

Numerical Investigation of Quantum Chaos in Transition State Systems

Ashot S. Gevorkyan (E-mail g_ashot@sci.am)

Institute for Informatics and Automation Problems, NAS ARMENIA

Ind. 375014, Parujr Sevak 1, Yerevan, Armenia

It is well known that the formation of a transition state plays an important role in wide variety of chemical processes. Less well reorganized is that the dynamics of transition formation is chaotic. In other words, the outcome of a collision in a system, which forms a transition state, is extremely sensitive to initial conditions. The first principle calculations of the quantum chaos were carried out in the framework of micro-irreversible multi-channel quantum scattering representation constructed by the authors of Ref. [1]. Based on intrinsic properties of scattering system the numerical problem was divided into independent subproblems. The parallel algorithm for numerical computations was developed and tested for massive-parallel systems Parsytec CC/16 and SPP-1600. This algorithm allowed us to carry out converging computations for three-body system for any values of the energy. It was shown, that even in the simple case of the three-body problem the principle of quantum determinism, in general, breaks down and one has a micro-irreversible quantum mechanics. The obtained result supports the transitional state theory, developed by Eyring and Polyani on the bases of heuristic considerations, the essence of the method being statistical descriptions of chemical reactions. In this work the ab initio calculations of quantum chaos (wave chaos) were carried out on the example of the elementary chemical reaction $Li + (FH) \rightarrow (LiFH)^* \rightarrow (LiF) + H$.

1. A.V.Bogdanov, A.S.Gevorkyan, Three-body Multi-Channel Scattering as a Model of Micro-Irreversible Quantum Mechanics, Proc. of the International Symposium on Nonlinear Theory and its Applications, Hilton Hawaiian Village, 1997, v.1, pp.693-696.