Variational Computation of the Total Ground-State Energy of the Helium Atom © Thursday, March 20, 2025, by James Pate Williams, Jr., BA, BS, MSwE, PhD

In this numerical effort Slater atomic orbitals and a Slater determinant were utilized. Two zetas were computed using an evolutionary hill climber with a population of twenty candidate solutions and twenty-five generations. Three components of the total energy are tabulated below (kinetic energy, potential energy, and electron-electron repulsion energy) in atomic units Hartree:

I	Kinetic	Potential	EE	Total	% Error
1	5.886711	-9.761734	0.970200	-2.904822	0.037968
2	6.189252	-9.961144	0.985115	-2.786778	4.027326
5	6.079653	-9.913087	0.966749	-2.866685	1.275432
8	6.057331	-9.877986	0.960937	-2.859718	1.515353
13	5.905317	-9.845930	0.956349	-2.984265	2.773840

I	Zeta(1)	Zeta(2)
1	1.538437	1.799712
2	1.570827	1.618974
5	1.593982	1.657364
8	1.637161	1.629210
13	1.748881	1.581915

runtime (in seconds): 56.139000

The index, I, is the candidate solution designator. The calculation was performed using a C++ program created by the Microsoft Visual Studio 2019 Community Version compiler in the x64 Release Configuration. The operating system was Windows 10 on an old Dell XPS 8900 desktop. The total ground-state energy value of -2.90372 Hartree was utilized in the percentage error calculation.