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Off-Center Thawed Gaussian Multi-Dimensional Approximation for Semiclassical Propagation LUCAS KOCIA, Harvard University, Department of Chemistry and Chemical Biology, ERIC HELLER, Harvard University, Department of Chemistry and Chemical Biology, Department of Physics — The Off-Center Thawed Gaussian Approximation's (OCTGA) performance in multi-dimensional coupled systems is shown in comparison to Herman-Kluk (HK), the current workhorse of semiclassical propagation in the field. As with the Heller-Huber method and Van Voorhis *et al.*'s nearly-real method of trajectories, OCTGA requires only a single trajectory and associated stability matrix at every timestep to compute Gaussian wave packet overlaps under any Hamiltonian. This is in sharp contrast to HK which suffers from the necessity of having to propagate thousands or more computationally expensive stability matrices at every timestep. Unlike similar methods, the OCTGA relies upon a single *real* guiding trajectory, which in general does not start at the center of the initial wave packet. This guiding "off-center" trajectory is used to expand the local potential, controlling the propagating "thawed" Gaussian wavepacket such that it is led to optimal overlap with a final state. Its simple and efficient performance in any number of dimensions heralds an exciting addition to the semiclassical tools available for quantum propagation.

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