

Abstract Submitted  
for the GEC12 Meeting of  
The American Physical Society

**Comparison of spherical and spheroidal expansions for energies and oscillator strengths of  $\text{H}_2^+$**  JEREMY SAVAGE, DMITRY FURSA, MARK ZAMMIT, IGOR BRAY, Curtin University — We calculate the bound state energies and oscillator strengths of the hydrogen molecule ion using configuration interaction expansions in both spherical and prolate spheroidal coordinates. States were built from similar Laguerre bases in the fixed nuclei approximation, allowing for the direct comparison of convergence rates and accuracy. Such a comparison will demonstrate the relative usefulness of spherical and spheroidal expansions for scattering on diatomic molecules. Specifically, this will assist in the implementation of the convergent close-coupling approach to scattering which is optimised by a smaller, more efficient set of configurations. It will be shown that the spheroidal basis is significantly faster to converge and more accurate for the low-lying states but this advantage gradually dissipates as state energy increases and the orbitals become more spherical.

Jeremy Savage  
Curtin University

Date submitted: 15 Jun 2012

Electronic form version 1.4