Title:	Time-dependent quantum mechanical wave packet dynamics
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Abstract:	Starting from a model study of the collinear (H, H2) exchange reaction in 1959, the time-dependent quantum mechanical wave packet (TDQMWP) method has come a long way in dealing with systems as large as Cl + CH4. The fast Fourier transform method for evaluating the second order spatial derivative of the wave function and split-operator method or Chebyshev polynomial expansion for determining the time evolution of the wave function for the system have made the approach highly accurate from a practical point of view. The TDQMWP methodology has been able to predict state-to-state differential and integral reaction cross sections accurately, in agreement with available experimental results for three dimensional (H, H2) collisions, and identify reactive scattering resonances too. It has become a practical computational tool in predicting the observables for many A + BC exchange reactions in three dimensions and a number of larger systems. It is equally amenable to determining the bound and quasi-bound states for a variety of molecular systems. Just as it is able to deal with dissociative processes (without involving basis set expansion), it is able to deal with multi-mode nonadiabatic dynamics in multiple electronic states with equal ease. We present an overview of the method and its strength and limitations, citing examples largely from our own research groups.
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