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A Wigner Distribution Analysis of Scattering Dynamics DAVID WEEKS, BRENT LACY, Air Force Institute of Technology — Using the time dependent Channel Packet Method (CPM),[1] a Fourier transformation of the correlation function between evolving wave packets is used to compute scattering matrix elements. The correlation function can also be used to compute a Wigner distribution as a function of time and energy. This scattering Wigner distribution is then used to investigate times at which various energetic contributions to the scattering matrix are made during a molecular collision. We compute scattering Wigner distributions for a variety of molecular systems and use them to characterize the associated molecular dynamics. In particular, the square well provides a simple and easily modified potential to study the relationship between the scattering Wigner distribution and wave packet dynamics. Additional systems that are being studied include the collinear H + H_2 molecular reaction, and the non-adiabatic B + H_2 molecular collision.

[1]D.E.Weeks, T.A.Niday, S.H.Yang, J Chem Phys. **125**, 164301 (2006).

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