Accurate nonrelativistic oscillator strengths for P-D transitions in the helium isoelectronic sequence

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Accurate Hylleraas-type wave functions have been used to calculate oscillator strengths for the transitions mP-nD, $m,n \leq 5$, in heliumlike ions with $Z = 3$-7. The uncertainty of the results estimated from the numerical convergence is less than 0.1% for most of the transitions studied. The results can be used to obtain reliable interpolated oscillator strengths for ions with $Z \geq 8$.

In our previous work,[1] we have calculated accurate oscillator strengths (f values) for a number of S-P and P-D transitions in neutral helium. In this paper we extend calculations to transitions in low-Z heliumlike ions. For S-P transitions between low-lying states, highly accurate f values have already been obtained by Schiff, Pekeris, and Accad,[2] while the data on P-D transitions available in the literature[3-6] are not on the same level of accuracy. We, therefore, carried out calculations for the transitions mP-nD, $m,n \leq 5$, in two-electron ions up to $Z = 7$. Reliable nonrelativistic f values for $Z \geq 8$ can be obtained by interpolation.

I. WAVE FUNCTIONS AND ENERGIES

We first briefly summarize the method to obtain wave functions; details were given in the previous paper.[1] The two-electron Schrödinger equation was solved variationally by use of trial functions consisting of symmetrized linear combinations of Hylleraas-type basis functions. To accelerate the convergence, we included in the expansions two sets of bases of the forms $r_1^i r_2^j r_{12}^k e^{-\xi r_1 - \eta r_2}$ and $r_1^i r_2^j r_{12}^k e^{-\zeta(r_1 + r_2)}$ multiplied by angular factors (in this paper

we refer to the former terms as "ξ terms" and the latter terms as "ζ terms"). Here r_1, r_2, and r_{12} have their usual meanings, and ξ, η, and ζ are the nonlinear parameters. We optimized only the value of ζ, and fixed the values of ξ and η so that ξ terms have the correct asymptotic form as $r_1, r_2 \to \infty$, i.e., $\xi = (-2E - Z^2)^{1/2}$ and $\eta = Z$ with E being the energy of the state in question.[7] An interpretation of the roles of ξ and ζ terms is that ξ terms roughly approximate the true wave function while ζ terms accurately compensate for the remaining discrepancy mainly in the range of middle and small values of r_1 and r_2. For P states, both ξ and ζ terms were given the angular factor of sp symmetry; for D states, ξ terms were given the sd angular factor while ζ terms were given the pp angular factor as well as the sd angular factor. (Thus, generally two ζ terms exist for given i, j, and k.)

The trial functions in the actual calculations included those expansion terms with the powers of r_1, r_2, and r_{12} satisfying the inequality

$$\nu_\xi, \nu_\zeta \geq i + j + k + |i - j|\delta_{k0} , \tag{1}$$

where δ_{k0} is the Kronecker δ, and ν_ξ and ν_ζ are certain integers specified for ξ and ζ terms, respectively; for ξ terms, the restriction $j,k \leq 1$ was further imposed. In order to see

TABLE I. Nonrelativistic energies for P and D states in the helium isoelectronic sequence. The optimum values of the nonlinear parameter ζ are given in terms of an empirical formula. All the values are given in atomic units.

