Blog Entry © Saturday, August 16, 2025, by James Pate Williams, Jr. Some More Elementary Quantum Chemistry

As I promised in yesterday's blog entry I have computed the ground state energy of the helium-hydrogen molecular ion (cation, positively charged ion) also known as hydrogen hydride or hydro-helium. I used an elitist evolutionary hill climber especially designed for the ion with four Gaussian type orbitals (GTOs) to model a Slater type 1s orbital (STO-1s). I used tournament selection with a tournament size of two and mutation every generation. Unlike most genetic algorithms I did not use crossover operators. I perturbed the orbital coefficients and orbital exponents every generation. By elitist I mean the worse candidate solution is replaced by a new child candidate solution every generation. The fitness function was the least squares fit of the GTOs to the STO-1s orbital.

Helium hydride was the among the first molecules formed in the early universe after the "Big Bang" according to theoretical cosmology. As the beginning universe's plasma cooled helium atoms captured protons to form helium hydride.

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STO-4G for Atomic Numbers 2.000000 and 1.000000
R = +1.463200e+00
Zeta A = +2.092500e+00   Zeta B = +1.240000e+00

Overlap integral = +5.501318e-01

Kinetic energy integrals:

T[1, 1] = +3.557584e+00  T[1, 2] = +1.294641e-01
T[2, 1] = +1.294641e-01  T[2, 2] = +1.249303e+00

Potential energy integrals on center A:

V[1, 1] = -5.658367e+00  V[1, 2] = -1.215918e+00
V[2, 1] = -1.215918e+00  V[2, 2] = -1.519294e+00

Potential energy integrals on center B:

V[1, 1] = -8.224971e-01  V[1, 2] = -5.126076e-01
V[2, 1] = -5.126076e-01  V[2, 2] = -1.676553e+00

Direct and exchange integrals:

V[1, 1, 1, 1] = +2.097420e+00 V[2, 1, 1, 1] = +5.995529e-01
V[2, 1, 2, 1] = +2.328304e-01 V[2, 2, 1, 1] = +8.941699e-01
V[2, 2, 2, 1] = +4.470363e-01 V[2, 2, 2, 2] = +1.242915e+00

Electronic energy =  0
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Convergence of density matrix = 1.01044

Electronic energy =  -3.72841

Convergence of density matrix = 0.697788

Electronic energy =  -4.24691

Convergence of density matrix = 0.0336876

Electronic energy =  -4.24845

Convergence of density matrix = 0.00249024

Electronic energy =  -4.24846

Convergence of density matrix = 0.000180803

Electronic energy =  -4.24846

Convergence of density matrix = 1.31446e-05

Electronic energy =  -4.24846

Convergence of density matrix = 9.5554e-07

Electronic energy =  -4.24846

Convergence of density matrix = 6.94628e-08

Electronic energy =  -4.24846

Convergence of density matrix = 5.04959e-09

Electronic energy =  -4.24846

Convergence of density matrix = 3.67079e-10

Electronic energy =  -4.24846

Convergence of density matrix = 2.6685e-11

Electronic energy =  -4.24846

Convergence of density matrix = 1.93979e-12
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Electronic energy =  -4.24846

Convergence of density matrix = 1.40844e-13

Calculation converged:

Electronic energy       = -4.248460325
Total molecular energy  = -2.881593184
Exp ground state energy = -2.97867
Percentage error        =  3.259065822

G Matrix:

-1.424285e+00  +3.898153e-02
-1.108214e+00  -6.256951e-01

F Matrix:

-1.235422e+00  -1.272397e+00
-1.272397e+00  -6.788978e-01

E Matrix:

-1.419374e+00  +0.000000e+00
+0.000000e+00  +6.818053e-01

C Matrix:

+7.200749e-01  -9.568083e-01
+4.028733e-01  +1.127689e+00

P Matrix:

+1.037016e+00  +5.801978e-01
+5.801978e-01  +3.246137e-01

Old P Matrix:

+1.356201e+00  +1.150693e+00
+7.587782e-01  +6.437990e-01

Coefficients:

2.654849e-01
5.008087e-01
3.102084e-01
2.557329e-01
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Exponents:

9.189877e-01
7.721183e-02
1.458565e+00
2.302927e-01