# Accurate oscillator strengths for neutral helium 

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#### Abstract

With use of variational wave functions, oscillator strengths have been calculated for all the allowed transitions between the states $n^{1} S, n^{1} P, n^{1} D, n^{3} S, n^{3} P$, and $n^{3} D, n \leq 9$, in neutral helium, with an estimated accuracy of better than $1 \%$ for most of the transitions and better than $0.1 \%$ for about a third of the transitions. The error estimate is based on numerical convergence as the number of expansion terms in the wave function is increased. By use of rapidly converging trial functions consisting of two sets of Hylleraas-type basis functions differing in the values of nonlinear parameters, the expansion lengths required are kept moderate (at most 140 terms). A discussion is given about the completeness of the Hylleraas-type basis.


## I. INTRODUCTION

Continuing efforts have been devoted to determine reliable atomic oscillator strengths ( $f$ values) and lifetimes. In the case of helium and heliumlike ions, accurate $f$ values have been calculated by Schiff et al. for the $m^{1} S-n^{1} P$ and $m^{3} S-n^{3} P$ transitions with $m, n \leq 5 .{ }^{1}$ They used variationally optimized wave functions containing hundreds of or about a thousand expansion terms, and attained an estimated accuracy of $1 \%$ or better for the large majority of the transitions. For neutral helium, however, the uncertainty of their results is still somewhat larger when transitions involve higher-lying excited states. In view of recent precision measurements of $f$ values and lifetimes with an accuracy of a fraction of a percent for selected atomic systems, ${ }^{2,3}$ it seems desirable to improve some of the results of Schiff et al. and to carry out precise calculations for a wider range of transitions. In this paper we report the results of such calculations for neutral helium; the transitions included are those between the $n^{1} S, n^{1} P, n^{1} D, n^{3} S, n^{3} P$, and $n^{3} D$ states with $n \leq 9$. The wave functions employed are truncated expansions based on complete Hylleraas-type basis functions, and the accuracy of the results is estimated from numerical convergence as the expansion length is increased. To accelerate convergence, we included in the expansion two sets of basis functions differing in the values of nonlinear parameters; although the expansion lengths employed are moderate (at most 140 terms), the present method improves the results of Schiff et al. for the majority of the transitions commonly treated.

## II. METHOD OF CALCULATION

The wave functions were obtained by variationally solving the Schrödinger equation with the usual nonrelativistic spin-independent Hamiltonian given in atomic units by

$$
\begin{equation*}
H=-\frac{1}{2} \Delta_{1}-\frac{1}{2} \Delta_{2}-\frac{Z}{r_{1}}-\frac{Z}{r_{2}}+\frac{1}{r_{12}} \tag{1}
\end{equation*}
$$

It is common to use a trial function consisting of a linear combination of the Hylleraas-type correlated basis of the
form

$$
\begin{equation*}
u_{i j k}=\left(1 \pm P_{12}\right) r_{1}^{i} r_{2}^{j} r_{12}^{k} e^{-\xi r_{1}-\eta r_{2}} P_{l}\left(\cos \theta_{1}\right) \tag{2}
\end{equation*}
$$

where $P_{12}$ is the permutation operator, $P_{l}$ is the Legendre polynomial giving the symmetry of the desired angular momentum state, $\xi$ and $\eta$ are adjustable parameters, and the + and - signs refer to the singlet and triplet states, respectively. (The basis employed by Schiff et al. was essentially of this form though they used perimetric coordinates.) One can attain a fairly high accuracy by using expansions containing a relatively small number of $u_{i j k}$ terms. For further improvement of the accuracy, however, it seems not very effective simply to increase the expansion length, as we consider below. Since the factor $r_{l}^{i} e^{-\xi r_{1}}$ has its maximum at $r_{1}=i / \xi$ and becomes zero when $r_{1} \rightarrow 0$ or $r_{2} \rightarrow \infty$, the terms involving this factor are considered to be suited for modifying the value of the wave function in the neighborhood of $r_{1}=i / \xi$. Consequently, if the value of $\xi$ is fixed at an optimum value for a short expansion, the terms involving higher powers of $r_{1}$, which are added as the expansion length is increased, will not effectively modify the value of the wave function in the range of middle and small $r_{1}$, where the wave function is expected to require more accurate representation; on the other hand, if the value of $\xi$ is increased in order to make such terms effective by decreasing the value of $i / \xi$, the accuracy attained by the terms with lower powers of $r_{1}$ will be deteriorated.

