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Mapped grid methods for Numerov propagation CHRISTOPHER MADRID, JUAN BLANDON, Angelo State University, GREGORY PARKER, University of Oklahoma — The Computational toll of solving the Schroedinger equation for certain atomic systems is sometimes prohibitively heavy. We present a grid-mapping method which decreases the number of points needed, and at the same time maintains or increases accuracy for three-atom scattering. By developing a hyperspherical mapping method for Numerov propagation, scattering cross-sections can be found for a large range of energies. This method is useful for systems with very shallow bound states where the mapping will give a large number of data points inside the potential well while decreasing the number of points at a large hyper-radius. The change in grid sizes is controlled by a mapping function that is easily modified. Results are shown for scattering in the HeH_2 and HNe_2 systems.

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