

1057-81-124

George A. Hagedorn* (hagedorn@math.vt.edu), Department of Mathematics, 460 McBryde Hall, Virginia Tech, Blacksburg, VA 24061-0123. *The Born–Oppenheimer Approximation for Diatomic Molecules with Large Angular Momentum.*

Almost everything that is known about molecular quantum mechanics is obtained from the Born–Oppenheimer approximation. The approximation is based on the smallness of the fourth root, ϵ , of the ratio of the electron mass divided by the mean nuclear mass, which is typically 10^{-1} . The standard approximation yields error bounds proportional to ϵ^5 if the vibrational and rotational quantum numbers belong to bounded sets. We describe an extension for diatomic molecules (obtained in work with Sharon Hughes) that has uniform error bounds proportional to ϵ^5 if the angular momentum quantum number is bounded by a constant times $\epsilon^{-3/2}$. In contrast to the standard approximation, one must include non-trivial couplings between the vibrational and rotational motions in this situation.

We compare the results of this approximation with published data for the H_2^+ and HD^+ ions. (Received January 16, 2010)