On the basis of the above consideration, the trial function in the present work were taken to be the expansion of the form

$$
\begin{equation*}
\psi=\sum_{i, j, k} a_{i j k} u_{i j k}+\sum_{i, j, k} b_{i j k} v_{i j k} \tag{3}
\end{equation*}
$$

for $S(l=0)$ and $P(l=1)$ states. Here $a_{i j k}$ and $b_{i j k}$ are the linear variational parameters, $u_{i j k}$ is given by Eq. (2), and $v_{i j k}$ is given by

$$
\begin{equation*}
v_{i j k}=\left(1 \pm P_{12}\right) r_{1}^{i} r_{2}^{j} r_{12}^{k} e^{-\xi\left(r_{1}+r_{2}\right)} P_{l}\left(\cos \theta_{1}\right) \tag{4}
\end{equation*}
$$

where $\zeta$ is the nonlinear variational parameter. The summations in (3) run over linearly independent terms with
$i \geq l$ and $j, k \geq 0$. The role of each term in (3) may be interpreted as follows. The first summation roughly approximates the true eigenfunction using a relatively small number of terms; the second summation accurately compensates for the remaining discrepancy, the value of $\zeta$ being chosen so as to make this compensation most effective without affecting the (fairly high) accuracy of the approximation by the $u_{i j k}$ terms.

In order to estimate the accuracy of the results correctly from convergence study, it is necessary to choose the trial function so that it can approximate the true eigenfunction to any desired degree as the number of expansion terms is increased. For $S$ and $P$ states, the $v_{i j k}$ terms form a complete set in the subspace of the functions of a given symmetry. For $D$ states, however, the $v_{i j k}$ terms must be supplemented by the terms given by

$$
\begin{equation*}
w_{i j k}=\left(1 \pm P_{12}\right) r_{1}^{i} r_{2}^{j} r_{12}^{k} e^{-\xi\left(r_{1}+r_{2}\right)}\left(3 \cos \theta_{1} \cos \theta_{2}-\cos \omega\right) \tag{5}
\end{equation*}
$$

to form a complete set, where $\omega$ is the angle between the radius vector of the two electrons. The trial function for $D(l=2)$ states was thus taken to be ${ }^{4}$

$$
\begin{equation*}
\psi=\sum_{i, j, k} a_{i j k} u_{i j k}+\sum_{i, j, k} b_{i j k} v_{i j k}+\sum_{i, j, k} c_{i j k} w_{i j k} \tag{6}
\end{equation*}
$$

where the first two summations run over linearly independent terms with $i \geq 2$ and $j, k \geq 0$, and the last summation with $i, j \geq 1$ and $k \geq 0$. We show the completeness of the expansion using $v_{i j k}$ and $w_{i j k}$ in the Appendix.

In the actual calculations, we truncated the expansion so that the powers of $r_{1}, r_{2}$, and $r_{12}$ satisfy the inequality

$$
\begin{equation*}
v_{u}, v_{v}, v_{w} \geq i+j+k+|i-j| \delta_{k 0} \tag{7}
\end{equation*}
$$

where $\delta_{k 0}$ is the Kronecker $\delta$, and $v_{u}, v_{v}$, and $v_{w}$ are certain integers specified for the $u_{i j k}, v_{i j k}$, and $w_{i j k}$ terms, respectively. For the $u_{i j k}$ terms, we further imposed the restrictions $j, k \leq 1$ and $j \leq i$. The term $|i-j| \delta_{k 0}$ in (7) is included in order to omit some of expansion terms which have nonzero $k$ and large $|i-j|$; the $r_{12}$ dependence of the terms with large $|i-j|$ is thought less important, since they have appreciable values only when the two electrons are far apart. Exclusion of such terms enables one to obtain larger values of $v_{u}, v_{v}$, and $v_{w}$ without unduly increasing the total number of terms in the expansion. In order to undertake a convergence study, we calculated the wave function of each level for four successive integral values of $v_{v}$ and $v_{w}$ with the value of $v_{u}$ fixed. The values of $v_{u}, v_{v}$, and $v_{w}$ associated with the longest expansion are summarized in Table I.

As in the usual manner, the linear variational parameters $a_{i j k}, b_{i j k}$, and $c_{i j k}$ were determined from matrix eigenvalue equations. In these calculations, the nonlinear parameters $\xi$ and $\eta$ were fixed at the values $\left(-2 E-Z^{2}\right)^{1 / 2}$ and $Z$, respectively, where $E$ is the energy eigenvalue of the state in question (thus the $u_{i j k}$ terms have the correct asymptotic form as $\left.r_{1}, r_{2} \rightarrow \infty\right)$; for this purpose, we used the eigenvalues calculated by Pekeris ${ }^{5}$ and Accad et al. ${ }^{6}$ when available and, otherwise, experimental energy values. ${ }^{7}$ The nonlinear parameter $\xi$ was optimized for the longest expansion for each state by solv-

TABLE I. Values of $v_{u}, v_{v}$, and $v_{w}$ associated with the longest expansion for each state.

| State |  | $v_{u}$ | $v_{v}$ | $v_{w}$ |
| :--- | :--- | :--- | :--- | :--- |
| $n^{1} S$ | $n=1,2$ | $n+1$ | 11 |  |
|  | $n=3-9$ | $n+2$ | 10 |  |
| $n^{3} S$ | $n=2$ | $n+2$ | 12 |  |
|  | $n=3-9$ | $n+2$ | 11 |  |
| $n^{1,3} P$ | $n=2$ | $n+1$ | 10 |  |
|  | $n=3-9$ | $n+2$ | 9 |  |
| $n^{1} D$ | $n=3-6$ | $n+2$ | 9 | 9 |
|  | $n=7-9$ | $n+2$ | 8 | 8 |
| $n^{3} D$ | $n=3-9$ | $n+2$ | 9 | 9 |

ing the eigenvalue equation for a series of $\zeta$ points taken at intervals of 0.1 (when $\zeta>1$ ) or 0.05 (when $\zeta<1$ ) in atomic units; further optimization was thought meaningless since the dependence of the energy eigenvalue on $\zeta$ was very small in the neighborhood of its optimum value. For expansions other than the longest ones, $\zeta$ was fixed at the value thus obtained.

