Calculations of Entanglement Entropy in Two-Electron Atomic Systems Using Highly-Correlated Hylleraas Functions[1] YEW KAM HO, Institute of Atomic and Molecular Sciences, Academia Sinica, CHIEN-HAO LIN, IAMS and National Taiwan University, YEN-CHANG LIN, IAMS and Catholic Fu-Jen University — We have calculated the linear entropy $L = 1 - Tr(\rho_A^2)$ of two-electron atomic systems as a practical quantitative measure for the amount of quantum entanglement in the helium atom, the hydrogen negative ion and the positronium negative ion, with $\rho_A = Tr_B(|\rangle_{AB\ AB}\langle\phi|)$ being the one-electron reduced density matrix, obtained after tracing the two-electron density matrix over the degrees of freedom of the other electron. We have used highly correlated Hylleraas-type wave functions (up to N =203 terms) with which the inter-electronic coordinates are explicitly included. Due to the use of r_{12} (the distance between the two electrons) factors in the wave functions, calculations of L would require the need to solve four-electron integrals. We will present our detailed calculations at the meeting, including investigations of systematic convergence of the linear entropy for increasing number of terms in the wave functions. Comparisons are made with other available results [1-3] for the helium atom.

[1] J. P. Coe and I. D'Amico, *J. Phys.: Conf. Ser.* **254**, 012010 (2010).
[2] J. S. Dehesa *et al*, *J. Phys. B* **45**, 015504 (2012).
[3] Y. C. Lin, C. Y. Lin, and Y. K. Ho, to be published.

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