Quantum chaos in chemistry: computational tools for strongly interacting dynamical systems

Svetlana Kotochigova

Temple University, Department of Physics

Computational efforts to describe complex molecular systems are often related to the amount of order and chaos in their dynamics. Consequently, as chaotic behavior of complex systems in chemistry is actually more common than ordered ones, the computation of collisional properties of atoms and molecules can have significant uncertainties. On the other hand, recognizing the chaotic or fractal nature of molecular dynamics can provide us with new insights and better understanding of the complex phenomena. Here, chaos theory can make predictions about extremely complex motion of many particles interacting with each other.

In this talk, I focus on two systems that are sufficiently complicated for quantum chaos to appear. I will demonstrate the emergence of chaos in the collisions of magnetic lanthanide atoms with their extremely large magnetic moments and orbital momenta as well as in reactive scattering between atoms and di-atomic molecules. Signatures of quantum chaos in these studies appear in the magnetic Feshbach resonance statistics and in the properties of adiabatic potentials in hyperspherical coordinates of the intermediate complex, respectively. For lanthanide atom collisions in an external magnetic field, we identified the key parameter that governs chaos and randomness. We were surprised to find that some states in the chaotic system are localized, whereas others are nonlocalized, making this system ``multifractal''. For the atom-dimer systems, the spacings between the potentials are chaotic for small hyperspherical radii and random for large ones. In essence, this confirms the extreme sensitivity to initial conditions as a defining feature of chaotic dynamical systems.