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Oscillator strengths for *S*-*P* and *P*-*D* transitions in heliumlike ions

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Explicitly correlated wave functions are constructed for the $n\,^1S$, $n\,^3S$, $n\,^1P$, $n\,^3P$,$n\,^1D$, and $n\,^3D$ states, with $n<7$, of the two-electron ions from He through Ne^{8+}. The variational energies are the best available for 180 of the 261 states. Electron-nuclear and electron-electron cusp checks are used to test the wave functions. For each ion, dipole oscillator strengths are calculated for 55 *S*-*P* and 40 *P*-*D* transitions. Our oscillator strengths are more accurate than previous values for 739 of the 855 transitions considered. Some coefficients for the $1/Z$ expansions of the energies and oscillator strengths have been estimated as an aid to extrapolating our results to higher nuclear charges.

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I. INTRODUCTION

Oscillator strengths are fundamental quantities in spectroscopy, but they are difficult to calculate by nonempirical quantum-mechanical methods. Hence, very many calculations of these quantities have been made for two-electron atoms, which are the simplest atomic species for which exact oscillator strengths are not known. However, most such studies have concentrated on a few select transitions with the aim of demonstrating that the method being used was generally useful. Only a few studies of high accuracy dealing with many transitions and many ions of the helium isoelectronic series have been reported.

Schiff, Pekeris, and Accad [1] used variationally determined wave functions to calculate oscillator strengths for 36 *S*-*P* transitions in each of the ions from He through Ne^{8+}. Kono and Hattori improved and extended [2] their work on He, and then reported oscillator strengths for 24 *P*-*D* transitions [3] in each of the ions from Li^+ through N^{5+}. A less accurate but much more extensive study was carried out by Sanders and Knight [4], who used *Z*-dependent, variational perturbation theory of low order to obtain oscillator strengths for 136 *S*-*P* and 112 *P*-*D* transitions for each of the ions through $Z=30$.

The purpose of this paper is to report calculated oscillator strengths for 55 *S*-*P* and 40 *P*-*D* transitions for each of the ions from He through Ne^{8+}. The accuracies of 739 of the 855 oscillator strengths considered have been improved. Moreover, our nonrelativistic energies are an improvement over current values for 180 of the 261 states considered. These calculations also enabled us to obtain estimates of coefficients in the $1/Z$ expansions of the oscillator strengths and energies.

The layout of this paper is as follows. Section II outlines our variational ansatz and method of calculation. Section III contains a comparison of our energies with previous work, and cusp and virial tests of our wave functions. A discussion of our oscillator strengths is contained in Sec. IV, and $1/Z$ expansion coefficients are contained in Sec. V. Hartree atomic units are used throughout.

II. WAVE FUNCTIONS

Our wave functions are variational approximations to the exact solutions of the Schrödinger equation with a nonrelativistic, infinite nuclear mass, spin-independent Hamiltonian given by

$$H=-\frac{\Delta_1}{2}-\frac{\Delta_2}{2}-\frac{Z}{r_1}-\frac{Z}{r_2}+\frac{1}{r_{12}}\ , \tag{1}$$

in which $\mathbf{r}_i=(r_i,\Omega_i)$ is the position vector of electron i for $i=1,2$, r_{12} is the interelectronic distance, and Z is the nuclear charge. Schiff, Pekeris, and Accad [1], Kono and Hattori [2,3], and Sanders and Knight [4] all used Hylleraas-type [5] wave functions containing several hundred and, in some cases, a few thousand terms. We have previously [6–8] shown that use of exponential correlation factors [5,9] can lead to compact wave functions of similar accuracy. Although our original work was restricted to low-lying states [6,7], the success of our ansatz for obtaining pseudospectra [8] encouraged us to expect that it would do well for more highly excited states as well. Thus, for the *S* and *P* states, we use spin free wave functions of the form [6–8]

$$\Psi=\sum_{k=1}^{N}c_k(1\pm P_{12})r_1^L\exp(-\alpha_k r_1-\beta_k r_2-\gamma_k r_{12})\times Y_{L,0}(\Omega_1)Y_{0,0}(\Omega_2)\ , \tag{2}$$

in which N is the number of terms, P_{12} is the permutation operator, the plus and minus signs refer to the singlet and triplet states, respectively, L is the total orbital angular

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momentum quantum number, c_k, α_k, β_k, and γ_k are variational parameters, and the $Y_{L,0}$ are spherical harmonics.

We had used [8] the above ansatz with $L=2$ for pseudospectral D states, but the expansion suffers from angular incompleteness in that case. Thus we include terms with the other factor required for angular completeness [10]. That is, our ansatz for D states is

$$\Psi=\sum_{k=1}^{N} c_k(1\pm P_{12})r_1^2\exp(-\alpha_k r_1-\beta_k r_2-\gamma_k r_{12})Y_{2,0}(\Omega_1)Y_{0,0}(\Omega_2)$$

$$+\sum_{k=N+1}^{N+M} d_k(1\pm P_{12})r_1r_2\exp(-\alpha_k r_1-\beta_k r_2-\gamma_k r_{12})\Upsilon(\Omega_1,\Omega_2)\ , \tag{3}$$

in which

$$\Upsilon(\Omega_1,\Omega_2)=2Y_{1,0}(\Omega_1)Y_{1,0}(\Omega_2)+Y_{1,1}(\Omega_1)Y_{1,-1}(\Omega_2)+Y_{1,-1}(\Omega_1)Y_{1,1}(\Omega_2)\ . \tag{4}$$

The two sets of terms in Eq. (3) will be referred to as *sd* and *pp* terms, respectively. Note that Bishop and Pipin [11] have recently used D state wave functions of this form.