After determining wave functions, we calculated $f$ values using both the length and velocity formulas ${ }^{8}$

$$
\begin{align*}
f_{l} & =C\left(E_{b}-E_{a}\right)\left|\int \psi_{b}^{*}\left(z_{1}+z_{2}\right) \psi_{a} d \tau\right|^{2}  \tag{8}\\
f_{v} & =\frac{C}{\left(E_{b}-E_{a}\right)}\left|\int \psi_{b}^{*}\left(\frac{\partial}{\partial z_{1}}+\frac{\partial}{\partial z_{2}}\right) \psi_{a} d \tau\right|^{2} \tag{9}
\end{align*}
$$

Here $C$ is equal to 2 for the $S-P$ transitions and is equal to $\frac{5}{3}$ for the $P-D$ transitions; $E_{a}$ and $E_{b}$ are the energy eigenvalues of the initial and final states, respectively. Each of these formulas was evaluated using the wave functions of four different expansion lengths (in such a way that the $n$th longest expansion of the initial wave function was used with the $n$th longest expansion of the final wave function). In these calculations, we always used the energy eigenvalues obtained from the longest expansions.

## III. RESULTS AND DISCUSSION

## A. Energy eigenvalues

In order to see the quality of the calculated wave functions, we first compare the obtained energy eigenvalues with those of the highly accurate calculations by Pekeris ${ }^{5}$ and Accad et al. ${ }^{6}$ These are listed in Table II in terms of the ionization energy $I$, converted from the energy eigenvalue $E$ using the relation $I=(-2 E-4) \mathscr{R}_{\mathrm{H}}$, where the value of $\mathscr{R}_{\mathrm{He}}$ used was $109722.267 \mathrm{~cm}^{-1}$. Also listed are the expansion lengths employed, the optimum values of $\zeta$, and the experimental ionization energies. ${ }^{7}$ Following Pekeris and co-workers, the number of digits given for the present results is determined so that the listed values differ from the extrapolated values (which one would obtain from the expansion of an infinite length) by not more than one or occasionally two in the last digits quoted, unless they are underlined. The expansion lengths employed by Pekeris and co-workers were more than 1000 (to 2300)
TABLE II. Comparison of the ionization energies for neutral helium. $N$ denotes the number of expansion terms used to obtain the present results and $\zeta_{\text {opt }}$ denotes the optimum value of the nonlinear parameter.

