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On the applicability of approximate methods in the elastic scattering between atoms and molecules near room temperature CONSTANTINOS MAKRIDES, Joint Quantum Institute, EITE TIESINGA, Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg, MD — Despite increases in computational capabilities, fully quantum numerical evaluation of scattering properties remains a computationally intensive problem. For atom-atom scattering, many simplified methods of computation have been used, which can often come to within a few percent of the true value of cross sections. Additionally, analytical models can also produce satisfactory results, such as the Born-approximation for the long-range phase shift between two alkali metals for room-temperature collisions. This particular approximation, has been rather robust and highlights the sensitivity of the cross section on the description of the long-range potential. The same model can be extended in certain regimes to atom-molecule scattering; however, the degree to which these models are applicable is not well understood. Our recent closed-coupled calculations on the Li+H_2 system have shown that elastic scattering properties are in disagreement with this Born-approximation, even for room-temperature collision energies, where one would expect the approximation to be applicable. Motivated by this discrepancy, we explain this difference. We additionally provide guidance for when the approximation is valid by studying the Li+Li and Li+He collisions.

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