Square integrability requires that the nonlinear parameters satisfy the following constraints:

$$\alpha_k+\beta_k>0\ , \tag{5}$$

$$\alpha_k+\gamma_k>0\ , \tag{6}$$

$$\beta_k+\gamma_k>0\ . \tag{7}$$

The nonlinear parameters were generated in a pseudorandom fashion, as in our previous work [6–8],

$$\alpha_k=\eta[(A_2-A_1)\langle\langle k(k+1)\sqrt{2}/2\rangle\rangle+A_1]\ , \tag{8}$$

$$\beta_k=\eta[(B_2-B_1)\langle\langle k(k+1)\sqrt{3}/2\rangle\rangle+B_1]\ , \tag{9}$$

$$\gamma_k=\eta[(G_2-G_1)\langle\langle k(k+1)\sqrt{5}/2\rangle\rangle+G_1]\ , \tag{10}$$

in which $\langle\langle x\rangle\rangle$ is defined to be the fractional part of x, A_1, A_2, B_1, B_2, G_1, and G_2 are variational parallelepiped parameters, and η is a virial scale factor [5,12]. This effectively reduces the problem of optimizing $3N$ nonlinear parameters to the much more tractable problem of optimizing six nonlinear parameters. All the linear parameters are found variationally.

On the basis of our previous work [6–8], we estimated that 100-term expansions would be sufficient to obtain an accuracy comparable to that achieved in previous work on oscillator strengths using conventional Hylleraas wave functions containing several hundred terms. For the sake of consistency, 100-term expansions were used for all states and ions, even though one can argue that neutral helium is sufficiently important that one should aim for higher accuracy in that case. Thus, we use $N=100$ in Eq. (2) for the S and P states. For the D states, we found by numerical experimentation on the $3\,^1D$ state of He that $M/(N+M)=0.3$ is a good mix of *sd* and *pp* terms; therefore, we use $N=70$ and $M=30$ with the constraint that the nonlinear parameters in the *pp* terms are the same as the nonlinear parameters in the first M *sd* terms.

The six parallelepiped parameters were independently optimized, subject to the square integrability conditions of Eqs. (5)–(7), for each of the 29 states of each ion using Powell's conjugate direction algorithm [13]. All optimization methods are plagued by local minima; hence it was not surprising that different initial estimates of the parameters often led to substantially different "optimized" values. Due to the large number of states we considered, only one initial estimate was considered for each state except when the optimized energies were higher than expected or the optimized parallelepiped parameters were clearly inconsistent with physical arguments. In such instances, up to 70 initial parameter estimates were tried. After the necessarily imperfect optimization, each wave function was scaled to satisfy the virial theorem [5,12]. Our scale factors never deviated from unity by more than 10^{-6} reflecting the fact that the optimizations had been allowed to continue until the energies were stable to at least 10^{-11} hartree—a threshold two orders of magnitude lower than the absolute accuracies of our wave functions. The optimized parallelepiped parameters are available from the authors upon request.

Following our earlier cautionary remarks [6], we performed *all* calculations in quadruple precision (≈ 32 decimal digits) to avoid computational linear dependence. The latter problem was most acute in the $6\,^1S$ state of He; in that case, the smallest eigenvalue of the Gram matrix, for normalized basis geminal functions was 1.2×10^{-30}.

III. ENERGIES AND QUALITY TESTS

The calculated energies for each of the bound S, P, and D states with $n<7$ are listed in Tables I–IV for He through Ne^{8+}. The ground-state energy of H^- is included for the sake of completeness. Consider the S states first. Our energies for 69 of the 100 S states considered are the lowest reported so far; the improvements range up to 12 μhartree for the $5\,^1S$ states of the ions with

TABLE I. Ground-state energies (in hartrees) of the two-electron ions.

Z	$-E$	Z	$-E$
1	0.527 751 011 8	6	32.406 246 598 0
2	2.903 724 373 6	7	44.781 445 145 0
3	7.279 913 409 6	8	59.156 595 119 0
4	13.655 566 234 0	9	75.531 712 357 5
5	22.030 971 574 2	10	93.906 806 507 2

TABLE II. Excited-state energies for He, Li^+, and Be^{2+}. The tabulated entries are $-E$ values in hartrees.

n	$n\,^1S$	$n\,^3S$	$n\,^1P$	$n\,^3P$	$n\,^1D$	$n\,^3D$
			He			
2	2.145 974 029 2	2.175 229 378 176	2.123 843 080 2	2.133 164 181 6		
3	2.061 271 972 0	2.068 689 067 283	2.055 146 357 0	2.058 081 077 2	2.055 620 732 0	2.055 636 308 8
4	2.033 586 699 5	2.036 512 082 933	2.031 069 646 4	2.032 324 334 3	2.031 279 844 5	2.031 288 846 2
5	2.021 176 830 9	2.022 618 871 382	2.019 905 984 9	2.020 551 176 5	2.020 015 829 7	2.020 021 022 8
6	2.014 563 084 7	2.015 377 452 422	2.013 833 970 5	2.014 207 945 5	2.013 898 212 5	2.013 901 405 8
			Li^+			
2	5.040 876 731 3	5.110 727 372 509	4.993 351 072 1	5.027 715 677 0		
3	4.733 756 077 8	4.752 076 455 858	4.720 206 872 8	4.730 459 664 1	4.722 390 988 4	4.722 526 912 4
4	4.629 783 597 3	4.637 136 594 629	4.624 151 390 4	4.628 463 556 3	4.625 074 124 1	4.625 150 773 2
5	4.582 427 952 7	4.586 092 669 796	4.579 566 513 6	4.581 768 403 5	4.580 038 695 6	4.580 082 425 7
6	4.556 953 177 0	4.559 038 618 569	4.555 305 067 2	4.556 576 783 9	4.555 578 166 8	4.555 604 868 4
			Be^{2+}			
2	9.184 873 877 5	9.297 166 589 741	9.110 771 614 2	9.174 973 137 9		
3	8.517 312 546 5	8.546 972 068 861	8.495 969 629 0	8.514 604 359 8	8.500 215 825 6	8.500 582 343 0
4	8.288 494 625 7	8.300 455 559 448	8.279 590 107 0	8.287 363 655 6	8.281 339 805 9	8.281 543 746 0
5	8.183 693 306 7	8.189 674 851 615	8.179 160 610 6	8.183 116 287 9	8.180 045 949 0	8.180 161 579 7
6	8.127 131 496 8	8.130 543 857 315	8.124 517 627 9	8.126 798 285 8	8.125 026 570 0	8.125 096 982 0

$Z > 3$. The energies for the remaining 31 S states are no more than 20 nhartree above the best available results as outlined below. The $1\,^1S$ and $2\,^1S$ energies, respectively, lie no more than 7.8 and 16.9 nhartree above the values obtained by Freund, Huxtable, and Morgan [14] and Frankowski [15] using wave functions containing logarithmic terms, and by Drake [16] from Hylleraas-type expansions containing several hundred terms. For neutral He, the higher ^1S and ^3S energies, respectively, lie no more than 20 and 0.9 nhartree above the results of Drake [16] and Kono and Hattori [17] obtained with Hylleraas-type expansions.