	ζ_{opt}	Energy[a]				
		$Z = 3$	$Z = 4$	$Z = 5$	$Z = 6$	$Z = 7$
2^1P	$0.98Z - 0.58$	4.993 351 06	9.110 771 61	14.477 283 25	21.093 332 30	28.959 116 38
3^1P	$0.85Z - 0.17$	4.720 206 9	8.495 969 6	13.382 714 9	19.380 521 3	26.489 416 0
4^1P	$0.78Z - 0.38$	4.624 151 4	8.279 590 1	12.997 492 1	18.777 882 9	25.620 770 2
5^1P	$0.77Z - 0.41$	4.579 566 5	8.179 160 6	12.818 739 8	18.498 315 4	25.217 890 4
2^3P	$0.95Z - 0.43$	5.027 715 67	9.174 973 13	14.573 137 68	21.221 710 69	29.120 501 74
3^3P	$0.80Z - 0.10$	4.730 459 7	8.514 604 4	13.410 068 5	19.416 735 1	26.534 560 8
4^3P	$0.74Z - 0.30$	4.628 463 5	8.287 363 6	13.008 846 1	18.792 864 7	25.639 402 1
5^3P	$0.73Z - 0.29$	4.581 768 4	8.183 116 3	12.824 505 4	18.505 912 6	25.227 329 3
3^1D	$0.70Z - 0.50$	4.722 391 0	8.500 215 8	13.389 100 3	19.389 059 1	26.500 103 2
4^1D	$0.75Z - 0.57$	4.625 074 1	8.281 339 8	13.000 080 6	18.781 303 8	25.625 014 8
5^1D	$0.82Z - 0.68$	4.580 038 7	8.180 046 0	12.820 039 8	18.500 024 2	25.220 002 1
3^3D	$0.70Z - 0.50$	4.722 526 9	8.500 582 3	13.389 771 6	19.390 083 5	26.501 513 1
4^3D	$0.75Z - 0.57$	4.625 150 8	8.281 543 7	13.000 451 0	18.781 865 9	25.625 785 4
5^3D	$0.83Z - 0.71$	4.580 082 4	8.180 161 6	12.820 249 0	18.500 341 0	25.220 435 7

[a]Negative signs are suppressed.

the convergence of the results, we calculated the wave function of each state for four successive integral values of ν_ζ with the value of ν_ξ fixed. For a given state, the largest value of ν_ζ was 9 or 10, and the value of ν_ξ was $n+2$ or $n+1$, where n is the principal quantum number of the state. The resulting total number of expansion terms was in the range from 112 to 140. We optimized ζ to two significant digits for the longest expansion for each state; the value of ζ thus obtained was used for shorter expansions.

The energy eigenvalues obtained are listed in Table I. These values are expected to have converged to within an uncertainty of a few units in the last decimal place quoted. Also listed, in terms of an empirical formula, are the optimum values of ζ.[8] The quality of the results for P states is slightly worse than, or comparable to, that of the calculations of Accade, Pekeris, and Schiff,[9] who employed 364-term correlated wave functions for the $2P$, $3P$, and $4P$ states and 560-term wave functions for the $5P$ state. The present results for D states improve the best literature data known to us.[10-12]

II. f VALUES

We also evaluated f values for wave functions of four different expansion lengths, both in length and velocity forms. The convergence of the f values is illustrated in Fig. 1 for some of the singlet transitions in Li II and N VI. It is seen that the convergence becomes better as the nuclear charge increases. We summarize the results in Table II by giving a single recommended f value for each transition, which is a
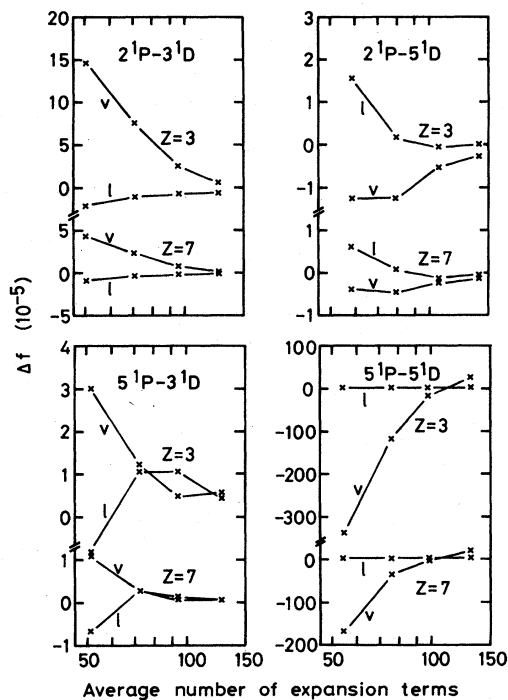

FIG. 1. Convergence of f values for ^1P-^1D transitions in Li II$(Z=3)$ and N VI$(Z=7)$. The value of $\Delta f \equiv f_{\text{cal}} - f_{\text{tab}}$, where f_{cal} and f_{tab} are, respectively, the calculated and tabulated (Table II) f values, is plotted as a function of the average expansion length for the P- and D-state wave functions. l and v on each curve refer to the length and velocity f values, respectively.

