

Abstract Submitted
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Mixed Quantum/Classical Theory (MQCT) to Study Inelastic Scattering of Molecules¹ BIKRAMADITYA MANDAL, DMITRI BABIKOV, Marquette University — Inelastic scattering of gas-phase molecules is important for analysis of molecular spectra observed by astronomers. These processes are rather complicated as one needs to have detailed description of state-to-state transition cross sections in a broad range of energy. Quantum mechanical treatment of these processes is computationally expensive while classical description is not always accurate. Solution is a mixed quantum/classical theory (MQCT) where translational motion (scattering) is treated classically whereas internal motion (rotation and/or vibration) is treated quantum mechanically. It makes the methodology computationally inexpensive, applicable even to larger molecules in broad range of collision energy. Computation of differential cross sections is also possible within MQCT using phase information to build the interference of partial waves. Moreover, MQCT can also provide some insight for the lower-energy regime dominated by scattering resonances. Detailed analysis of differential and integral cross sections for elastic and inelastic scattering of $\text{Na} + \text{N}_2$ is explored using this methodology, and accuracy is confirmed in a broad range of energy.

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