Semiclassical Analysis of Quantum Mechanical Calculations of Rotationally Inelastic Collisions of He and Ar with NaK[†]

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Abstract

Recent quantum mechanical calculations and laboratory experiments at Lehigh University have provided detailed information about rotationally inelastic collisions of He and Ar with NaK in a cell at thermal energies. The purpose of this project was to develop a semiclassical model for these collisions based on the well-known vector model. In the quantum mechanical theory, Grawert coefficients $B_\lambda(j, j')$ (where λ is an integer) give the probability that a discrete amount $\lambda\hbar$ of angular momentum is transferred from the projectile to the target in a transition between rotational levels j and j'. Derouard showed that one can develop a semiclassical model by transforming from λ to the continuous variable α, the angle between initial and final angular momentum vectors $\boldsymbol{j}$ and $\boldsymbol{j'}$. In the present work we invoked the vector model, which relates the polar angle θ of the angular momentum vector to the azimuthal quantum number m, and showed that the distribution $P(\theta, \theta') \sin\theta'$ of final polar angles θ' could be expressed as a convolution of the semiclassical Grawert coefficient $B(j, j'; \cos\alpha)$. Using this expression we calculated the expected distribution of values of $\Delta\theta = \theta' - \theta$ and compared it with the quantum mechanical result. The semiclassical model agreed very well with the quantum mechanical theory, especially when the quantum number j was large. The distribution of projections of j onto the z axis before and after collision (in a transition $jm \to j'm'$) demonstrated (as others have also noticed) that m changes in such a way that θ tends to be preserved. The semiclassical model also predicts the propensity for collision-induced changes in j to be even numbers, in agreement with quantum mechanical theory and experiment.

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