| State | Ionization energy ${ }^{\text {a }}\left(\mathrm{cm}^{-1}\right)$ |  |  |  |  | State | $N$ | $\zeta_{\text {opt }}$ | Ionization energy ( $\mathrm{cm}^{-1}$ ) |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $N$ | $\zeta_{\text {opt }}$ | Present work | PAS ${ }^{\text {b }}$ | Expt. ${ }^{\text {c }}$ |  |  |  | Present work | PAS | Expt. |
| $1^{1} S$ | 138 | 2.9 | 198317.3741 | $198317.374 \underline{3}$ | 198310.81 |  |  |  |  |  |  |
| $2^{1} S$ | $140^{\text {d }}$ | 1.8 | 32033.203 | 32033.206 | 32033.26 | $2^{3} S$ | 123 | 1.5 | 38453.12917 | 38453.12925 | 38454.74 |
| $3{ }^{1} S$ | 121 | 1.6 | 13445.80 | 13445.8 | 13445.87 | $3^{3} S$ | 106 | 1.4 | 15073.440 | 15073.439 | 15073.92 |
| $4{ }^{1} S$ | 123 | 1.6 | 7370.42 | 7370.4 | 7370.48 | $4^{3} S$ | 108 | 1.2 | 8012.377 | 8012.377 | 8012.60 |
| $5^{1} S$ | 127 | 1.6 | 4647.14 | 4647.1 | 4647.18 | $5^{3} S$ | 112 | 1.3 | 4963.588 | 4963.59 | 4963.72 |
| $6^{1} S$ | 129 | 1.4 | 3195.79 | 3195.78 | 3195.81 | $6^{3} S$ | 114 | 1.2 | 3774.498 | 3374.498 | 3374.58 |
| $7^{1} S$ | 133 | 1.5 | 2331.77 | 2331.75 | 2331.77 | $7{ }^{3} S$ | 118 | 1.2 | 2442.400 | 2442.400 | 2442.46 |
| $8^{1} S$ | 135 | 1.3 | 1776.10 | 1776.08 | 1775.93 | $8^{3} S$ | 120 | 1.1 | 1849.285 | 1849.285 | 1849.39 |
| $9^{1} S$ | 139 | 1.3 | 1397.76 | 1397.74 | 1397.83 | $9^{3} S$ | 124 | 1.1 | 1448.666 | 1448.666 | 1448.77 |
| $2^{1} P$ | $140{ }^{\text {d }}$ | 1.4 | $27176.68 \underline{5}$ | 27176.688 | 27175.81 | $2^{3} P$ | $140{ }^{\text {d }}$ | 1.4 | 29222.151 | 29222.1537 | 29223.80 |
| $3^{1} P$ | 118 | 1.4 | 12101.57 | 12101.57 | 12101.34 | $3^{3} P$ | 118 | 1.5 | $12745.57 \underline{4}$ | 12745.576 | 12746.12 |
| $4^{1} P$ | 120 | 1.3 | 6818.06 | 6818.1 | 6817.99 | $4^{3} P$ | 120 | 1.2 | 7093.40 | 7093.40 | 7093.67 |
| $5^{1} P$ | 124 | 1.2 | 4368.26 | 4368.2 | 4368.24 | $5^{3} P$ | 124 | 1.2 | 4509.84 | 4509.8 | 4510.03 |
| $6{ }^{1} P$ | 126 | 0.95 | 3035.78 |  | 3055.77 | $6^{3} P$ | 126 | 1.0 | 3117.85 |  | 3117.90 |
| $7^{1} P$ | 130 | 1.0 | 2231.60 |  | 2231.57 | $7^{3} P$ | 130 | 1.0 | 2283.31 |  | 2283.41 |
| $8^{1} P$ | 132 | 1.0 | 1709.28 |  | 1709.30 | $8^{3} P$ | 132 | 1.1 | 1743.93 |  | 1743.99 |
| $9^{1} P$ | 136 | 1.0 | 1350.98 |  | 1351.02 | $9^{3} P$ | 136 | 1.1 | 1375.32 |  | 1375.39 |
| $3{ }^{1} D$ | 132 | 0.90 | 12205.66 |  | 12205.75 | $3^{3} \mathrm{D}$ | 112 | 0.90 | 12209.08 |  | 12209.16 |
| $4^{1} D$ | 134 | 0.90 | 6864.19 |  | 6864.25 | $4^{3} \mathrm{D}$ | 114 | 0.90 | 6866.16 |  | 6866.22 |
| $5^{1} D$ | 138 | 1.0 | 4392.36 |  | 4392.42 | $5^{3} \mathrm{D}$ | 118 | 1.0 | 4393.50 |  | 4393.57 |
| $6^{1} D$ | 140 | 0.75 | 3049.88 |  | 3049.95 | $6^{3} \mathrm{D}$ | 120 | 0.70 | 3050.58 |  | 3050.64 |
| $7^{1} D$ | 107 | 0.80 | 2240.53 |  | 2240.65 | $7^{3} D$ | 124 | 0.75 | 2240.99 |  | 2241.08 |
| $8^{1} D$ | 109 | 0.75 | 1715.28 |  | 1715.27 | $8^{3} \mathrm{D}$ | 126 | 0.70 | 1715.60 |  | 1715.63 |
| $9^{1} D$ | 113 | 0.80 | 1355.21 |  | 1355.29 | $9^{3} \mathrm{D}$ | 130 | 0.70 | 1355.44 |  | 1355.53 |

[^0]

FIG. 1. Convergence of ionization energies for the $2^{1} P$ and $5^{1} P$ states as the number of expansion terms is increased. Present results $(\times)$ are compared with those of Accad et al. ( $\square$, Ref. 6). Right-hand-side scale for the $5^{1} P$ state should be used for the latter results.
for $S$ states and 560 for $P$ states. In spite of the quite moderate expansion lengths used in this work, the accuracy of our results compares favorably with that attained by Pekeris and co-workers. The results for $P$ states indicate that in the method of Pekeris and co-workers the convergence of the energy eigenvalues becomes rapidly poor as one deals with higher excited states, while in the present method this effect is not as serious. Such a tendency is more clearly seen in Fig. 1, where as a typical example of the convergence the ionization energies of the $2^{1} P$ and $5^{1} P$ states are plotted as a function of the (logarithmic) expansion length employed.

The estimated uncertainties of the calculated ionization
energies are comparable to, or smaller than, the experimental uncertainties. Any discrepancy between the calculated and experimental ionization energies therefore suggests the effect of various correction terms for nonrelativistic ionization energies. ${ }^{9}$

## B. $f$ values

The results of $f$-value calculations are summarized in Tables III and IV. The listed $f$ values are "recommended" values and are selected from "length $f$ values," "velocity $f$ values," and occasionally values lying between these. The estimated uncertainties of the listed $f$ values are $\pm 1$ in the last digits quoted when these are not underlined, and $\pm 3$ when underlined. The estimation of the accuracy is based on the following requirements: For each transition, both the length and velocity $f$ values lie in the range specified by the above error estimate when they are calculated using the longest expansion, and at the same time both are expected to converge on some value in this range. In Figs. 2 and 3 we illustrate the convergence of the results for some of the ${ }^{1,3} S_{-}{ }^{1,3} P$ and ${ }^{1} P_{-}{ }^{1} D$ transitions (the convergence for the ${ }^{3} P_{-}{ }^{3} D$ transitions would show similar features and is not given here).

