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Two-electron S and P term values with smooth Z dependence

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Perturbation and extrapolation techniques based on expansion in inverse powers of the atomic number Z have recently been used to estimate term values for S and P states of heliumlike atoms in the intermediate range of values of Z. The coefficients in these expansions are determined by utilizing the accurate data currently available for values of $Z \leq 10$. In order to obtain optimum results from such techniques, the data for low values of Z should exhibit a smooth variation with atomic number. To meet this requirement, the paper lists smooth values for the nonrelativistic energy and the relativistic corrections for the ground state and the states $n\ ^1S$, $n\ ^3S$, $n\ ^1P$, and $n\ ^3P$, $n = 2$–5 for $Z = 2$–10. Smooth behavior with Z has been ensured by quoting, for a given state, values obtained using the same type and length of expansion for the wave function. Also, the effect of rounding errors has been minimized by quoting the original values obtained in atomic units, and by listing the numbers to one or two digits more than would be justified by convergence arguments.

Much experimental data, derived from both laboratory[1-8] and extraterrestrial[9-11] sources, has become available in recent years on the spectra of heliumlike ions for a wide range of the nuclear charge Z. On the theoretical side, accurate term values have been computed for the low-lying S and P states for atoms up to $Z=10$.[12,13] These values have been used,[14,15] together with perturbation and extrapolation procedures based on expansions in powers of Z^{-1}, to estimate the values of the ionization energies for larger values of Z. For the low-lying D states up to $Z=10$, Blanchard and Drake[16] have computed term values and used them to estimate coefficients in the Z^{-1} expansion. As these authors point out, in order to obtain the best possible results from such extrapolation schemes, the data used should be of sufficient accuracy, and should also vary smoothly with Z.

The published data for the S and P states up to $Z=10$, consisting as it does of the most accurate values obtained in each case, is not necessarily the most suitable for use in an extrapolation procedure, for the following reasons. First, three different types of wave-function expansions (which we refer to as types B,[12,17] C,[13] and D[13]) were used. Thus, the values quoted for a given state for various values of Z are sometimes based on different types of expansions, or on similar expansions containing differing numbers of terms. This introduces a certain lack of smoothness in the data. Secondly, the results are listed only to the number of digits which were felt to be significant (judging by the convergence of the value as the number of terms in the wave-function expansion was increased), resulting in a possible loss of accuracy in the quoted values due to rounding off. Last, while the calculations were carried out in atomic units, the results are listed in cm^{-1}. The conversion to cm^{-1} is performed by multiplying by $2R_M$, where R_M is the Rydberg constant for the given nuclear mass. The value of R_M does not vary smoothly with Z, depending as it does on the nuclear mass rather than the atomic number. The extrapolation should therefore be carried out on the data in atomic units, and rounding errors are again liable to be introduced on reconverting the published values to atomic units.

In order to remedy this deficiency, we list below values in atomic units for the nonrelativistic energy parameter $\epsilon = (-E)^{1/2}$ and the relativistic corrections E_J which fulfill the requirements mentioned above in the following way. For a given state, the value quoted for each Z is obtained from the same type of expansion containing an equal number of terms. The number of figures to which each value is listed is one or two more than would be justified on the ground of convergence with expansions of increasing length. Also, all of the values are given in atomic units as originally calculated. Thus the effect of rounding errors is minimized.

Table I contains values for ϵ for the $1\,^1S$ state and the states $n\,^1S$, $n\,^3S$, $n=2-5$. The values for the $1\,^1S$ and $2\,^1S$ states were obtained using a type-B expansion containing 1078 terms, for the $2\,^3S$ state using a type-C expansion containing 120

TABLE I. Values for the nonrelativistic energy parameter $\epsilon = (-E)^{1/2}$ (where E is the energy in atomic units) for the S states. Each column heading includes the type and number of terms in the wave-function expansion.