The energies of the 48 P states with $n=4$, 5, and 6 for the cations lie below the best available values. Our ^1P and ^3P energies for He lie no more than 10 and 14 nhartree, respectively, above the values obtained by Drake and Makowski [18], and Kono and Hattori [17]. Most of the $2\,^1P$, $2\,^3P$, $3\,^1P$, and $3\,^3P$ energies for the cations lie above the values of Accad, Pekeris, and Schiff [20], but never by more than 30 nhartree.

Our ^1D and ^3D energies for helium lie no more than 15 and 10 nhartree, respectively, above those of Drake [19]. Our energies for the D states of the cations are in all cases as good as or better than those in the literature [3].

TABLE III. Excited-state energies for B^{3+}, C^{4+}, and N^{5+}. The tabulated entries are $-E$ values in hartrees.

n	$n\,^1S$	$n\,^3S$	$n\,^1P$	$n\,^3P$	$n\,^1D$	$n\,^3D$
			B^{3+}			
2	14.578 528 014 0	14.733 897 348 781	14.477 283 253 6	14.573 137 685 5		
3	13.411 996 931 7	13.453 104 279 643	13.382 714 879 9	13.410 068 480 2	13.389 100 300 3	13.389 771 590 0
4	13.009 726 826 2	13.026 336 958 201	12.997 492 052 7	13.008 846 136 5	13.000 080 558 2	13.000 451 012 3
5	12.824 972 647 7	12.833 292 190 279	12.818 739 792 6	12.824 505 426 0	12.820 039 768 9	12.820 249 042 8
6	12.725 096 643 3	12.729 848 532 224	12.721 500 515 9	12.724 821 231 6	12.722 244 756 6	12.722 371 938 0
			C^{4+}			
2	21.222 017 684 6	21.420 755 902 276	21.093 332 300 9	21.221 710 689 9		
3	19.417 808 525 6	19.470 403 018 010	19.380 521 287 2	19.416 735 089 9	19.389 059 129 7	19.390 083 504 7
4	18.793 472 876 6	18.814 746 155 889	18.777 882 958 4	18.792 864 670 2	18.781 303 774 6	18.781 865 933 5
5	18.506 260 618 2	18.516 925 265 508	18.498 315 415 8	18.505 912 632 5	18.500 024 180 1	18.500 341 010 0
6	18.350 845 016 0	18.356 940 714 471	18.346 259 740 7	18.350 632 330 1	18.347 235 242 6	18.347 427 451 3
			N^{5+}			
2	29.115 415 693 9	29.357 681 737 453	28.959 116 388 4	29.120 501 738 3		
3	26.534 742 571 1	26.598 842 151 505	26.489 416 031 7	26.534 560 787 9	26.500 103 284 7	26.501 513 187 1
4	25.639 727 620 1	25.665 670 121 432	25.620 770 176 3	25.639 402 115 9	25.625 014 784 5	25.625 785 417 7
5	25.227 553 793 9	25.240 566 728 042	25.217 890 422 9	25.227 329 314 6	25.220 002 095 0	25.220 435 655 2
6	25.004 374 460 8	25.011 815 871 593	24.998 796 797 6	25.004 226 664 1	24.999 999 643 7	25.000 262 436 4

TABLE IV. Excited-state energies for O^{6+}, F^{7+}, and Ne^{8+}. The tabulated entries are $-E$ values in hartrees.

n	$n\,^1S$	$n\,^3S$	$n\,^1P$	$n\,^3P$	$n\,^1D$	$n\,^3D$
O^{6+}						
2	38.258 757 285 8	38.544 647 320 047	38.074 735 221 6	38.269 422 709 9		
3	34.762 795 528 4	34.838 409 733 347	34.709 410 232 8	34.763 525 857 8	34.722 240 109 8	34.724 058 155 7
4	33.548 488 006 4	33.579 102 862 297	33.526 156 282 4	33.548 450 694 2	33.531 217 100 8	33.532 207 822 1
5	32.988 850 381 8	33.004 213 186 445	32.977 465 633 8	32.988 751 591 3	32.979 975 410 1	32.980 532 032 2
6	32.685 683 781 2	32.694 471 907 219	32.679 111 956 6	32.685 601 986 2	32.680 539 052 3	32.680 876 234 4
F^{7+}						
2	48.652 061 617 4	48.981 638 329 481	48.440 244 265 5	48.668 427 287 7		
3	44.101 965 058 9	44.189 099 531 881	44.040 509 034 4	44.103 620 061 9	44.055 474 517 7	44.057 717 033 7
4	42.519 752 173 8	42.555 041 240 113	42.494 042 049 7	42.520 006 368 7	42.499 913 067 1	42.501 132 218 2
5	41.790 149 243 0	41.807 862 859 144	41.777 041 255 1	41.790 177 441 4	41.779 945 329 5	41.780 629 577 8
6	41.394 772 284 7	41.404 907 718 164	41.387 205 279 1	41.394 757 153 1	41.388 854 301 5	41.389 268 509 8
Ne^{8+}						
2	60.295 340 024 1	60.668 646 584 034	60.055 676 728 0	60.317 488 814 7		
3	54.552 249 617 8	54.650 907 980 593	54.482 715 091 1	54.554 837 569 3	54.499 809 847 9	54.502 488 978 1
4	52.553 519 041 0	52.593 483 453 112	52.524 428 097 6	52.554 066 852 7	52.531 104 267 4	52.532 558 033 1
5	51.631 449 632 5	51.651 514 721 700	51.616 617 303 3	51.631 605 691 2	51.619 912 692 8	51.620 727 944 7
6	51.131 639 509 0	51.143 122 668 823	51.123 076 728 3	51.131 691 464 4	51.124 945 808 2	51.125 439 135 9