TABLE II. f values for P-D transitions in the helium isoelectronic sequence. P states are assumed to be the initial states. Estimated uncertainties are ± 1 in the last digits quoted if these are not underlined, and ± 3 if underlined.

	$Z=3$	$Z=4$	$Z=5$	$Z=6$	$Z=7$
2^1P-3^1D	0.71161	0.70879	0.70633	0.70449	0.70313
2^1P-4^1D	0.11927	0.11917	0.11931	0.11950	0.11968
2^1P-5^1D	0.042732	0.042749	0.042873	0.043007	0.043129
3^1P-3^1D	0.02432	0.02105	0.01783	0.01528	0.01329
3^1P-4^1D	0.65172	0.64670	0.64204	0.63845	0.63570
3^1P-5^1D	0.14141	0.14105	0.14073	0.14049	0.14031
4^1P-3^1D	0.01501	0.01550	0.01595	0.016299	0.016570
4^1P-4^1D	0.04397	0.03711	0.03092	0.02617	0.02257
4^1P-5^1D	0.6511	0.6443	0.6383	0.6337	0.6303
5^1P-3^1D	0.00306	0.00316	0.003249	0.003315	0.003365
5^1P-4^1D	0.03878	0.03999	0.04107	0.04188	0.04250
5^1P-5^1D	0.06162	0.05141	0.04251	0.03578	0.03072
2^3P-3^3D	0.62465	0.63912	0.64926	0.65647	0.66180
2^3P-4^3D	0.12321	0.12328	0.12321	0.12310	0.12300
2^3P-5^3D	0.046796	0.046449	0.046157	0.045927	0.045746
3^3P-3^3D	0.09076	0.07112	0.05778	0.04848	0.04169
3^3P-4^3D	0.5034	0.52726	0.54376	0.55541	0.56400
3^3P-5^3D	0.12784	0.13063	0.13243	0.13363	0.13448
4^3P-3^3D	0.03278	0.02930	0.02705	0.02554	0.02446
4^3P-4^3D	0.16059	0.12523	0.10150	0.08503	0.07305
4^3P-5^3D	0.4706	0.4995	0.5194	0.5335	0.5438
5^3P-3^3D	0.00620	0.005610	0.005227	0.004966	0.004778
5^3P-4^3D	0.07872	0.07089	0.06587	0.06249	0.06008
5^3P-5^3D	0.22266	0.17335	0.14038	0.11754	0.10095

TABLE III. Comparison of the f values in the present work with those of Weiss (Ref. 3) and those of Godefroid and Verhaegen (Ref. 6).

			$Z=3$	$Z=5$	$Z=7$	$Z=8$	$Z=9$	$Z=10$
$2^1P\text{-}3^1D$	Present work	len.	0.711604	0.706327	0.703129			
		vel.	0.711615	0.706331	0.703132			
		int.[a]				0.7021	0.7013	0.7007
	Weiss	len.	0.7108	0.7065	0.7034	0.7024	0.7016	0.7009
		vel.	0.7173	0.7121	0.7078	0.7065	0.7050	0.7042
	Godefroid and	len.			0.7034			
	Verhaegen	vel.			0.7038			
$3^1P\text{-}3^1D$	Present work	len.	0.024318	0.017833	0.013292			
		vel.	0.024321	0.017831	0.013291			
		int.				0.0117	0.0105	0.0095
	Weiss	len.	0.0244	0.0178	0.0132	0.0117	0.0105	0.0095
		vel.	0.0288	0.0221	0.0165	0.0147	0.0131	0.0118
$2^3P\text{-}3^3D$	Present work	len.	0.624653	0.649262	0.661801			
		vel.	0.624662	0.649266	0.661803			
		int.				0.6659	0.6691	0.6717
	Weiss	len.	0.6243	0.6493	0.6618	0.6659	0.6691	0.6717
		vel.	0.6263	0.6504	0.6626	0.6667	0.6696	0.6723
	Godefroid and	len.			0.6619			
	Verhaegen	vel.			0.6616			
$3^3P\text{-}3^3D$	Present work	len.	0.090761	0.057781	0.041692			
		vel.	0.090789	0.057790	0.041697			
		int.				0.0365	0.0325	0.0293
	Weiss	len.	0.0906	0.0577	0.0417	0.0365	0.0325	0.0293
		vel.	0.0901	0.0578	0.0420	0.0368	0.0328	0.0294