Figure 2 also shows the convergence of the results of Schiff et al., ${ }^{1}$ who used wave functions containing up to 364 terms ( 1078 terms for the $1{ }^{1} S$ state). It is seen that the present results generally give better convergence than those of Schiff et al. A full comparison between the two sets of results shows that the present results give improved $f$ values for the majority of the transitions commonly studied (and of course that all of the two sets of $f$ values agree within the uncertainties specified by Schiff et al.).

For $P-D$ transitions, the present results also give sys-

TABLE III. $f$ values for $S$ - $P$ transitions in neutral helium. $S$ states are assumed to be the initial states. Estimated uncertainties are $\pm 1$ in the last digits quoted if these are not underlined, and $\pm 3$ if underlined.

|  | $2^{1} P$ | $3^{1} P$ | $4^{1} P$ | $5^{1} P$ | $6^{1} P$ | $7^{1} P$ | $8^{1} P$ | $9^{1} P$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $1^{1} S$ | 0.27616 | 0.07344 | 0.029863 | 0.015039 | 0.008628 | 0.005405 | 0.003610 | 0.002530 |
| $2^{1} S$ | 0.37644 | 0.15134 | 0.04916 | 0.02234 | 0.01213 | $0.00736 \underline{0}$ | 0.004813 | 0.003325 |
| $3^{1} S$ | 0.14547 | 0.6262 | 0.14390 | 0.0505 | 0.02419 | 0.01368 | 0.00857 | 0.00576 |
| $4^{1} S$ | 0.02587 | 0.3075 | 0.858 | 0.1463 | 0.0528 | 0.02588 | 0.01495 | 0.00954 |
| $5^{1} S$ | 0.009652 | 0.05548 | 0.476 | 1.083 | 0.1526 | 0.0556 | 0.02760 | 0.01613 |
| $6^{1} S$ | 0.004769 | 0.02111 | 0.0862 | 0.647 | 1.305 | 0.1609 | $0.058 \underline{8}$ | 0.0293 |
| $7^{1} S$ | 0.002739 | 0.01064 | 0.03305 | 0.1172 | 0.819 | 1.53 | 0.1705 | 0.0623 |
| $8^{1} S$ | 0.001730 | 0.00623 | 0.01681 | 0.0451 | 0.1482 | 0.993 | 1.745 | 0.181 |
| $9^{1} S$ | 0.001167 | 0.003999 | 0.00994 | 0.02305 | 0.0571 | 0.1793 | 1.166 | 1.963 |
|  | $2^{3} P$ | $3^{3} P$ | $4^{3} P$ | $5^{3} P$ | $6^{3} P$ | $7^{3} P$ | $8^{3} P$ | $9^{3} P$ |
| $2^{3} S$ | 0.539086 | 0.064461 | 0.025769 | 0.012491 | $0.00698 \underline{2}$ | 0.004299 | 0.002836 | 0.001970 |
| $3^{3}$ S | 0.20853 | 0.8909 | 0.05008 | 0.02292 | 0.01199 | 0.00707 | 0.00454 | 0.00309 |
| $4^{3}$ S | $0.0317 \underline{2}$ | 0.4357 | 1.215 3 | 0.04423 | 0.02163 | 0.01178 | 0.00716 | 0.00471 |
| $5^{3} \mathrm{~S}$ | 0.01134 | 0.06761 | 0.668 | 1.531 | 0.0415 | 0.02111 | 0.01174 | 0.00727 |
| $6^{3} S$ | $0.00548 \underline{8}$ | 0.02470 | 0.1040 | 0.903 | 1.842 | 0.0403 | 0.0210 | 0.0118 |
| $7^{3} S$ | 0.003113 | 0.01221 | 0.0382 | $0.140 \underline{3}$ | 1.139 | 2.151 | 0.0399 | 0.0212 |
| $8^{3} S$ | 0.001949 | 0.00707 | $0.0191 \underline{10}$ | 0.0517 | 0.176 | $1.37 \underline{6}$ | 2.458 | $0.040 \underline{0}$ |
| $9^{3} S$ | 0.001306 | 0.00451 | 0.01117 | 0.0260 | $0.065 \underline{0}$ | 0.212 | $1.61 \underline{3}$ | 2.764 |

TABLE IV. $f$ values for $P-D$ transitions in neutral helium. $P$ states are assumed to be the initial states. Estimated uncertainties are $\pm 1$ in the last digits quoted if these are not underlined, and $\pm 3$ if underlined.

