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Semiclassical treatment of high-lying electronic states of H_2^+ and an approach for computing electronic spectra of long-range diatomic Rydberg molecules[1] CHRIS H. GREENE, T. J. PRICE, Purdue University — A comparison between quantum mechanical and semiclassical WKB calculations for energies and wave functions of high-lying $^2\Sigma$ states of H_2^+ is presented. Some of the states shown lie in an unexplored regime, corresponding asymptotically to $H(n \leq 145)$ plus a proton, with $R \leq 120,000\ a_0$. For all but the lowest lying states, reasonable agreement with quantum mechanical results is obtained by using a straightforward WKB approximation that neglects some barrier effects; these semiclassical calculations are about two orders of magnitude faster than the quantum calculations. In addition, a method is presented in which electronic states of H_2^+ are used as a starting point for calculating long-range potential energy curves of diatomic Rydberg molecules with charged atomic cores. This method utilizes the fact that the Rydberg electron moves in a two center Coulomb potential when it is well outside of both cores. Interactions between the Rydberg and core electrons mix in irregular wave functions of H_2^+; these effects are incorporated via the Green's function for H_2^+ and the quantum defects associated with each atom.

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