The stability of Coulomb three-body systems

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Three-body Coulomb systems are the simplest that incorporate both atomic and molecular ions and are therefore of considerable interest not only for atomic and molecular theory but also for light isotopes containing various elementary particles, such as muons and positrons.

High accuracy non-relativistic quantum chemical calculations of the energy levels and wavefunctions of three-particle systems of the form $\{m_1^{\pm}m_2^{\pm}m_3^{\mp}\}$ are calculated using a fast and efficient series solution method in a triple orthogonal Laguerre basis set [1]. The results are presented in the form of a reciprocal mass fraction ternary diagram [2], [3] and used to calculate accurate values of g, the fractional additional binding

$$g = \frac{E_0 - E_{th}}{E_{th}}$$

where E_0 is the three-body energy and E_{th} is the lowest threshold energy.

The topology of the stability and instability domains, based on the knowledge that all symmetric systems with $m_1 = m_2$ are stable against spontaneous dissociation, has been discussed and an expression for the width of the stability band formulated in terms of the binding g as a function of the reciprocal mass fraction for the uniquely charged particle [2]. Here we present a functional fit to g and use it to define a lower bound to the stability zone of three-particle Coulomb systems.

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[2] Martin, A., Richard, J-M., Wu, T. T. Phys. Rev. A, 46:3697-3703, 1992.

[3] Armour, E.A.G., Richard, J-M., Varga, K. Phys. Rep., 413:1-90, 2005.