SOME FIRST-ORDER PERTURBATION ENERGY VALUES*

by

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In the conventional perturbation study of the two-electron atom the perturbation is chosen to be the electron-electron interaction term in the potential energy¹:

$$H = H_0 + Z^{-1} r_{12}^{-1}$$

where H_0 is the zero-order Hamiltonian with eigenfunctions Ψ_{Op} , say, and Z is the nuclear charge. Then, as is well known, the first-order perturbation energy correction is given by

$$\epsilon_1(p) = \int d\tau \Psi_{Op}^* \Psi_{Op} / Z r_{12}.$$

In this note, the $\epsilon_1(p)$ are computed for a number of the singly-excited singlet and triplet S, P, and D symmetry states of the helium iso-electronic sequence. By a singly-excited state is meant one whose correct zero-order wavefunction is of the form of a properly symmetrized product $\Psi_{Op} = \Psi_{100}(1) \Psi_{nlm}(2)$ where the Ψ_{nlm} are the hydrogen problem eigenfunctions. These ϵ_1 values are needed for the calculation of the higher-order energy coefficients.

In the standard spectroscopic notation for Ψ_{nlm} ,

$$\epsilon_1 = [1s1s|nl\bar{n}l] + [1s\bar{n}l|1s\bar{n}l],$$

where, for example, the first integral is the coulomb energy of interaction between the charge distribution $1s1s$ and $nl\bar{n}l$.

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In terms of the hypergeometric function

$$F(a, b | c | z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n n!} z^n,$$

$$a_n = \Gamma(a+n)/\Gamma(a),$$

it follows that

$$\begin{aligned} [1s1s | nlnl] = Z n^{-2} \{ 1 + \frac{(n+l)! n^{2n-2l-2}}{(2l+1)! (n-l-1)! (n+1)^{2n+1}} [F(1+l-n, 2+l-n | 2l+2 | n^{-2}) \\ - \frac{(n^2+n+1)}{(n-l-1)(n+1)} F(1+l-n, 1+l-n | 2l+2 | n^{-2})] \} \end{aligned}$$

and

$$\begin{aligned} [1snl | 1snl] = \frac{4Zn(n+l)!}{[(2l+1)!]^2 (2l+1)(n-l-1)! (n+1)^{2l+5}} \sum_{r=0}^{\infty} \frac{(1+l-n)_r (r+1)}{(2l+2)_r} \left(\frac{2}{n+1}\right)^r \\ \times \sum_{s=0}^{r+1} \frac{(2l+2+s)!}{2^s s!} F(l+1-n, 2l+3+s | 2l+2 | \frac{1}{n+1}) \end{aligned}$$

These integrals are presented in Table I.

The ϵ_1 values for the singlet and triplet NS, NP and ND states of the helium isoelectronic series ($N < 20$) are presented in Tables II-IV. The calculations were performed in double precision (27 significant decimal figures) on the CDC 1604 located on this campus. Pilot calculations indicate an accuracy of at least 24 figures, and the data have been rounded accordingly.

¹In order to obtain this form of the hamiltonian, atomic units of length Za_0 and of energy $2RhcZ^2$ are used. However, in the discussion that follows and in the tables, units of a_0 and $2Rhc$ respectively are used.

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TA Electron Interaction Integrals in Atomic Units

N	[1S1S/NSNS] /Z	[1SNS/1SNS] /Z
2	2.098765432098765432098765E-01	2.194787379972565157750342E-02
3	9.948730468750000000000000E-02	5.767822265625000000000000E-03
4	5.763328000000000000000000E-02	2.339635199999999999999999E-03
5	3.751685901221866585378245E-02	1.176828733692921697799003E-03
6	2.634345980290449722025098E-02	6.745767083359918115890088E-04
7	1.950593356320950988447294E-02	4.223879156839416282309685E-04
8	1.502101619964298119102841E-02	2.819243622938868681764002E-04
9	1.192169312241013900000000E-02	1.975053306445844399999998E-04
10	9.691024274974534320044353E-03	1.437221255687173670056111E-04
11	8.032385851295680375616647E-03	1.078368520567764693717119E-04
12	6.765721845597162605382153E-03	8.297782420348613097774282E-05
13	5.776611470279517232169509E-03	6.521296732919522089882602E-05
14	4.989523873553340520904901E-03	5.218057877323045356154086E-05
15	4.352973108614080811222551E-03	4.240339975897315788043595E-05
16	3.830886080597473619003433E-03	3.492494356599942695316096E-05
17	3.397380464078058030277007E-03	2.910722227831226138464248E-05
18	3.033495829100864268230069E-03	2.451353282818590902125846E-05
19	2.725085645881544465818405E-03	2.083807561043771273671047E-05
20	2.461421881674201149921885E-03	1.786235793481188266559361E-05

