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The classical H_2^+ ion

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Abstract

The aim of this project was to use purely classical physics to simulate the orbital motion of the positive molecular hydrogen ion, H_2^+ . This was achieved by using various numerical integration techniques, namely the leapfrog and Runge-Kutta 4th order methods, to solve Newton's equations of motion. The numerical accuracy of these integration techniques was considered throughout. The simulations increased in complexity; beginning with a simple two-body model of the ion, up to the general three-body model. Where possible, comparisons with the analytic solution were explored.