LANCZOS WAVEPACKET PROPAGATION IN A CLASSiCALLY MOVING BASIS SET

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We present our recent work on generalized wavepacket techniques, in which a wavepacket is propagated exactly using a time-dependent orthogonal basis set that is translated in phase space to follow the classical time evolution of a fiducial point. Such methods can be used to simulate phenomena ranging from infrared spectra to cross sections for photodissociative and reactive processes. Application of Lanczos propagation methods has been found to yield a scheme which scales favorably, and may be particularly useful for large systems.