Z \ State	$1\,^1S\,(B\,1078)$	$2\,^1S\,(B\,1078)$	$3\,^1S\,(C\,364)$	$4\,^1S\,(C\,364)$	$5\,^1S\,(C\,364)$	$2\,^3S\,(C\,120)$	$3\,^3S\,(C\,364)$	$4\,^3S\,(C\,364)$	$5\,^3S\,(C\,364)$
2	1.704 031 799 83	1.464 914 347 45	1.435 710 9	1.426 035 0	1.421 676 2	1.474 865 85	1.438 293 792	1.427 064 129	1.422 188 042
3	2.698 131 466 46	2.245 189 690 02	2.175 718 7	2.151 691 1	2.140 657 5	2.260 691 777	2.179 925 787	2.153 401 156	2.141 516 426 7
4	3.695 343 858 97	3.030 655 687 04	2.918 442 9	2.878 973 1	2.860 713 3	3.049 125 537	2.923 520 489 7	2.881 051 112	2.861 760 782 5
5	4.693 716 179 94	3.818 183 865 48	3.662 238 85	3.606 898 8	3.581 195 3	3.838 475 909	3.667 847 361 4	3.609 201 700	3.582 358 456 6
6	5.692 648 469 70	4.606 736 122 11	4.406 563 87	4.335 143 0	4.301 888 9	4.628 256 244	4.412 527 960 9	4.337 596 813	4.303 129 696 6
7	6.691 893 987 98	5.395 870 246 10	5.151 188 14	5.063 567 9	5.022 702 6	5.418 272 944	5.157 406 532 4	5.066 129 694 2	5.023 999 069 3
8	7.691 332 467 15	6.185 366 384 03	5.895 997 99	5.792 105 0	5.743 591 1	6.208 433 561	5.902 407 112 6	5.794 747 865 2	5.744 929 338 7
9	8.690 898 248 25	6.975 102 983 91	6.640 930 80	6.520 716 6	6.464 529 2	6.998 688 326	6.647 488 211 4	6.523 422 506 6	6.465 899 997 6
10	9.690 552 435 88	7.765 007 407 80	7.385 949 26	7.249 380 1	7.185 501 9	7.789 008 059	7.392 625 242 1	7.252 136 472 4	7.186 898 819 5

TABLE II. Values for the nonrelativistic energy parameter $\epsilon = (-E)^{1/2}$ (where E is the energy in atomic units) for the P states. Type-D expansions were used, containing the number of terms indicated in the column heading.

Z \ State	$2\,^1P\,(364)$	$3\,^1P\,(364)$	$4\,^1P\,(364)$	$5\,^1P\,(560)$	$2\,^3P\,(364)$	$3\,^3P\,(364)$	$4\,^3P\,(364)$	$5\,^3P\,(560)$
2	1.457 341 100 3	1.433 578 155	1.425 155 91	1.421 233 87	1.460 535 583 1	1.434 601 362 9	1.425 596 077	1.421 460 88
3	2.234 580 738 0	2.172 603 705	2.150 383 96	2.139 992 12	2.242 256 827 4	2.174 961 992 7	2.151 386 412	2.140 506 567
4	3.018 405 476 3	2.914 784 662	2.877 427 65	2.859 923 16	3.029 021 812 7	2.917 979 502 1	2.878 778 146	2.860 614 666
5	3.804 902 529 9	3.658 239 315	3.605 203 45	3.580 326 75	3.817 477 922 8	3.661 976 037 7	3.606 777 801	3.581 131 862
6	4.592 747 795 1	4.402 331 348	4.333 345 45	4.300 966 78	4.606 702 800 85	4.406 442 455 3	4.335 073 776	4.301 849 907
7	5.381 367 519 1	5.146 786 963	5.061 696 35	5.021 741 758	5.396 341 514 74	5.151 170 819 6	5.063 536 520	5.022 681 486
8	6.170 472 853 2	5.891 469 277	5.790 177 55	5.742 600 935	6.186 228 472 60	5.896 060 200 0	5.792 102 440	5.743 583 515
9	6.959 902 605 1	6.636 302 363	6.518 745 43	6.463 516 158	6.976 276 033 26	6.641 055 645 5	6.520 736 642	6.464 532 268
10	7.749 559 776 9	7.381 240 757	7.247 373 87	7.184 470 556	7.766 433 468 43	7.386 124 667 1	7.249 418 379	7.185 513 600

TABLE III. Values of $-E_J/\alpha^2$ (E_J in atomic units) for the S states. Type-C expansions were used, containing the number of terms indicated in the column heading.

