Time-Dependent Three-Body Reactive Scattering in Hyperspherical Coordinates JEFFREY CRAWFORD, University of Oklahoma, GREGORY PARKER, Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma — A time-dependent wave packet method for extracting state-to-state reactive S matrix elements is presented using hyperspherical coordinates. This method expresses the wave packet in the adiabatically adjusting, principal axes hyperspherical (APH) coordinates during propagation, since they treat all arrangement channels equivalently. This allows efficient conversion from mass-scaled Jacobi reactant channel coordinates to APH coordinates and from APH coordinates to Delves' product channel coordinates. The final state analysis is carried out by projecting the product channel eigenfunctions onto the propagated wave packet along a fixed asymptotic hyperradius at each time step. The S matrix elements are proportional to the Fourier transform of the projection coefficients. Comparisons with other results are given. Future work to include collision-induced dissociation and recombination is discussed.

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