

Contribution Title:	TRANSITIONS THROUGH AVOIDED CROSSINGS IN MOLECULAR QUANTUM DYNAMICS
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We are interested in the dynamics of a molecule's nuclear wave function near an avoided crossing of two electronic energy levels. More precisely, we study the time development of the wave function's component in an initially unoccupied energy subspace, when the wave packet crosses the transition region. In the optimal superadiabatic representation, which we define, this component builds up monotonously, and has the approximate shape of an error function; thus, its norm displays the same behaviour as observed by Michael Berry in a simplified, time-adiabatic model in 1990. Finally, we give a simple, explicit formula for the transmitted wave packet in the scattering region, which is in excellent agreement with high precision ab initio numerical computations.