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An approximate semiclassical method that uses real valued trajectories for time dependent tunneling calculations

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A semiclassical method will be presented that describes the time dependent tunneling of a quantum wave packet encountering a barrier. Tunneling through barriers plays a significant role in many reactions. The method described in this talk uses an approximation to the standard semiclassical stationary phase method. The approximation employed in this work leads to real valued tunneling trajectories, while most methods for this problem employ complex valued trajectories. Using only real valued trajectories will have significant advantages in applications to larger systems. It is found that there are typically three of these approximate stationary phase contributions to the wave function for each point in the transmitted region. Two of these have energies very close to the barrier top, one slightly above the barrier top and the other slightly below it. The third approximate stationary phase contribution is at a lower energy. Difficulties in obtaining accurate values for the contributions from trajectories with energy very close to the barrier top will be considered, and the accuracy of the approximate stationary phase wave function will be discussed.

Biography

Michael F Herman received his PhD in Chemistry from the University of Chicago in 1980. He then did his Post-doctoral research at Columbia University in New York before joining the Chemistry faculty at Tulane University in New Orleans in the Fall of 1981. He is best known for the development of semiclassical methods for the calculations of the properties and dynamics of chemical systems.

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