A VARIATIONAL METHOD OF THE ROVIBRATIONAL ENERGIES OF POLYATOMIC MOLECUES

H.-G. YU, *Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973-5000, USA*.

A two-layer Lanczos algorithm has been developed for calculating the rovibrational energy levels of polyatomic molecules in terms of a partitioned Hamiltonian. Such a Hamiltonian is formed in a set of orthogonal polyspherical coordinates. This algorithm solves the full-dimensional eigenvalues problem in a reduced-dimensional (RD) manner. By splitting the coordinates into radial and angular groups, one obtains a small RD Hamiltonian in each coordinate group. The eigenstates of each RD system are computed using either a standard or guided spectral transform (GST) Lanczos method. These two subsystems are exactly coupled via a set of diabatic basis functions in the angular degrees of freedom without any dynamical approximation. Finally, we will discuss its application for some polyatomic molecules up to six-atom ones.