Atomic Structure Database for Helium and He-like Ions

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Abstract

High precision variational calculations in Hylleraas coordinates for helium and heliumlike ions have now reached a high degree of refinement. The technique of using a double basis set overcomes problems of numerical linear dependence in the basis set, and a drastic loss of accuracy for the more highly excited Rydberg states. As a result, nonrelativistic eigenvalues exceeding spectroscopic accuracy are available for the singly excited spectrum up to at least n = 10 and L = 7. Relativistic and quantum electrodynamic corrections have also been calculated, along with the associated wave functions. Results are also available for the heliumlike ions up to Z = 18, for a total of 1751 atomic states, not counting fine structure.

The purpose of this paper is to describe a project to make this very large data base of high precision calculations for wave functions and energies available on the internet through a convenient user interface, located at the web site http://www.sharcnet.ca/drake/downloads. The web site will also include sample programs to make use of the wave functions to calculate other atomic properties.

Method for Generating The Wave Functions

Schrödinger's variational method is used for generating the wave functions.

$$E(\Psi) = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \min$$

The trial function used is of the following form:

$$\Psi(r_1, r_2) = \sum_{i,j,k} a_{ijk} r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2}$$

This gives a system of homogeneous linear equations whose solution is an upper bound to the true ground state energy

$$\frac{\partial E}{\partial a_{ijk}} = 0$$

Data files

Information is stored in 3 types of files: 2 are Wave function files (.POW for infinite mass, .POL for finite mass) while .MAT files store energy information.

Wave Functions:

Here is an example wave function file to illustrate how the information is organized…

```
 2  0  0 44  1   211S044.POW  QZ=2 1 1S    FROM QPOLD ON W-STATION         ,OK
-2.018620655007659047 6D-01-2.903724131001531809 5D+00 0.000000000000000000 0D+00
   3    1   22   44    4    4    4    4    3
   1    1    0 0   1.000000000000000    .500000000000000
   2   22    0 0   1.139160156250000   1.092407226562500
  23   44    0 0   1.521789550781250   1.438049316406250
 0 0 0  0 1 0  0 0 1  0 2 0  1 1 0  0 1 1  0 0 2  0 3 0  1 2 0  0 2 1
 1 1 1  0 1 2  0 0 3  0 4 0  1 3 0  2 2 0  0 3 1  1 2 1  0 2 2  1 1 2
 0 1 3  0 0 4  0 0 0  0 1 0  0 0 1  0 2 0  1 1 0  0 1 1  0 0 2  0 3 0
 1 2 0  0 2 1  1 1 1  0 1 2  0 0 3  0 4 0  1 3 0  2 2 0  0 3 1  1 2 1
 0 2 2  1 1 2  0 1 3  0 0 4
-3.372798360600937548 2D-02 5.961792235355249895 9D+01-2.513957293108295581 5D+01
-1.168000829652199672 3D+01-7.765860116047592070 8D+00 9.177096656780231610 9D+00
-1.135085133442205078 3D+00 8.922347817537192709 2D-01 1.477198956736120878 2D+00
-8.714987718717856438 9D-01-4.892579011630532314 2D-01 3.892322255158205967 4D-01
-2.890469959055818913 6D-02-3.252740550479487485 8D-02-6.996007030911390415 6D-02
-1.085557392457882629 5D-02 3.319949492916605212 4D-02 3.697215847058611610 3D-02
-2.515295274272837440 3D-02-1.051978519570535918 1D-02 5.029729906155465416 6D-03
-5.456203409695817240 3D-05-1.025884520139332951 6D+00-6.060594781523401962 5D+01
 2.488778313287987164 8D+01-9.319187679079722045 8D+00-1.525758006795367669 2D+01
 8.826553443124250194 5D+00 1.226332589229543762 2D+00-5.334945675467258329 8D-01
-3.666650667240334097 5D+00 2.778613299696640232 0D-01 9.450770059021142724 5D-01
 4.670438599409769678 5D-01-6.308939671578493592 6D-04-3.363953658064347019 1D-03
-4.771862343113018325 4D-02-3.166742399512395631 6D-01 4.354867150419412094 0D-03
 3.037154319453072079 7D-02-1.075836084309890710 1D-02 7.811513192974761577 9D-02
 2.215596084098619604 0D-02 2.827174800891976247 7D-03
```

Header

α,β information

radial exponents

coefficients

This particular file would yield a 44 term wave function. Here are the first 5 terms and 44th term of the function…

$$\Psi = -3.3727\times10^{-2} r_1^0 r_2^0 r_{12}^0 e^{-r_1-0.5r_2} +$$
$$5.9617\times10^{+1} r_1^0 r_2^1 r_{12}^0 e^{-1.1392r_1-1.0924r_2} +$$
$$-2.5139\times10^{+1} r_1^0 r_2^0 r_{12}^1 e^{-1.1392r_1-1.0924r_2} +$$
$$-1.1680\times10^{+1} r_1^0 r_2^2 r_{12}^0 e^{-1.1392r_1-1.0924r_2} +$$
$$-7.7658\times10^{+0} r_1^1 r_2^1 r_{12}^0 e^{-1.1392r_1-1.0924r_2} +$$
$$9.1770\times10^{+0} r_1^0 r_2^1 r_{12}^1 e^{-1.1392r_1-1.0924r_2} +$$
$$\ldots +$$
$$2.8271\times10^{-3} r_1^0 r_2^0 r_{12}^4 e^{-1.5217r_1-1.4380r_2}$$

Atomic Energies:

Contained in every .MAT energy file is a table containing a detailed energy breakdown for different electron configurations in a given state. The following example is the 5P state of Helium.

```
Contributions to the 5 P state energies of 4He relative to He+(1s) (MHz.).
-------------------------------------------------------------------------
Term          5 1P1            5 3P0            5 3P1            5 3P2
-------------------------------------------------------------------------
Enr   -130957168.320   -135201781.077   -135201781.077   -135201781.077
EM(1)       2912.781        -3436.617        -3436.617        -3436.617
EM(2)         -2.701           -2.740           -2.740           -2.740
Erel       -1287.022         1849.394          190.426           53.482
Eanom           .000            1.934           -1.083            .263
Est             .260             .000            -.260            .000
(ERR)M          .688             .073             .288             .137
(ERR)X        .3761(10)        .6691(18)        .3080(18)        .2760(18)
Enuc            .005             .047             .047             .047
EL(1)         7.74(27)       -72.03(27)       -72.04(27)       -72.04(27)
EL(2)        -4.364           -2.529           -2.529           -2.529
EL(2)'          .017             .000             .000             .000
Eho           .00(69)           .0(1.6)          .0(1.2)          .00(21)
Total -130955541.91(74)  -135203443.1(1.7)  -135205105.4(1.2)  -135205240.89(34)
-------------------------------------------------------------------------
```

non-relativistic energy as calculated from the expectation value of the non-relativistic Hamiltonian

correction for g factor not exactly 2

singlet/triplet relativistic energy correction

contribution due to finite size of nucleus

QED terms

Total Energy after all relativistic and QED corrections considered