CONICAL INTERSECTIONS IN THE PRESENCE OF SPIN-ORBIT COUPLING

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Conical intersections do not exist as isolated points but as continuous seams of dimension $N^{int} - 2$ for the nonrelativistic Coulomb hamiltonian, where N^{int} is the number of internal coordinates. Including the spin-orbit interaction can change the situation qualitatively. For odd-electron systems the hamiltonian is complex causing the dimension to reduce to $N^{int} - 3$ or even $N^{int} - 5$ when there is no spatial symmetry present. In order to be able to study the effect of the spin-orbit interaction quantitatively we have implemented an algorithm that can locate conical intersections in the presence of the spin-orbit interaction.
The system H_2 + OH has been found to have conical intersections between $^2\Sigma - ^2\Pi$ states in linear symmetry or $1^2A' - 2^2A'$ states in C_s symmetry, in the nonrelativistic case. Points of the seam including the spin-orbit coupling have been located and compared with the nonrelativistic results.