Z \ State	$2\,^1S\,(220)$	$3\,^1S\,(364)$	$4\,^1S\,(364)$	$5\,^1S\,(364)$	$2\,^3S\,(120)$	$3\,^3S\,(220)$	$4\,^3S\,(364)$	$5\,^3S\,(364)$
2	0.034 289 2	0.011 996	0.005 428	0.002 905	0.164 468	0.045 091 5	0.018 290 5	0.009 144 2
3	0.557 44	0.199 88	0.091 06	0.048 63	1.445 04	0.438 118 4	0.186 202	0.095 632
4	2.892 05	1.044 31	0.477 84	0.255 90	5.723 3	1.813 340	0.786 471	0.408 698
5	9.301 3	3.362 44	1.540 37	0.825 66	15.818 7	5.138 272	2.254 12	1.179 138
6	22.986 8	8.305 24	3.805 77	2.040 5	35.488 6	11.713 76	5.176 51	2.719 347
7	48.087 9	17.357 13	7.953 52	4.264 5	69.427 4	23.173 98	10.293 34	5.423 32
8	89.681 3	32.335 8	14.815 4	7.943 4	123.267 4	41.486 44	18.496 66	9.766 66
9	153.781 5	55.392 4	25.375 6	13.604 6	203.578 2	68.951 99	30.830 9	16.306 56
10	247.340 4	89.011 3	40.770 5	21.857 0	317.866 9	108.204 81	48.492 7	25.681 81

TABLE IV. Values of $-E_J/\alpha^2$ (E_J in atomic units) for the P states. Type-D expansions containing 220 terms were used.

Z \ State	$2\,^1P$	$3\,^1P$	4^1P	5^1P	2^3P	3^3P	4^3P	5^3P
2	0.040 017	0.014 84	0.006 95	0.003 9	−0.026 934	−0.004 850	−0.001 51	−0.000 68
3	0.482 271	0.180 45	0.084 11	0.045 13	0.129 772	0.090 125	0.047 39	0.027 17
4	2.106 768	0.803 93	0.377 37	0.203 3	1.411 15	0.659 71	0.323 3	0.179 3
5	6.116 702	2.372 47	1.120 8	0.607 1	5.442 96	2.335 71	1.122 9	0.616 6
6	14.149 82	5.557 98	2.638 2	1.435	14.536 89	6.008 76	2.864 0	1.566
7	28.280 55	11.217 5	5.343	2.914	31.691 81	12.828 7	6.085 3	3.319
8	51.020 53	20.393 2	9.739	5.322	60.593 97	24.204 7	11.447	6.234
9	85.318 8	34.312 6	16.418	8.985	105.617 10	41.804 9	19.729	10.733
10	134.561 7	54.388 1	26.065	14.281	171.822 41	67.557 1	31.835	17.307

terms, and for the remaining states using a type-C expansion containing 364 terms. In Table II we list ϵ for the states $n\,^1P$, $n\,^3P$, $n=2-5$. They were obtained using type-D expansions containing 364 terms for $n=2$, 3, and 4, and 560 terms for $n=5$. Table III contains the values of $-E_J/\alpha^2$ for the states $n\,^1S$, $n\,^3S$, $n=2-5$. They were obtained using type-C expansions containing 120 terms in the case of $2\,^3S$, 220 terms in the case of $2\,^1S$ and $3\,^3S$, and 364 terms in the case of the remaining states. In Table IV, we list $-E_J/\alpha^2$ for the P states, the results listed all having been obtained from type-D expansions containing 220 terms.

On differencing the values given in Tables I to IV, we see that the results behave smoothly with Z. In fact, the values of ϵ can be almost exactly reproduced by an expression of the form $Z(a_0+a_1/Z+\cdots+a_6/Z^6)$, while the values of $-E_J/\alpha^2$ fit almost exactly to an expression of the form $Z^4(a_0+a_1/Z+\cdots+a_4/Z^4)$.

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