[a]Interpolated values, see text.

length f value, a velocity f value, or occasionally some value lying between these. The estimated uncertainties of the listed f values are ± 1 in the last digits quoted when these are not underlined, and ± 3 when underlined. Except for the transitions between the states of the same principal quantum numbers, this estimation is based on the following requirements: for each transition, both the length and velocity f values lie in the range stated above when calculated using the longest expansion, and at the same time both are expected to converge on some value in this range. In the case of the transitions between the states of the same principal quantum numbers, the length f values are much more stable than the velocity f values as the expansion length is increased (see Fig. 1), and are thus expected to be more reliable. The uncertainty of the results for these transitions is, therefore, estimated from the convergence of the length f values only; the length-velocity discrepancies for the $3^{1,3}P\text{-}3^{1,3}D$ transitions are at most three and those for $4^{1,3}P\text{-}4^{1,3}D$ and $5^{1,3}P\text{-}5^{1,3}D$ transitions are at most 30, in the last decimal places quoted in Table II.

In Table III, we compare the present results with those of Weiss,[3] who employed 52-term Hylleraas-type wave functions similar to our "ξ terms", and those of Godefroid and Verhaegen,[6] who employed multiconfiguration Hartree-Fock (MCHF) wave functions; these are the most accurate previous calculations for the $2P\text{-}3D$ and $3P\text{-}3D$ transitions. As is seen, agreement between the length and velocity f values is significantly better in the present results.

One can use the present results to obtain interpolated f values for ions with $Z \geq 8$ on the basis of the well-known Z expansion[13]

$$f = f_0 + f_1 Z^{-1} + f_2 Z^{-2} + \cdots \; . \tag{2}$$

Here, f_0 is essentially the hydrogenic f value and f_1 has been calculated by Laughlin for the transitions $mP\text{-}nD$, $m,n \leq 4$.[14] If we fix f_0 and f_1 (or only f_0 if f_1 is unknown) at these known values and adjust three or four additional f_i's by a standard least-squares-fitting procedure, the resulting expressions reproduce our "recommended" f values to the last significant digits (for all the transitions studied and for all $Z = 2$–7).[15] Interpolated f values for $Z = 8$–10 obtained from these expressions are included in Table III to the digits we feel reliable. Except for the $2^1P\text{-}3^1D$ transition, these are in exact agreement with Weiss's length f values, which are expected to be accurate since his length f values for $Z \leq 7$ are also in close agreement with our "recommended" f values. It may, therefore, be concluded that the interpolation procedure described above give highly reliable (nonrelativistic) f values for ions with $Z \geq 8$.

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[7]For P states ξ was fixed using the energy values given in Ref. 9.

For D states, the eigenvalue equation was first solved with ξ fixed using the energy values given in Refs. 10 and 11. The resulting more accurate energy was used to obtain new ξ, and the eigenvalue equation was re-solved.

8The formulas for some of the transitions do not give the correct optimum values for $Z = 2$.

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15In the course of the least-squares-fitting calculations, we found that the values of f_1 given by Laughlin (Ref. 14) are in error (by 0.1–10%). We used the values of f_1 rederived from his Z expansion coefficients for the reduced dipole matrix elements. Also found was an overlooked typesetting error in our previous paper (Table IV in Ref. 1); the f values for the 3^3P-4^3D transition in neutral helium is 0.4776 instead of being 0.4476.