Independent checks of the accuracies of our wave functions can be made with the help of cusp conditions [21–25]. In particular, the electron-nuclear cusp condition [21–23] states

$$C_{en}=\left[\frac{-\rho'(r)}{2Z\rho(r)}\right]_{r=0}=-1\ , \tag{11}$$

in which $\rho(r)$ is the spherically averaged electron number density. The electron-electron cusp condition [21,22,24] reads

$$C_{ee}=[h'(u)/h(u)]_{u=0}=1\ , \tag{12}$$

in which $h(u)$ is the spherical average of the interelectronic density [26]. Equation (12) is satisfied trivially by virtue of the Pauli principle for states of maximum spin multiplicity (i.e., triplet states in two-electron systems). In such cases, there is a higher-order cusp condition [25],

$$C_{ee}=\left[\frac{2h^{(3)}(u)}{3h''(u)}\right]_{u=0}=1\ . \tag{13}$$

Exact wave functions satisfy the cusp conditions exactly, and thus a measure of the quality of an approximate wave function is the degree to which it satisfies them. The one-electron cusp condition of Eq. (11) is easier to satisfy than the two-electron cusp conditions of Eqs. (12) and (13). For our wave functions, the largest deviation of C_{en} from unity is only 7.1×10^{-5} for the $2\,^1S$ state of B^{3+}, whereas the largest deviation of C_{ee} from unity is 0.20 for the $6\,^1D$ state of B^{3+}. Our wave functions have average deviations from unity of 9×10^{-6} for C_{en} and 0.045 for C_{ee}. The average C_{ee} deviations for states of the same symmetry are 0.037, 0.016, 0.031, 0.060, 0.067, and 0.071 for the ^1S, ^3S, ^1P, ^3P, ^1D, and ^3D states, respectively. Similarly, the average C_{en} deviations for states of the same symmetry are 1.4×10^{-5}, 2.2×10^{-6}, 1.3×10^{-5}, 1.1×10^{-5}, 6.7×10^{-6}, and 5.2×10^{-6} for the ^1S, ^3S, ^1P, ^3P, ^1D, and ^3D states, respectively. For each state, the deviations averaged over all the ions tend to increase as the principal quantum number increases. For each symmetry, the deviations averaged over principal quantum number tend to remain constant as the nuclear charge increases.

Neither accurate energies nor accurate cusp ratios guarantee accurate oscillator strengths. However, they do attest to the overall quality of the wave functions.

IV. OSCILLATOR STRENGTHS

Optical oscillator strengths were calculated for the dipole-allowed S-P and P-D transitions using both the length form [27]

$$f_l=C(E_m-E_n)|\langle m|z_1+z_2|n\rangle|^2 \tag{14}$$

and the velocity form [28]

$$f_v=\frac{C}{E_m-E_n}\left|\left\langle m\left|\frac{\partial}{\partial z_1}+\frac{\partial}{\partial z_2}\right|n\right\rangle\right|^2\ , \tag{15}$$

in which $C=2$ and $\frac{5}{3}$, respectively, for S-P and P-D transitions between states m and n, and z_i is the z coordinate of electron i. The f values were also computed in quadruple precision to reduce roundoff errors arising from cancellation among contributing terms that in turn is a consequence of the near linear dependence of our basis functions. Interestingly, the length and velocity forms proved to be equally susceptible to roundoff errors. The length and velocity forms are equivalent if both wave functions are exact, but give different results if approximate wave functions are used. There is no consensus in the literature [1–3] as to which approximate value is more reliable and under what circumstances. We chose to use the average of the length and velocity results: $f=(f_l+f_v)/2$. Moreover, we use, as others [1–3] do, the difference between the two values, $\delta f=f_l-f_v$, as an estimate of the accuracy of the mean. Thus, in Tables V–VIII, we list mean f values rounded on the basis of δf. A regular entry indicates that δf was between 0.7 and 2.99 units in the last quoted digit, whereas an underlined last digit indicates that δf was between 3 and 6.99 units in that digit. Since agreement between the two forms is not an infallible indicator of accuracy [1], the tabulated values are limited to six decimal digits whenever the length and velocity values agree to more than six digits.

We find that δf is generally smaller for transitions involving lower-lying states and for the more highly charged ions. However, in contrast to previous work [1], we find that δf is *not* always smaller for the triplet than for the corresponding singlet transition. For instance, δf values for transitions originating from the $6\,^1S$, $4\,^1P$, and $5\,^1P$ states are smaller than for the corresponding triplet transitions.

For each $m\,^1S-n\,^1P$ and $m\,^3S-n\,^3P$ transition, the oscillator strengths are monotonic functions of the nuclear charge; they increase monotonically with Z when $n>m$ and decrease monotonically otherwise. Moreover, the oscillator strengths are monotonic functions of Z for all $m\,^3P-n\,^3D$ transitions except 2^3P-4^3D for which a maximum occurs at $Z=4$. On the other hand, the oscillator strengths for the $m\,^1P-n\,^1D$ transitions are unimodal functions of Z; the extremum is usually a maximum if $n\geq m$.

