannel R-matrix method and test it on model potentials before applying it to ab initio scattering calculations. I follow up on my bachelor thesis where we described the Siegert states and their influence on the cross section and did the analysis for a short-range potential in one channel. In this work, we implement the multichannel approach within the one-particle R-matrix method. The method is tested for multichannel potentials and the long-range dipole and Coulombic potentials. Then we implement our approach into the multi-electron R-matrix UKRmol+ codes and apply our method to real molecular systems. We analyze the results of electronically elastic and inelastic calculations.