N	[1S1S/NPNP] /Z	[1SNP/1SNP] /Z
2	2.427983539094650205761317E-01	1.707056851089772900472489E-02
3	1.088256835937500000000000E-01	4.531860351562500000000000E-03
4	6.151628800000000000000000E-02	1.844183040000000000000000E-03
5	3.949193016604853596165896E-02	9.289450202112955363080965E-04
6	2.748240234691903906133370E-02	5.328924321889143609294211E-04
7	2.022164709708818008948583E-02	3.338240609647158407824462E-04
8	1.549983003603115530178243E-02	2.228776227973291730106337E-04
9	1.225766340961948720000000E-02	1.561708216970136000000000E-04
10	9.935782217938511249290656E-03	1.136598080518734269094758E-04
11	8.216184878356343689608994E-03	8.528966879770779620046936E-05
12	6.907240510689810470474531E-03	6.563358979306275799677071E-05
13	5.887887085405890578326985E-03	5.158520951538110765011771E-05
14	5.078596634067437059217319E-03	4.127828349314895148930006E-05
15	4.425378975421500552688861E-03	3.354522808282623751897562E-05
16	3.890537518528209559800097E-03	2.762994127110355393587759E-05
17	3.447105929963256022627927E-03	2.302802837411850376255617E-05
18	3.075381148107272601011308E-03	1.939419406443346833316350E-05
19	2.760696253017178852227367E-03	1.648662518977304692227173E-05
20	2.491951175820291650664087E-03	1.413253427087888894706960E-05

TABLE I. Continued

N	[LSIS/NDNC]/Z	[LSND/1SND]/Z
3	1.110229492187500000000000E-01	2.471923828125000000000000E-04
4	6.245017600000000000000000E-02	1.318584320000000000000000E-04
5	3.497153714499822181578011E-02	7.341110654804578495072831E-05
6	2.776038433772337620692570E-02	4.424851106405615903871695E-05
7	2.039636130584072998317424E-02	2.351689447815886069292901E-05
8	1.561727735122057729961021E-02	1.938273451465877879803398E-05
9	1.234018245635709040000000E-02	1.374576762479011200000001E-05
10	9.995955149323494311687540E-03	1.008929042069964351783517E-05
11	8.261402824972751094603408E-03	7.618162753599473045534251E-06
12	6.942075165212680036381447E-03	5.890050409762642926303856E-06
13	5.915288728730418172120338E-03	4.646162425873358511605765E-06
14	5.100537977912009114469100E-03	3.728546906562507276037555E-06
15	4.443219444614686444459242E-03	3.037045285275432557929287E-06
16	3.905238516610295941495060E-03	2.506217312123009302173383E-06
17	3.459362871371720056865816E-03	2.092050328456574608710269E-06
18	3.085707094256108967058436E-03	1.764221244421282263896754E-06
19	2.769476408418814786285643E-03	1.501382230564176059753297E-06
20	2.499479292690519923496315E-03	1.288211828203079740686713E-06