Oscillator strengths for 503 of the 855 transitions we considered have been calculated previously [1–3] using variationally determined Hylleraas-type wave functions. An unequivocal comparison is not always possible because the previously tabulated values are sometimes the f_l values, sometimes the f_v values, and sometimes extrapolations based on both length and velocity values obtained from a series of wave functions. Nevertheless, detailed comparison of our f_l and f_v values with the older work [1–3] reveals several trends. Generally, when a discrepancy occurs, one of our f_l and f_v values (usually the latter) lies outside the error margins cited whereas the other agrees closely with the older value. For each ion,

TABLE V. Optical oscillator strengths for the $m\,^1S$ to $n\,^1P$ transitions in the two-electron ions.

m	n	He	Li^+	Be^{2+}	B^{3+}	C^{4+}	N^{5+}	O^{6+}	F^{7+}	Ne^{8+}
1	2	0.276 17	0.456 62$\underline{7}$	0.551 555	0.608 915	0.647 067	0.674 198	0.694 449	0.710 131	0.722 625
	3	0.073 43	0.110 637	0.126 850	0.135 37$\underline{3}$	0.140 479	0.143 817	0.146 149	0.147 857	0.149 158
	4	0.029 86$\underline{1}$	0.043 66$\underline{7}$	0.049 227	0.051 970	0.053 529	0.054 505	0.055 161	0.055 626	0.055 971
	5	0.015 039	0.021 697	0.024 273	0.025 501	0.026 178	0.026 591	0.026 862	0.027 050	0.027 186
	6	0.008 627	0.012 358	0.013 767	0.014 426	0.014 782	0.014 996	0.015 134	0.015 228	0.015 296
2	2	0.376 4$\underline{8}$	0.212 58	0.148 56	0.114 37	0.093 05$\underline{7}$	0.078 48	0.067 860	0.059 783	0.053 430
	3	0.151 35	0.257 08$\underline{5}$	0.305 89	0.333 730	0.351 69	0.364 24$\underline{2}$	0.373 502	0.380 615	0.386 25$\underline{1}$
	4	0.049 15	0.072 7	0.082 13	0.087 0$\underline{4}$	0.090 08$\underline{9}$	0.092 1$\underline{2}$	0.093 6$\underline{0}$	0.094 7$\underline{2}$	0.095 6$\underline{0}$
	5	0.022 34	0.031 55	0.034 97	0.036 70$\underline{7}$	0.037 74$\underline{6}$	0.038 444	0.038 939	0.039 312	0.039 600
	6	0.012 13$\underline{6}$	0.016 77	0.018 41	0.019 237	0.019 72$\underline{1}$	0.020 044	0.020 272	0.020 44$\underline{3}$	0.020 575
3	2	0.145 46$\underline{0}$	0.094 67$\underline{1}$	0.077 37$\underline{2}$	0.068 542	0.063 160	0.059 52$\underline{8}$	0.056 911	0.054 936	0.053 391
	3	0.626 3	0.362 $\underline{7}$	0.256 2	0.198 2	0.161 7	0.136 5	0.118 1	0.104 1	0.093 1
	4	0.143 9	0.265 0$\underline{6}$	0.323 1$\underline{7}$	0.357 1	0.379 2$\underline{4}$	0.394 87	0.406 4$\underline{8}$	0.415 4$\underline{1}$	0.422 5$\underline{3}$
	5	0.050 5	0.079 76	0.092 0$\underline{3}$	0.098 6	0.102 9	0.105 7$\underline{4}$	0.107 8	0.109 4$\underline{3}$	0.110 6$\underline{7}$
	6	0.024 1	0.036 2	0.040 95	0.043 46	0.045 00	0.046 05	0.046 81	0.047 37	0.047 81
4	2	0.025 865	0.018 748	0.015 950	0.014 428	0.013 466	0.012 800	0.012 312	0.011 939	0.011 645
	3	0.307 5$\underline{3}$	0.205 3$\underline{2}$	0.170 0$\underline{1}$	0.152 02	0.141 10	0.133 77	0.128 52	0.124 56	0.121 48
	4	0.858 1	0.501 3	0.355 4	0.275 5	0.224 9	0.190 0	0.164 4$\underline{2}$	0.145 0	0.129 6
	5	0.146 28	0.284 2$\underline{4}$	0.351 83	0.391 6$\underline{2}$	0.417 83	0.436 38	0.450 20	0.460 88	0.469 39
	6	0.052 8	0.087 2	0.101 893	0.110 1$\underline{2}$	0.115 2$\underline{9}$	0.118 8$\underline{6}$	0.121 4$\underline{7}$	0.123 45	0.125 011
5	2	0.009 66	0.007 21$\underline{7}$	0.006 210	0.005 65$\underline{5}$	0.005 297	0.005 047	0.004 863	0.004 721	0.004 609
	3	0.055 50	0.041 32	0.035 64	0.032 575	0.030 649	0.029 328	0.028 366	0.027 636	0.027 06$\underline{2}$
	4	0.475 8$\underline{0}$	0.322 95$\underline{0}$	0.269 6$\underline{2}$	0.242 39	0.225 84	0.214 74	0.206 78	0.200 80	0.196 14
	5	1.083 3	0.635 8	0.451 6	0.350 3	0.286 1$\underline{7}$	0.241 8$\underline{3}$	0.209 3$\underline{7}$	0.184 5$\underline{9}$	0.165 0$\underline{4}$
	6	0.152 64$\underline{6}$	0.308 0$\underline{0}$	0.385 15	0.430 9	0.461 08	0.482 52	0.498 5	0.510 89	0.520 8
6	2	0.004 77$\underline{1}$	0.003 618	0.003 132	0.002 859	0.002 683	0.002 560	0.002 468	0.002 397	0.002 341
	3	0.021 0$\underline{9}$	0.016 23	0.014 157	0.013 021	0.012 29$\underline{9}$	0.011 80$\underline{1}$	0.011 43$\underline{7}$	0.011 17	0.010 941
	4	0.086 20	0.065 4$\underline{4}$	0.056 98	0.052 39	0.049 51	0.047 53	0.046 09	0.044 99	0.044 13
	5	0.646 7$\underline{7}$	0.443 7$\underline{1}$	0.372 45	0.335 96	0.313 79	0.298 89	0.288 20$\underline{2}$	0.280 16$\underline{2}$	0.273 89$\underline{7}$
	6	1.305 3$\underline{7}$	0.768 3	0.546 4	0.424 2	0.346 6	0.292 9$\underline{5}$	0.253 6$\underline{7}$	0.223 6$\underline{6}$	0.199 9$\underline{9}$

TABLE VI. Optical oscillator strengths for the $m\ {}^3S$ to $n\ {}^3P$ transitions in the two-electron ions.

