Finite-mass effects beyond the Born-Oppenheimer approximation in the spectroscopy of three-body systems — •René Jestädt[1], Heiko Appel[1], Alison Crawford Uranga[2], Lorenzo Stella[2]Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Nano-Bio Spectroscopy group, Departamento Física de Materiales, Universidad del País Vasco, Centro de Física de Materiales CSIC-UPV/EHU-MPC and DIPC, San Sebastiàn, Spain

In this work we utilize a Lagrange-Laguerre variational method [1] to construct highly accurate numerical solutions for non-relativistic three-body systems (Helium atom, H_2^+, HD^+ and dtμ in 3D). Our approach does not rely on the Born-Oppenheimer approximation. This allows us to investigate the mass-dependence of optical dipole absorption spectra. For the molecular systems H_2^+, HD^+ and dtμ, we find a rather pronounced mass dependence of the dipole transiton matrix elements close to the second ionization threshold. We compare our 3D results to one-dimensional model calculations and provide a mechanism in terms of non-adiabatic coupling elements.

[1] Hesse and Baye, J. Phys. B, **34**, 1425 (2001)

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