Full Quantum Dynamics of Atom-Diatom Chemical Reactions in Hyperspherical Elliptic Coordinates

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Explicit expressions of the full Hamiltonian of tri-atomic system in the hyperspherical elliptic [1] (HSE) coordinates are derived [2]. The derivation is made from the expressions in the Delves coordinates [3].

An efficient numerical algorithm is also presented in order to evaluate the surface eigenfunctions including all the effects of Coriolis coupling terms. The SDT (sequential diagonalization truncation) technique is employed with Legendre-based DVR basis functions that are supplemented with dumping factor to give adjustable boundary condition. In order to get better performance, not only the HSE coordinates but also the Delves coordinates are employed in non-reactive region. The close-couping calculation along hyperradius is carried out with use of the R-matrix propagation method.

The whole formalism is numerically tested by using the $Cl + DH$ and $O(^1D) + HCl$ reaction system. The correctness of the formulation and the developed computer code are demonstrated by comparing the results with another existing code *ABC* [4].

This new methodology is expected to give all the scattering information with better numerical efficiency and physical understanding of reaction dynamics, especially for systems with heavy-light-heavy mass combination.

Cl + HD --> H + DCl, D + HCl on BW4 PES

Cl + HD(v=0, j=1, Ω=0) --> H + DCl (v=0, j=2, Ω=0)
J=3⁻ on BW4 PES
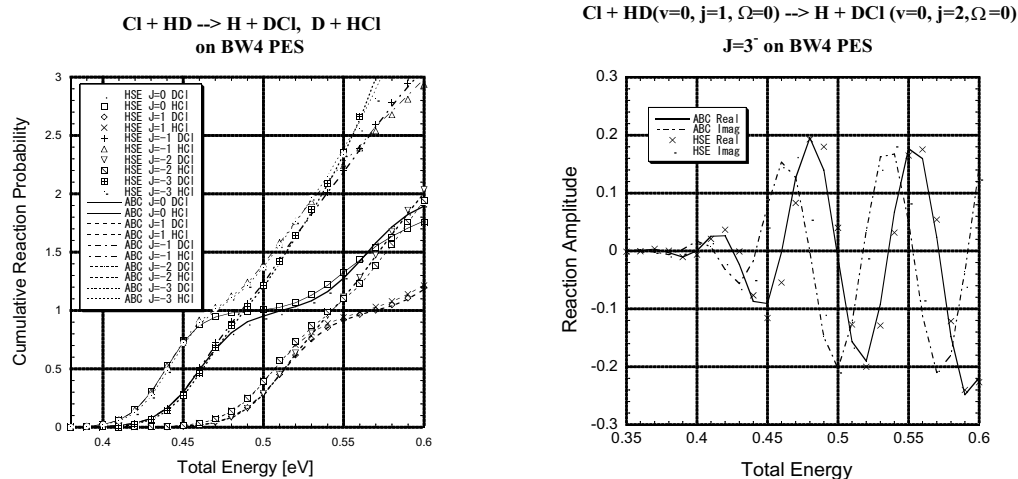
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