m	n	He	Li^{+}	Be^{2+}	B^{3+}	C^{4+}	N^{5+}	O^{6+}	F^{7+}	Ne^{8+}
2	2	0.539 1	0.307 944	0.213 139	0.162 626	0.131 381	0.110 178	0.094 856	0.083 267	0.074 199
	3	0.064 47	0.187 07	0.252 58	0.291 22	0.316 48	0.334 23	0.347 366	0.357 482	0.365 507
	4	0.025 76	0.057 54	0.071 52	0.079 03	0.083 665	0.086 803	0.089 063	0.090 765	0.092 095
	5	0.012 493	0.025 60	0.030 955	0.033 733	0.035 409	0.036 526	0.037 320	0.037 911	0.038 370
	6	0.006 981	0.013 745	0.016 411	0.017 769	0.018 578	0.019 112	0.019 489	0.019 770	0.019 985
3	2	0.208 52	0.117 09	0.088 70	0.075 437	0.067 845	0.062 951	0.059 543	0.057 035	0.055 116
	3	0.891 0	0.513 0	0.355 8	0.271 8	0.219 8	0.184 4	0.158 8	0.139 43	0.124 3
	4	0.050 06	0.186 83	0.264 06	0.310 27	0.340 67	0.362 11	0.378 02	0.390 30	0.400 04
	5	0.022 91	0.061 42	0.079 30	0.089 09	0.095 20	0.099 37	0.102 38	0.104 662	0.106 450
	6	0.011 985	0.028 719	0.035 918	0.039 72	0.042 045	0.043 607	0.044 721	0.045 563	0.046 215
4	2	0.031 715	0.021 472	0.017 328	0.015 221	0.013 962	0.013 131	0.012 541	0.012 104	0.011 764
	3	0.435 71	0.255 01	0.197 46	0.170 16	0.154 37	0.144 13	0.136 958	0.131 663	0.127 597
	4	1.215 4	0.703 7	0.489 1	0.373 9	0.302 5	0.253 9	0.218 8	0.192 1	0.171 3
	5	0.044 22	0.196 15	0.285 20	0.339 00	0.374 54	0.399 67	0.418 35	0.432 78	0.444 24
	6	0.021 63	0.065 88	0.087 20	0.098 99	0.106 41	0.111 48	0.115 16	0.117 950	0.120 14
5	2	0.011 32	0.008 061	0.006 623	0.005 876	0.005 423	0.005 120	0.004 903	0.004 742	0.004 617
	3	0.067 59	0.047 99	0.039 62	0.035 29	0.032 674	0.030 921	0.029 67	0.028 74	0.028 010
	4	0.668 35	0.400 05	0.313 28	0.271 78	0.247 69	0.231 99	0.220 98	0.212 823	0.206 555
	5	1.530 8	0.889 8	0.619 1	0.473 7	0.383 4	0.321 9	0.277 4	0.243 6	0.217 2
	6	0.041 51	0.209 30	0.310 34	0.371 77	0.412 49	0.441 34	0.462 80	0.479 38	0.492 57
6	2	0.005 492	0.003 990	0.003 308	0.002 947	0.002 727	0.002 579	0.002 475	0.002 396	0.002 335
	3	0.024 68	0.018 45	0.015 528	0.013 963	0.012 998	0.012 352	0.011 88	0.011 533	0.011 267
	4	0.103 97	0.075 88	0.063 5	0.056 980	0.053 0	0.050 31	0.048 40	0.046 98	0.045 86
	5	0.903 3	0.548 28	0.432 33	0.376 62	0.344 17	0.323 00	0.308 12	0.297 09	0.288 601
	6	1.841 9	1.073 7	0.747 7	0.572 4	0.463 3	0.389 1	0.335 3	0.294 5	0.262 6

TABLE VII. Optical oscillator strengths for the $m\ {}^1P$ to $n\ {}^1D$ transitions in the two-electron ions.

m	n	He	Li^{+}	Be^{2+}	B^{3+}	C^{4+}	N^{5+}	O^{6+}	F^{7+}	Ne^{8+}
2	3	0.710 17	0.711 61	0.708 792	0.706 33	0.704 492	0.703 132	0.702 101	0.701 303	0.700 672
	4	0.120 27	0.119 270	0.119 178	0.119 314	0.119 497	0.119 678	0.119 844	0.119 990	0.120 119
	5	0.043 28	0.042 74	0.042 746	0.042 875	0.043 008	0.043 129	0.043 235	0.043 325	0.043 405
	6	0.020 952	0.020 654	0.020 675	0.020 752	0.020 833	0.020 907	0.020 969	0.021 024	0.021 071
3	3	0.021 1	0.024 3	0.021 0	0.017 8	0.015 25	0.013 27	0.011 71	0.010 46	0.009 45
	4	0.648 10	0.651 706	0.646 698	0.642 046	0.638 449	0.635 702	0.633 569	0.631 878	0.630 512
	5	0.141 32	0.141 406	0.141 040	0.140 730	0.140 492	0.140 313	0.140 176	0.140 071	0.139 98
	6	0.056 26	0.056 23	0.056 183	0.056 161	0.056 15	0.056 140	0.056 136	0.056 15	0.056 132
4	3	0.015 305	0.015 01	0.015 50	0.015 95	0.016 299	0.016 570	0.016 780	0.016 951	0.017 087
	4	0.040 04	0.043 9	0.037 08	0.030 90	0.026 16	0.022 56	0.019 77	0.017 55	0.015 77
	5	0.647 66	0.651 1	0.644 29	0.638 28	0.633 710	0.630 271	0.627 627	0.625 54	0.623 869
	6	0.152 82	0.153 14	0.152 40	0.151 73	0.151 23	0.150 84	0.150 55	0.150 30	0.150 119
5	3	0.003 114	0.003 067	0.003 163	0.003 249	0.003 316	0.003 366	0.003 405	0.003 437	0.003 462
	4	0.039 300	0.038 78	0.039 99	0.041 067	0.041 883	0.042 505	0.042 985	0.043 364	0.043 670
	5	0.057 31	0.061 59	0.051 415	0.042 51	0.035 77	0.030 72	0.026 83	0.023 79	0.021 32
	6	0.669 83	0.673 10	0.664 842	0.657 73	0.652 406	0.648 425	0.645 381	0.642 992	0.641 080
6	3	0.001 190	0.001 173	0.001 210	0.001 243	0.001 267	0.001 286	0.001 301	0.001 312	0.001 321
	4	0.008 38	0.008 29	0.008 532	0.008 72	0.008 896	0.009 012	0.009 104	0.009 175	0.009 232
	5	0.068 42	0.067 711	0.069 746	0.071 516	0.072 84	0.073 85	0.074 629	0.075 238	0.075 728
	6	0.073 60	0.078 3	0.064 8	0.053 5	0.044 87	0.038 4	0.033 5	0.029 6	0.026 54

