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Abstract

The work of Noid et al. [J. Chem. Phys., 67, 404 (1977)] has shown that sharp molecular spectra can be obtained through a Fourier transform of the autocorrelation function of a classical trajectory. In the present work, we extend this idea to obtain a spectrum by Fourier transform of the dipole moment function of collision product trajectories. We show that this "classical collision spectrum" (CCS) is related to the cross section for creating the product times an Einstein A factor. As a test case, we analyze product CO trajectories obtained from O + CO collisions at 8 km/sec and focus on the spectral resolution of the CCS. The CCS of these trajectories shows rich quantum-like features, including well-separated vibrational overtones and rotational band-heads, which become more pronounced with particular trajectory weighting methods. For polyatomic cases, the hope is that the CCS can be deconvolved into ro-vibrational specific probabilities and cross sections for quasi-periodic trajectories, which would otherwise overlap in a conventional classical trajectory energy analysis. Chaotic trajectories are expected to broaden and decrease the achievable resolution of the CCS. Chaotic motion will therefore impact the ability to separate ro-vibrational specific cross sections, an issue that will be addressed in future work.