|  | $3^{1} \mathrm{D}$ | $4^{1} \mathrm{D}$ | $5^{1} D$ | $6^{1} D$ | $7{ }^{1} D$ | $8^{1} D$ | $9^{1} D$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $2^{1} P$ | 0.71016 | 0.12026 | 0.04326 | 0.02095 | 0.01190 | 0.007464 | 0.005015 |
| $3^{1} P$ | 0.02114 | 0.6481 | 0.1413 | 0.05629 | $0.0289 \underline{0}$ | 0.01708 | 0.01104 |
| $4^{1} P$ | 0.01531 | 0.0401 | 0.648 | 0.1529 | 0.0636 | 0.0336 | 0.02034 |
| $5^{1} P$ | 0.00311 | 0.0393 | $0.057 \underline{3}$ | 0.670 | 0.1632 | 0.0693 | 0.0373 |
| $6^{1} P$ | $0.00118 \underline{8}$ | 0.00838 | 0.0684 | 0.074 | 0.703 | 0.1732 | 0.0745 |
| $7^{1} P$ | 0.000594 | 0.00327 | 0.01501 | $0.100 \underline{8}$ | 0.089 | 0.741 | 0.1837 |
| $8^{1} P$ | 0.000345 | 0.001664 | 0.00595 | 0.0226 | 0.135 | 0.105 | 0.784 |
| $9^{1} P$ | 0.000220 | $0.00097 \underline{9}$ | 0.00306 | 0.00903 | 0.0307 | 0.171 | 0.120 |
|  | $3^{3} \mathrm{D}$ | $4^{3} \mathrm{D}$ | $5^{3} \mathrm{D}$ | $6^{3} \mathrm{D}$ | $7^{3} D$ | $8^{3} D$ | $9^{3} \mathrm{D}$ |
| $2^{3} P$ | $0.6102 \underline{2}$ | 0.12285 | 0.04701 | 0.02347 | 0.01356 | 0.008603 | 0.005823 |
| $3^{3} P$ | 0.1121 | 0.4476 | 0.1246 | 0.05301 | 0.02816 | 0.01698 | 0.01112 |
| $4^{3} P$ | 0.0370 | $0.200 \underline{9}$ | 0.439 | 0.1240 | 0.0552 | 0.0303 | 0.01871 |
| $5^{3} P$ | 0.00690 | 0.0883 | 0.2801 | 0.430 | 0.1254 | 0.0571 | 0.0318 |
| $6^{3} P$ | 0.00258 | 0.0170 | 0.1470 | 0.354 | 0.434 | 0.128 | 0.0589 |
| $7^{3} P$ | 0.001284 | 0.00650 | 0.0289 | 0.210 | 0.426 | 0.445 | 0.132 |
| $8^{3} P$ | 0.000743 | 0.00327 | 0.01116 | $0.042 \underline{0}$ | 0.276 | 0.496 | 0.460 |
| $9^{3} P$ | 0.000474 | 0.001919 | 0.00567 | 0.01627 | $0.055 \underline{5}$ | 0.343 | 0.564 |



FIG. 2. Convergence of $f$ values for $S-P$ transitions. The value of $\Delta \equiv\left(f_{\text {cal }}-f_{\text {tab }}\right) / f_{\text {tab }}$, where $f_{\text {cal }}$ and $f_{\text {tab }}$ are, respectively, the calculated and tabulated (Table III) $f$ values, is plotted as a function of the average expansion length for the $S$ - and $P$-state wave functions. Present results $(\times)$ are compared with those of Schiff et al. ( $\quad$, Ref. 1). $l$ and $v$ on each curve refer to the length and velocity $f$ values, respectively. Left-hand-side scale for $\Delta$ should be used for the present results, and the right-hand-side scale for those of Schiff et al.


FIG. 3. Convergence of $f$ values for ${ }^{1} P_{-}{ }^{1} D$ transitions. The value of $\Delta \equiv\left(f_{\text {cal }}-f_{\text {tab }}\right) / f_{\text {tab }}$, where $f_{\text {cal }}$ and $f_{\text {tab }}$ are, respectively, the calculated and tabulated (Table IV) $f$ values, is plotted as a function of the average expansion length for the $P$ - and $D$-state wave functions [ $\times$, the present results obtained using expansions given by Eq. (6); $\quad$, expansions with $w_{i j k}$ terms omitted]. $l$ and $v$ on each curve refer to the length and velocity $f$ values, respectively. Also plotted, regardless of the expansion length, are the results of Green et al. ( $\bullet$, length formula; $\bigcirc$, velocity formula; see Ref. 11). Left-hand-side scale for $\Delta$ should be used for the present results associated with full-term expansions $(\times)$, and the right-hand-side scale for the rest.
tematically closer agreement between the length and the velocity $f$ values than the best theoretical data in the literature. ${ }^{10-14}$ We include in Fig. 3 the results of extensive calculations by Green et al. ${ }^{11}$ For $2^{1,3} P-3^{1,3} D$ transitions, Davis and Chung ${ }^{14}$ have compared their results with those of other authors; ${ }^{10-13}$ we refer the reader to their paper for comparison with the present results: $f_{l}\left(2^{1} P-3^{1} D\right)=0.71016, \quad f_{v}\left(2^{1} P-3^{1} D\right)=0.71018, \quad f_{l}\left(2^{3} P\right.$ $\left.3^{3} D\right)=0.61022, f_{v}\left(2^{3} P-3^{3} D\right)=0.61024$.