TABLE VIII. Optical oscillator strengths for the *m* ^3P to *n* ^3D transitions in the two-electron ions.

m	*n*	He	Li^+	Be^{2+}	B^{3+}	C^{4+}	N^{5+}	O^{6+}	F^{7+}	Ne^{8+}
2	3	0.610 24	0.624 659	0.639 126	0.649 263	0.656 473	0.661 802	0.665 883	0.669 098	0.671 696
	4	0.122 850	0.123 21$\underline{4}$	0.123 27$\underline{5}$	0.123 20	0.123 10	0.123 00$\underline{0}$	0.122 90$\underline{3}$	0.122 824	0.122 748
	5	0.047 0	0.046 79$\underline{5}$	0.046 44$\underline{7}$	0.046 16$\underline{0}$	0.045 93	0.045 74$\underline{9}$	0.045 602	0.045 482	0.045 384
	6	0.023 472	0.023 277	0.023 016	0.022 808	0.022 647	0.022 524	0.022 427	0.022 347	0.022 282
3	3	0.112 2	0.090 8	0.071 2	0.057 8$\underline{1}$	0.048 5$\underline{0}$	0.041 7$\underline{1}$	0.036 55	0.032 52	0.029 29
	4	0.477 6$\underline{0}$	0.503 38	0.527 27	0.543 77	0.555 417	0.563 999	0.570 55$\underline{4}$	0.575 71$\underline{4}$	0.579 876
	5	0.124 531	0.127 8$\underline{5}$	0.130 6$\underline{0}$	0.132 4$\underline{1}$	0.133 63$\underline{1}$	0.134 484	0.135 12	0.135 61	0.135 988
	6	0.052 9$\underline{8}$	0.053 88	0.054 55	0.054 95	0.055 19$\underline{6}$	0.055 36$\underline{6}$	0.055 48	0.055 57	0.055 64$\underline{5}$
4	3	0.036 960	0.032 79	0.029 30	0.027 05	0.025 54$\underline{0}$	0.024 46$\underline{2}$	0.023 66$\underline{0}$	0.023 040	0.022 548
	4	0.200 947	0.160 6	0.125 2$\underline{6}$	0.101 5$\underline{2}$	0.085 0$\underline{5}$	0.073 0$\underline{6}$	0.063 99	0.056 90	0.051 22
	5	0.438 3$\underline{9}$	0.470 5$\underline{4}$	0.499 4$\underline{9}$	0.519 40	0.533 46	0.543 81	0.551 72	0.557 94	0.562 96
	6	0.123 97$\underline{2}$	0.129 22	0.133 7	0.136 65	0.138 6	0.140 0$\underline{6}$	0.141 1$\underline{4}$	0.141 9$\underline{8}$	0.142 6$\underline{4}$
5	3	0.006 90$\underline{2}$	0.006 20$\underline{2}$	0.005 61$\underline{3}$	0.005 229	0.004 967	0.004 779	0.004 639	0.004 529	0.004 442
	4	0.088 31	0.078 73	0.070 90	0.065 873	0.062 492	0.060 085	0.058 294	0.056 911	0.055 813
	5	0.280 0$\underline{9}$	0.222 7	0.173 3$\underline{7}$	0.140 4$\underline{0}$	0.117 5$\underline{6}$	0.100 9$\underline{6}$	0.088 41	0.078 60	0.070 73
	6	0.429 44	0.466 48	0.499 46	0.522 13	0.538 14$\underline{4}$	0.549 94	0.558 95	0.566 04$\underline{4}$	0.571 77
6	3	0.002 586	0.002 331	0.002 114	0.001 975	0.001 878	0.001 809	0.001 757	0.001 717	0.001 685
	4	0.017 043	0.015 44	0.014 11	0.013 23	0.012 648	0.012 22$\underline{1}$	0.011 902	0.011 656	0.011 458
	5	0.146 98	0.131 57	0.119 085	0.111 08$\underline{9}$	0.105 70$\underline{5}$	0.101 873	0.099 018	0.096 816	0.095 066
	6	0.354 3$\underline{2}$	0.281 1	0.218 6$\underline{5}$	0.177 0$\underline{2}$	0.148 19	0.127 2$\underline{6}$	0.111 42	0.099 06	0.089 14

there are more discrepancies between our results and older work [1–3] for the triplet rather than the singlet transitions. In general, an observed discrepancy for a given transition tends to occur for several of the ions.

For He, our f_l and f_v values lie within the recommended error margins of the values of Kono and Hattori [2] for 72 of the 95 transitions considered. If we take energies and suggested error margins in the oscillator strengths as criteria, then we find that our results are "more accurate" than theirs [2] for 60 transitions, comparable for 22, and "less accurate" for 13 transitions. For the *S*-*P* transitions of the cations with $Z>2$, a similar comparison with the work of Schiff, Pekeris, and Accad [1] suggests that our recommended oscillator strengths are more accurate than theirs [1] for 255 transitions and less accurate for 33 transitions. Most of the latter involve the $3\,^1S$ and $3\,^3S$ states. Similarly, our values are more accurate than those of Kono and Hattori [3] for 72, comparable for 19, and less accurate for 29 *P*-*D* transitions for the cations from Li^+ through N^{5+}. There are also 152 *S*-*P* and 200 *P*-*D* transitions that we considered for which no previous high accuracy values are available.

