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Absence of Bound States in Extremely Asymmetric Positive Diatomic Molecules

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Abstract. It is shown that the Hamiltonian for a diatomic molecule consisting of N electrons and two dynamic nuclei with charges Z_1 and Z_2 has no bound states if one of the charges is sufficiently large. The nuclear motion is completely unrestricted, and the kinetic energy of both nuclei can be included in the Hamiltonian. One of the nuclear charges can be arbitrarily small, provided that the other is sufficiently large.

I. Introduction

For atomic systems, it is well-known that all positive ions are so stable that they have infinitely many bound states [1–4], but that extremely negative ions are unstable with respect to expulsion of at least one electron [5–8]. (See [9] for a complete, up-to-date list of references.) However, one expects that molecular systems will be unstable if the nuclear charges are either very large, or very small, relative to the number of electrons. Proofs of both of these phenomena were recently given [9, 10] for diatomic molecules in which the nuclei are completely dynamic, i.e., the nuclear motion is unrestricted and the kinetic energy of the nuclei is included in the Hamiltonian. In particular, it was shown in [10] that a positive diatomic molecule will be unstable with respect to breakup into atomic subsystems when *both* nuclear charges are large compared to the number of electrons; however, this argument was unable to preclude the existence of bound states for systems in which one of the nuclear charges was less than the total number of electrons, even if the other charge was absurdly large. In this paper we remedy this defect, i.e., it is shown that a positive diatomic molecule is unstable if *one* of the nuclear charges is sufficiently large.

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