TABLE II. The ϵ_1 in Atomic Units. S-States

N	$\epsilon_1(N^1S)$	$\epsilon_1(N^3S)$
2	2.318244170096021947873800E-01	1.879236694101508916323731E-01
3	1.052551269531250000000000E-01	9.371948242187500000000000E-02
4	5.997291520000000000000000E-02	5.529364480000000000000000E-02
5	3.869368774591158755158146E-02	3.634003027852574415598345E-02
6	2.701803651124048903183999E-02	2.566888309456650540866197E-02
7	1.992832147889345151270390E-02	1.908354564752556825624197E-02
8	1.530294056193686805920481E-02	1.473909183734909432285201E-02
9	1.211919845305472344000000E-02	1.172418779176555456000000E-02
10	9.834746400543251687049965E-03	9.547302149405816953038742E-03
11	8.140222703352456844983359E-03	7.924548999238903906244936E-03
12	6.848699669800648736359896E-03	6.682744021393676474404410E-03
13	5.841824437608712453068335E-03	5.711398502950322011270684E-03
14	5.041704452326570974466442E-03	4.937343294780110067343360E-03
15	4.395376508373053969102987E-03	4.310569708855107653342114E-03
16	3.865811024163473045956594E-03	3.795961137031474192050272E-03
17	3.426487686356370291661650E-03	3.368273241799745768892365E-03
18	3.058009361929050177251328E-03	3.008982296272678359208811E-03
19	2.745923721491982178555116E-03	2.704247570271106753081695E-03
20	2.479284239609013032587478E-03	2.443559523739389267256291E-03

TABLE III. The ϵ_1 in Atomic Units. P-States

N	$\epsilon_1(N^1P)$	$\epsilon_1(N^3P)$
2	2.598689224203627495808566E-01	2.257277853985672915714068E-01
3	1.133575439453125000000000E-01	1.042938232421875000000000E-01
4	6.336047104000000000000000E-02	5.967210496000000000000000E-02
5	4.042087518625983149796706E-02	3.856298514583724042535086E-02
6	2.801529477910795342226312E-02	2.694950991473012470040428E-02
7	2.055547115805289593026828E-02	1.988782303612346424870339E-02
8	1.572270765882848447479306E-02	1.527695241323382612877180E-02
9	1.241383423131650080000000E-02	1.210149258792247360000000E-02
10	1.004944202599038467620013E-02	9.822122409886637822381181E-03
11	8.301474547154051485809463E-03	8.130895209558635893408524E-03
12	6.972874100482873228471302E-03	6.841606920896747712477760E-03
13	5.939472294921271685977102E-03	5.836301875890509470676867E-03
14	5.119874917560586010706619E-03	5.037318350574288107728019E-03
15	4.458924203504326790207836E-03	4.391833747338674315169885E-03
16	3.918167459799313113735975E-03	3.862907577257106005864220E-03
17	3.470133958337374526390483E-03	3.424077901589137518865370E-03
18	3.094775342171706069344471E-03	3.055986954042839132678144E-03
19	2.777182878206951899149639E-03	2.744209627827405805305095E-03
20	2.506083710091170539611157E-03	2.477818641549412761717018E-03

TABLE IV. The ϵ_1 in Atomic Units. D-States

N	$\epsilon_1(N^1D)$	$\epsilon_1(N^3D)$
3	1.112701416015625000000000E-01	1.107757568359375000000000E-01
4	6.258203443200000000000000E-02	6.231831756800000000000000E-02
5	4.004494825154626760073084E-02	3.989812603845017603082939E-02
6	2.780463284878743236596441E-02	2.771613582665932004788698E-02
7	2.042537820031888884386717E-02	2.036834441136257112248131E-02
8	1.563666008573523607840824E-02	1.559789461670591852081218E-02
9	1.235392822398188051200000E-02	1.232643668873230028800000E-02
10	1.000604443974419395520537E-02	9.985865858902794668169705E-03
11	8.269020987726350567648942E-03	8.253784662219151621557873E-03
12	6.947965215622442679307751E-03	6.936185114802917393455144E-03
13	5.919934911156291530631944E-03	5.910642546304544813608733E-03
14	5.104266524818571621745137E-03	5.096809431005446607193062E-03
15	4.446256489899961877017172E-03	4.440182399329411011901313E-03
16	3.907744733922418950797233E-03	3.902732299298172932192887E-03
17	3.461454921700176631474527E-03	3.457270821043263482257106E-03
18	3.087471315500530249322333E-03	3.083942873011687684794539E-03
19	2.770977790649378962345397E-03	2.767975026188250610225890E-03
20	2.500767504518723093237002E-03	2.498191080862316843755628E-03