V. 1/*Z* EXPANSION COEFFICIENTS

Z scaling of the coordinates and treatment of the interelectronic repulsion as a perturbation leads to so-called $1/Z$ perturbation theory [29]. Within this context, the $1/Z$ expansion for the energy is given by

$$E/Z^2=\varepsilon_0+\varepsilon_1/Z+\varepsilon_2/Z^2+\cdots \qquad (16)$$

and the $1/Z$ expansion of the transition moment *M*, which is simply the integral appearing in Eq. (14), is given by

$$M=M_0+M_1/Z+M_2/Z^2+\cdots \ . \qquad (17)$$

The first two coefficients in these expansions are well known and have been tabulated for the energies [30] of very many states and transition moments [4] of many transitions. Higher-order coefficients have been calculated for the energies of some states by variational perturba-

TABLE IX. Energy $1/Z$ expansion coefficients. The ε_1 coefficients are from Ref. [30].

State	ε_1	ε_2	ε_3	ε_4
$6\,^1S$	0.027 018 04	−0.012 902	−0.000 24	−0.0006
$6\,^3S$	0.025 668 88	−0.010 880	−0.000 40	−0.0002
$6\,^1P$	0.028 015 29	−0.014 317	−0.000 26	0.0001
$6\,^3P$	0.026 949 51	−0.012 256	−0.000 39	−0.0003
$3\,^1D$	0.111 270 14	−0.057 486	0.006 09	−0.0084
$4\,^1D$	0.062 582 03	−0.032 170	0.002 81	−0.0038
$5\,^1D$	0.040 044 95	−0.020 492	0.001 49	−0.0020
$6\,^1D$	0.027 804 63	−0.014 180	0.000 9	−0.0012
$3\,^3D$	0.110 775 76	−0.054 620	−0.000 71	0.0000
$4\,^3D$	0.062 318 32	−0.030 687	−0.000 56	0.0001
$5\,^3D$	0.039 898 13	−0.019 677	−0.000 34	0.0001
$6\,^3D$	0.027 716 14	−0.013 691	−0.000 21	0.0001

TABLE X. Second-order coefficients for the $1/Z$ expansion of the transition moments for the mS to nP transitions.

m	n	Singlet	Triplet	m	n	Singlet	Triplet
1	2	−0.359		4	2	0.53	0.68
1	3	−0.209		4	3	4.14	5.0
1	4	−0.103		4	4	−12.9	−10.7
1	5	−0.0609		4	5	−0.81	−3.4
1	6	−0.044		4	6	−0.5	−0.94
2	2	−3.13	−2.054	5	2	0.28	0.372
2	3	−0.15	−0.977	5	3	1.4	1.4
2	4	0.1	−0.25	5	4	8.3	10
2	5	0.18	−0.11	5	5	−20.42	−17.46
2	6	0.14	−0.062	5	6	−1	−5.3
3	2	1.7	2.0	6	2	0.19	0.25
3	3	−7.167	−5.626	6	3	0.8	0.874
3	4	−0.4	−2.03	6	4	2	2.8
3	5	0.09	−0.530	6	5	12.6	14.3
3	6	0.3	−0.22	6	6	−30.5	−25.90

TABLE XI. Second-order coefficients for the $1/Z$ expansion of the transition moments for the mP to nD transitions.

m	n	Singlet	Triplet	m	n	Singlet	Triplet
2	3	2.4	1.86	5	3	0.04	0.48
2	4	0.720	0.74	5	4	1.2	3.42
2	5	0.36	0.45	5	5	−17	−18
2	6	0.23	0.31	5	6	10.7	3.8
3	3	−2	−5.21	6	3	−0.08	0.28
3	4	4.95	2.3	6	4	−2.4	1.0
3	5	1.6	1.1	6	5	2.7	5.93
3	6	0.85	0.74	6	6	−26.3	−26.0
4	3	0.1	1.52				
4	4	−10.3	−10.7				
4	5	7.37	3.0				
4	6	2.3	1				

tion methods [31–35] and by fitting [31,36] variationally calculated energies [20,37].

We determine some higher-order energy coefficients by fitting our calculated energies using a least-squares procedure in which the first two coefficients were constrained to the known values [30]. Table IX lists our estimates of ε_i, $i=2,3,4$ for the 6S and 6P states which were not considered by Blanchard [36], and for all the D states we calculated. The latter are included because the existing variational perturbation estimates [35] were based on wave functions that did not include pp-type terms which are necessary for angular completeness [10]. Our expansion coefficients for these D states should be more accurate.

We also estimated the third coefficient M_2 in Eq. (17) from our calculated transition moments M in both the length and velocity forms. We used both differencing and least-squares fitting of M^2, with M_0 and M_1 constrained to their known values [4]. Our estimated coefficients are listed in Tables X and XI for the S-P and P-D transitions, respectively. Most of our estimates should be more accurate than previous values [4] obtained by differencing calculated transition moments themselves; the latter procedure is not as reliable because the moments often change sign over the range of nuclear charges considered.

VI. CONCLUSIONS

Explicitly correlated wave functions have been constructed for the $n\,^1S$, $n\,^3S$, $n\,^1P$, $n\,^3P$, $n\,^1D$, and $n\,^3D$ states, with $n<7$, of the two-electron ions from He through Ne^{8+}. The variational energies are the best available for 180 of the 261 states considered even though all our wave functions are limited to 100 terms. This constitutes a clear-cut demonstration of the advantages of the exponentially correlated ansatz and pseudorandom exponent generating scheme advocated by us [6–8] provided that care is taken to ensure angular completeness [10] as in this work. For each ion, dipole oscillator strengths have been calculated for 55 S-P and 40 P-D transitions. Our oscillator strengths are more accurate than previous values for 739 of the 855 transitions considered. These calculations should serve as a challenge to recently reported techniques [38] for measuring oscillator strengths. The coefficients obtained for the $1/Z$ expansions of the energies and oscillator strengths may prove useful in extrapolating our results to higher nuclear charges.

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