Blog Entry © Friday, August 15, 2025, by James Pate Williams, Jr. Some Elementary Quantum Chemistry

I recently reimplemented a translation of a FORTRAN program whose source code is in Appendix B of "Modern Quantum Chemistry Introduction to Advanced Electronic Structure Theory" © 1996 by Attila Szabo and Neil S. Ostlund which is online at:

modern-quantum-chemistry.pdf

The first result is an ab initio calculation of the ground state energy of the helium-hydrogen cation also known as helium hydride or hydro-helium. This ion was very important in the short time after the “Big Bang”. My calculation is nearly the same as the results in Appendix B of the previously cited research textbook.

Elapsed milliseconds = 449

The percentage of error is **3.980015117%.**

```
STO-3G for Atomic Numbers 2.000000 and 1.000000
R = +1.463200e+00
Zeta A = +2.092500e+00   Zeta B = +1.240000e+00

Overlap integral = +4.502970e-01

Kinetic energy integrals:

T[1, 1] = +2.167518e+00  T[1, 2] = +1.666923e-01
T[2, 1] = +1.666923e-01  T[2, 2] = +7.611584e-01

Potential energy integrals on center A:

V[1, 1] = -4.142359e+00  V[1, 2] = -1.102230e+00
V[2, 1] = -1.102230e+00  V[2, 2] = -1.265152e+00

Potential energy integrals on center B:

V[1, 1] = -6.770699e-01  V[1, 2] = -4.110003e-01
V[2, 1] = -4.110003e-01  V[2, 2] = -1.227366e+00

Direct and exchange integrals:

V[1, 1, 1, 1] = +1.307654e+00 V[2, 1, 1, 1] = +4.369535e-01
V[2, 1, 2, 1] = +1.769633e-01 V[2, 2, 1, 1] = +6.055646e-01
V[2, 2, 2, 1] = +3.084422e-01 V[2, 2, 2, 2] = +7.749059e-01

Electronic energy =  0
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Convergence of density matrix = 0.882369

Electronic energy =  -4.1409

Convergence of density matrix = 0.279484

Electronic energy =  -4.22592

Convergence of density matrix = 0.0299869

Electronic energy =  -4.22698

Convergence of density matrix = 0.00237178

Electronic energy =  -4.22699

Convergence of density matrix = 0.000180541

Electronic energy =  -4.22699

Convergence of density matrix = 1.37005e-05

Electronic energy =  -4.22699

Convergence of density matrix = 1.03942e-06

Electronic energy =  -4.22699

Convergence of density matrix = 7.88572e-08

Electronic energy =  -4.22699

Convergence of density matrix = 5.9826e-09

Electronic energy =  -4.22699

Convergence of density matrix = 4.53877e-10

Electronic energy =  -4.22699

Convergence of density matrix = 3.44336e-11

Electronic energy =  -4.22699

Convergence of density matrix = 2.61228e-12

Electronic energy =  -4.22699
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```
Convergence of density matrix = 1.98234e-13

Calculation converged:

Electronic energy       = -4.226985624
Total molecular energy  = -2.860118484
Exp ground state energy = -2.97867
Percentage error        =  3.980015117

G Matrix:

-1.473114e+00  -3.878860e-01
-1.093934e+00  -2.280139e-01

F Matrix:

-1.457794e+00  -1.051086e+00
-1.051086e+00  -8.120075e-01

E Matrix:

-1.507652e+00  +0.000000e+00
+0.000000e+00  -1.520900e-01

C Matrix:

+8.010989e-01  -7.826747e-01
+3.381012e-01  +1.067720e+00

P Matrix:

+1.283519e+00  +5.417050e-01
+5.417050e-01  +2.286248e-01

Old P Matrix:

+1.527447e+00  +1.119670e+00
+6.446540e-01  +4.725530e-01
```

Results for the hydrogen molecule:

Elapsed milliseconds = 11806

The percentage of error is: **2.11517738%**

STO-5G for Atomic Numbers 1.000000 and 1.000000

```
R = +1.401100e+00
Zeta A = +1.240000e+00   Zeta B = +1.240000e+00

Overlap integral = +7.627331e-01

Kinetic energy integrals:

T[1, 1] = +7.711687e-01  T[1, 2] = +3.178841e-01
T[2, 1] = +3.178841e-01  T[2, 2] = +7.711687e-01

Potential energy integrals on center A:

V[1, 1] = -1.289190e+00  V[1, 2] = -6.962884e-01
V[2, 1] = -6.962884e-01  V[2, 2] = -7.672652e-01

Potential energy integrals on center B:

V[1, 1] = -7.672652e-01  V[1, 2] = -6.962884e-01
V[2, 1] = -6.962884e-01  V[2, 2] = -1.289190e+00

Direct and exchange integrals:

V[1, 1, 1, 1] = +1.018021e+00 V[2, 1, 1, 1] = +6.079188e-01
V[2, 1, 2, 1] = +4.188139e-01 V[2, 2, 1, 1] = +7.727169e-01
V[2, 2, 2, 1] = +6.080437e-01 V[2, 2, 2, 2] = +1.018021e+00

Electronic energy =  0

Convergence of density matrix = 0.567301

Electronic energy =  -1.86336

Convergence of density matrix = 7.37953e-05

Electronic energy =  -1.86336

Convergence of density matrix = 1.18093e-05

Electronic energy =  -1.86336

Convergence of density matrix = 1.88982e-06

Electronic energy =  -1.86336

Convergence of density matrix = 3.02425e-07

Electronic energy =  -1.86336
```

```
Convergence of density matrix = 4.83965e-08

Electronic energy =  -1.86336

Convergence of density matrix = 7.7448e-09

Electronic energy =  -1.86336

Convergence of density matrix = 1.23939e-09

Electronic energy =  -1.86336

Convergence of density matrix = 1.98336e-10

Electronic energy =  -1.86336

Convergence of density matrix = 3.17397e-11

Electronic energy =  -1.86336

Convergence of density matrix = 5.07913e-12

Electronic energy =  -1.86336

Convergence of density matrix = 8.12798e-13

Calculation converged:

Electronic energy       = -1.863358613
Total molecular energy  = -1.149633682
Exp Ground state energy = -1.174475931
Percentage error        =  2.11517738

G Matrix:

-4.924671e-01  +3.781357e-01
-4.924221e-01  -3.782581e-01

F Matrix:

-3.320915e-01  -5.925757e-01
-5.925757e-01  -3.320072e-01

E Matrix:

-5.245406e-01  +0.000000e+00
```

```
+0.000000e+00  +1.098030e+00

C Matrix:

+5.326468e-01  -1.451644e+00
+5.325301e-01  +1.451686e+00

P Matrix:

+5.674251e-01  +5.673009e-01
+5.673009e-01  +5.671766e-01

Old P Matrix:

+1.000124e+00  +1.000095e+00
+9.999052e-01  +9.998758e-01
```

Tomorrow I will perform calculations on the He-H+ ion (cation) for STO-4G and STO-5G.