Hylleraas-B-spline basis set and its application of energies, polarizability and Bethe-logarithm of helium

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For solving the Hamiltonian eigenvalue problem of a two-electron atomic system, the Hylleraas-B-spline, H-B-spline, basis set is constructed through coupling the correlation term r_{12} and the traditional B-spline basis set [1]. This basis overcomes the ground state difficulty of using the traditional B-spline-type basis and inherits the property of fitting a wider range of initial states in one diagonalization. In the energy calculation for ground state of helium, the accuracy of our result using H-B-spline basis has 7 significant digits higher than using traditional B-spline basis. Combing the sum over pseudostates approach, we calculated the polarizability of helium. In two gauges, the results of polarizabilities for low-lying states of helium reached 8 significant digits at least. And the relative difference of the results of two gauges reached 10^{-11}. Recently, we extend this basis to the non-relativistic Bethe-logarithm, BL, calculations. Using H-B-spline basis, our preliminary results of BL arrived 7 significant digits for the $2\ ^3S - 10\ ^3S$ states of helium.

States	Hyllerass-B-splines	Ref. [2]	Ref. [3]
$2\ ^3S$	4.3640364*(1)*	4.36403682(1)	4.3640354
$3\ ^3S$	4.3686666*(1)*	4.36866692(2)	4.3686665
$4\ ^3S$	4.3697230*(2)*	4.36972344(5)	4.3697229
$5\ ^3S$	4.3700782(2)	4.37007831(8)	4.3700791
$6\ ^3S$	4.3702286*(4)*		4.3702300
$7\ ^3S$	4.370302(1)		4.3703043
$8\ ^3S$	4.3703442*(2)*		4.3703450
$9\ ^3S$	4.370367(1)		4.3703690
$10\ ^3S$	4.370382(1)		4.3703841

Table 1: Comparison of BL for the $n\ ^3S$, n up to 10, states of helium. Units are a.u.

[1] S.-J. Yang, X.-S. Mei, T.-Y. Shi, and H.-X. Qiao, Physical Review A 95, 062505 (2017).
[2] G. W. F. Drake and S. P. Goldman, Canadian Journal of Physics 77, 835 (1999).
[3] G. W. F. Drake, Physica Scripta 2001, 22 (2001).