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Solving the Schrödinger equation for Hydrogen Molecular ion (H2+) using Sinc functions and empolying both Python and Numpy

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In this contribution, we present the results of calculations for the ground state energy of H2+ employing Sinc functions as a basis set as discussed for a number of
examples in [1]. The modifications required to the basis functions to make them suitable for calculating the ground state energy of H2+ as well as the application of the cusp factor formulism [2] are outlined. Finally the resulting energies are investigated as a function of the number of basis functions and double-logarithmic fits are performed. It is found that they converge with an order of at least six.
[1] Proceedings of 64th SAIP Conference 2019, ISBN: 978-0-620-88875-2, edited by Prof. Makaiko Chithambo, p 347
[2] Eur. Phys. J. B. (2019) 92: 230

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

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