Abstract Submitted
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Probing Collins conjecture with correlation energies and entanglement entropies for the ground state of the helium isoelectronic sequence[1] YEW KAM HO, YEN-CHANG LIN, Institute of Atomic and Molecular Sciences, Academia Sinica — Correlation energy of a quantum system is defined as the difference between its exact energy $E_{\rm ex}$, and its Hartree-Fock energy $E_{\rm HF}$. In a recent related development, entanglement measures can be quantified with von Neumann entropy $S_{vN}(\rho) = -Tr(\rho \log_2 \rho)$ or linear entropy $S_L(\rho) = 1 - Tr(\rho^2)$, where ρ is the one-particle reduced density matrix, and $Tr(\rho^2)$ is defined as the purity of state. In the present work we calculate S_L and S_{vN} for the ground $1s^2\,^1S$ states in helium-like ions for $Z = 2$ to 15, using configuration interaction (CI) with B-Spline basis up to about 6000 terms to construct the wave functions, and with which density matrix, linear and von Neumann entropies are calculated [1]. We have found close relationship between the reduced correlation energy, defined as $E_{\rm corr} = (E_{\rm CI} - E_{\rm HF})/E_{\rm CI}$ (with $E_{\rm CI}$ being our calculated energy), and S_L or S_{vN}. Our results support Collins conjecture [2] that there is a linear relationship between correlation energy and entanglement entropy, i.e., $E_{\rm corr} = CS$, where C is called Collins constant. Using the calculated ground state energies for $Z = 2$ to $Z = 15$, and the entanglement measured with linear entropy S_L for such states, C is determined as 0.90716. At the meeting, we will present result for Collins constant determined from von Neumann entropy, and details of our calculations. [1] Y.-C. Lin, C.-Y. Lin, and Y. K. Ho, *Phys. Rev. A* **87**, 022316 (2013); *Can. J. Phys.* **93**, 646 (2015). [2] D. M. Collins, *Z. Naturforsch*, **48,** 68 (1993).

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