

C9930, 8. lekce, 7. 5. 2020

Hartreeho metoda SCF: dokončení, Slaterovy determinanty

Lowe, Quantum Chemistry, Kapitola 5:

5-6, 5-3 (v tomto pořadí)

5-6 Hartreeho metoda selfkonzistentního pole (Hartree SCF)



Douglas Rayner Hartree (1897 –1958)

An illustration showing a young boy kneeling on the floor, focused on assembling a Meccano bridge. A young girl stands beside him, looking on. The bridge is a suspension-style structure with two tall towers and cables. Various Meccano parts like gears, axles, and beams are scattered on the floor around them.

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nebyly komentovány.

- Jejich obsah komentuji přímo na jednotlivých
snímcích.

Problém započtení interakce dvojice elektronů v atomu He ($1s^2$)

TABLE 5-1 ▶ Average Values for Energy Calculated from Helium Atom Ground State Approximate Wavefunctions^a

Wavefunction description	\bar{E} (eV)
1) Product of He ⁺ orbitals	-74.83
2) Product of hydrogenlike orbitals with ζ fixed by SCF method	-77.48
3) Best product-type wavefunction	-77.870917
4) Nonorbital wavefunction of Pekeris [9]. This wavefunction uses functions of r_1 , r_2 and r_{12} as coordinates and has the form of an exponential times a linear combination of 1078 terms	-79.00946912

^a $\bar{E} = \int \psi^* H \psi d\tau / \int \psi^* \psi d\tau$, where H is given by Eq. (5-2).

V přednášce jsme z této tabulky uvedli první hodnotu, jako hodnotu získanou se započtením repulze pro neoptimalizované, „raw“ orbitaly iontu typu vodíku.

Další výsledky ilustrují, jak blízko k experimentální hodnotě z přednášky (-79.0143) se lze dostat, a co to stojí.

Tento obrázek pro atom He porovná vstupní a výstupní orbital
precedury SCF.

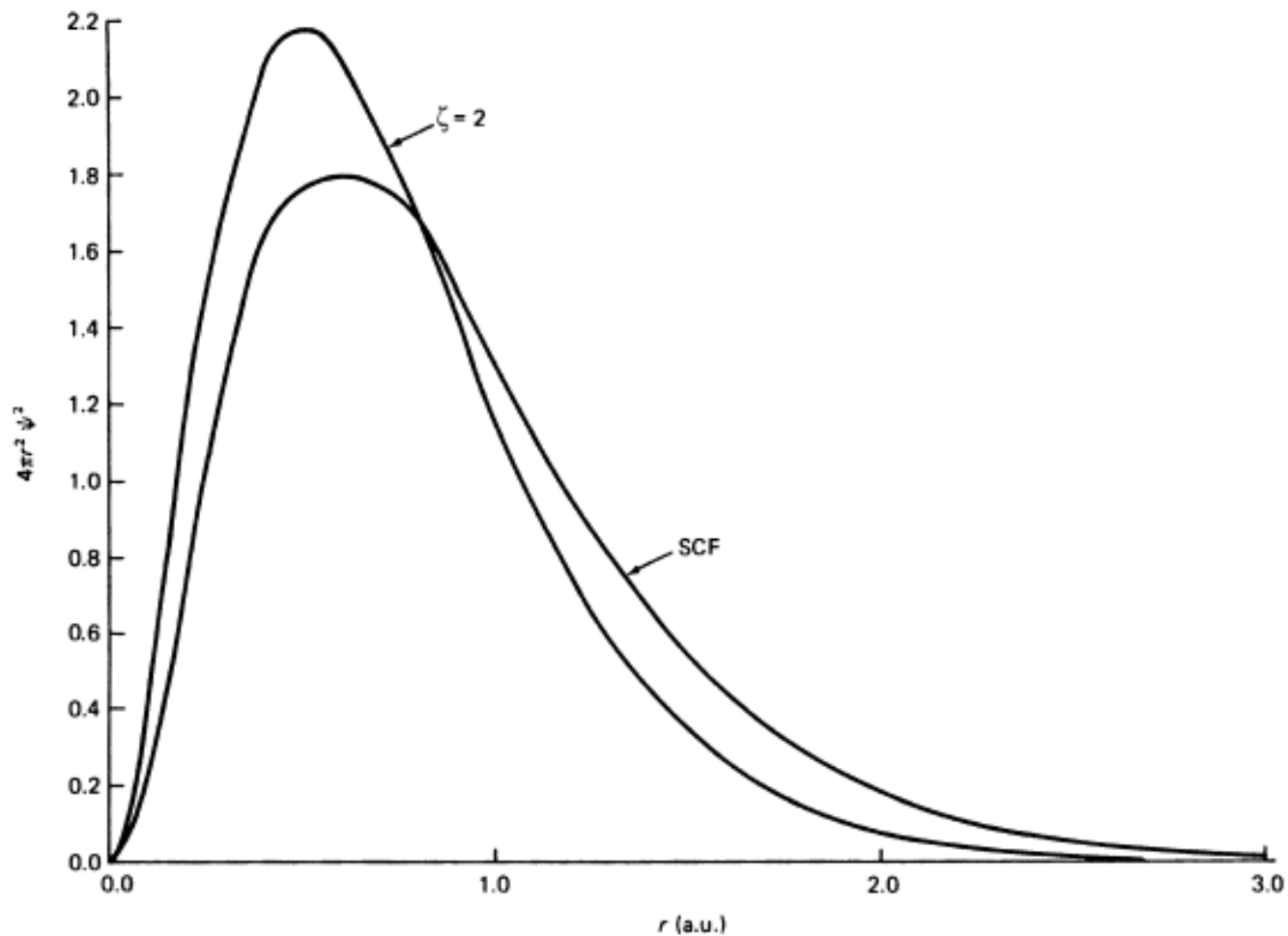


Figure 5-5 ► Electron distribution in helium as given by SCF and unshielded independent electron approximations.