It may be of interest to see how results are affected if we omit the $w_{i j k}$ terms from the expansion for $D$ states (the Hylleraas-type trial function used in Ref. 10 involved no terms similar to $w_{i j k}$ ). We made such calculations for the $2^{1} P-3^{1} D$ and $3^{1} P-3^{1} D$ transitions. The results for the $2^{1} P-3^{1} D$ transition are plotted in Fig. 3. It is seen that the length and velocity $f$ values appear to converge on different limits whose discrepancy is $0.5 \%$. The calculations for the $3^{1} P-3^{1} D$ transition show that the length $f$ value appears to converge on 0.02114 while the velocity $f$ value converges on 0.0241 , the discrepancy being $14 \%$. Thus the importance of the $w_{i j k}$ terms for accurate $f$-value calculations is clear.

To summarize, we have calculated accurate $f$ values in neutral helium for the transitions between the $S, P$, and $D$ states with the principal quantum number of the running electron $n \leq 9$. By using rapidly converging variational wave functions consisting of two sets of Hylleraas-type bases differing in the values of the nonlinear parameters, we were able to keep the number of expansion terms moderate. Judging from the convergence of the results as the number of expansion terms was increased up to

106-140, we may conclude that the accuracy of the $f$ values obtained is better than $1 \%$ for most of the transitions and better than $0.1 \%$ for about a third of the transitions.

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## APPENDIX: COMPLETENESS OF THE EXPANSION USING $v_{i j k}$ AND $w_{i j k}$

Coolidge and James showed the completeness of the series

$$
\sigma=\sum_{i, j, k} a_{i j k} r_{1}^{i} r_{2}^{j} r_{12}^{k} e^{-\xi\left(r_{1}+r_{2}\right)}
$$

in the subspace of the $S$-state functions, which depend only on $r_{1}, r_{2}$, and $r_{12} .{ }^{15}$ Combining this result with the fact that any $P$-state function with $M=0$ and odd parity ( $M$ denotes the projection of the total orbital angular momentum on the quantization axis) can be written as ${ }^{16}$

$$
\psi=R_{1}\left(r_{1}, r_{2}, r_{12}\right) \cos \theta_{1}+R_{2}\left(r_{1}, r_{2}, r_{12}\right) \cos \theta_{2},
$$

we readily deduce the completeness of the $P$-state expansion using $v_{i j k}$. Here we show the completeness of the present $S$-, $P$-, and $D$-state expansions in a somewhat different way by giving an explicit relation between the expansion using a correlated basis and that using an uncorrelated basis.

Let us consider the following functions for $L=0,1$, or 2:

$$
\begin{gather*}
F_{L ; i j l}=r_{1}^{i} r_{2}^{j} e^{-\xi\left(r_{1}+r_{2}\right)} \sum_{m=-l}^{l} C(l+L, l, m,-m ; L, 0) \\
\\
\times Y_{l+L}^{m}\left(\theta_{1}, \varphi_{1}\right) Y_{l}^{-m}\left(\theta_{2}, \varphi_{2}\right)  \tag{A1}\\
(i \geq l+L, j \geq l, l \geq 0) \quad(\mathrm{A} 1) \\
\widetilde{F}_{L ; i j l}=r_{1}^{i} r_{2}^{j} e^{-\xi\left(r_{1}+r_{2}\right)} \sum_{m=-l}^{l} C(l, l+L, m,-m ; L, 0) \\
 \tag{A2}\\
\times Y_{l}^{m}\left(\theta_{1}, \varphi_{1}\right) Y_{l+L}^{-m}\left(\theta_{2}, \varphi_{2}\right) \\
(i \geq l, j \geq l+L, l \geq 0) \quad(\mathrm{A} 2) \\
G_{i j l}=r_{1}^{i} r_{2}^{j} e^{-\xi\left(r_{1}+r_{2}\right) \sum_{m=-l}^{l} C(l, l, m,-m ; 2,0)}  \tag{A3}\\
\times Y_{l}^{m}\left(\theta_{1}, \varphi_{1}\right) Y_{l}^{-m}\left(\theta_{2}, \varphi_{2}\right) \\
(i, j \geq l, l \geq 1)
\end{gather*}
$$

$$
\begin{align*}
& f_{L ; i j k}=r_{1}^{i} r_{2}^{j} r_{12}^{k} e^{-\xi\left(r_{1}+r_{2}\right)} P_{L}\left(\cos \theta_{1}\right) \\
& \quad(j, k \geq 0, i \geq L)  \tag{A4}\\
& \widetilde{f}_{L ; i j k}=r_{1}^{i} r_{2}^{j} r_{12}^{k} e^{-\xi\left(r_{1}+r_{2}\right)} P_{L}\left(\cos \theta_{2}\right) \\
& \quad(i, k \geq 0, j \geq L)  \tag{A5}\\
& g_{i j k}=r_{1}^{i} r_{2}^{j} r_{12}^{k} e^{-\xi\left(r_{1}+r_{2}\right)}\left(3 \cos \theta_{1} \cos \theta_{2}-\cos \omega\right) \\
& \quad(i, j \geq 1, k \geq 0) . \tag{A6}
\end{align*}
$$

Here the $C$ 's are the Clebsch-Gordan coefficients and the $Y_{l}^{m}$ 's are the normalized spherical harmonics. We know the fact that $F_{0 ; i j l}$ form a complete set in the subspace of the $S$-state functions, $F_{1 ; i j l}$ and $\widetilde{F}_{1 ; i j l}$ in the subspace of the $P$-state functions with $M=0$ and odd parity, and $F_{2 ; i j l}, \widetilde{F}_{2 ; i j l}$, and $G_{i j l}$ in the subspace of the $D$-state function with $M=0$ and even parity. Our purpose is to find a relation between ( $F_{L ; i j l}, \widetilde{F}_{L ; i j l}, G_{i j l}$ ) and ( $f_{L ; i j k}, \widetilde{f}_{L ; i j k}, g_{i j k}$ ). Using the spherical harmonic addition theorem

$$
\begin{equation*}
P_{l}(\cos \omega)=\frac{4 \pi}{2 l+1} \sum_{m=-l}^{l} Y_{l}^{m}\left(\theta_{1}, \varphi_{1}\right) Y_{l}^{-m}\left(\theta_{2}, \varphi_{2}\right) \tag{A7}
\end{equation*}
$$

together with a recurrence relation

$$
\begin{equation*}
Y_{l+1}^{m}(\theta, \varphi)=\left[\frac{(2 l+1)(2 l+3)}{(l+m+1)(l-m+1)}\right]^{1 / 2} Y_{l}^{m}(\theta, \varphi) \cos \theta-\left[\frac{(2 l+3)(l+m)(l-m)}{(2 l-1)(l+m+1)(l-m+1)}\right]^{1 / 2} Y_{l-1}^{m}(\theta, \varphi) \tag{A8}
\end{equation*}
$$

and some recurrence formulas for the Legendre polynomials, ${ }^{17}$ we can reduce the summations in Eqs. (A1)-(A3) as follows:

$$
\begin{align*}
& s_{0}=\frac{(-1)^{l}}{4 \pi}(2 l+1)^{1 / 2} P_{l}(\cos \omega)  \tag{A9}\\
& s_{1}=\frac{(-1)^{l}}{4 \pi}\left[\frac{3}{l+1}\right]^{1 / 2}\left[P_{l+1}^{\prime}(\cos \omega) P_{1}\left(\cos \theta_{1}\right)-P_{l}^{\prime}(\cos \omega) P_{1}\left(\cos \theta_{2}\right)\right],  \tag{A10}\\
& s_{2}=\frac{(-1)^{l}}{4 \pi}\left[\frac{40(2 l+1)!}{3(2 l+4)!}\right]^{1 / 2}\left[P_{l+2}^{\prime \prime}(\cos \omega) P_{2}\left(\cos \theta_{1}\right)+P_{l}^{\prime \prime}(\cos \omega) P_{2}\left(\cos \theta_{2}\right)-P_{l+1}^{\prime \prime}(\cos \omega)\left(3 \cos \theta_{1} \cos \theta_{2}-\cos \omega\right)\right],  \tag{A11}\\
& s_{3}=\frac{(-1)^{l}}{4 \pi}\left[\frac{80(2 l-2)!}{(2 l+3)!}\right]^{1 / 2}\left\{(2 l+1) P_{l}^{\prime \prime}(\cos \omega)\left[P_{2}\left(\cos \theta_{1}\right)+P_{2}\left(\cos \theta_{2}\right)\right]\right.
\end{align*}
$$

$$
\begin{equation*}
\left.-\left[(2 l-1) P_{l+1}^{\prime \prime}(\cos \omega)+(2 l+3) P_{l-1}^{\prime \prime}(\cos \omega)\right]\left(3 \cos \theta_{1} \cos \theta_{2}-\cos \omega\right) / 2\right\} \tag{A12}
\end{equation*}
$$

Here $s_{0}, s_{1}, s_{2}$, and $s_{3}$ denote the summations associated, respectively, with $F_{0 ; i j l}, F_{1 ; i j l}, F_{2 ; i j l}$, and $G_{i j l}$, and the first and second derivatives of the $P_{l}$ 's are written, respectively, as $P_{l}^{\prime}$ and $P_{l}^{\prime \prime}$. The summations associated with $\widetilde{F}_{1 ; i j l}$ and $\widetilde{F}_{2 ; i j l}$ are obtained by exchanging $\theta_{1}$ and $\theta_{2}$ in Eqs. (A10) and (A11). Derivation of these relations is straightforward though somewhat tedious, and we do not give details here. Substituting

$$
\begin{equation*}
\cos \omega=\left(r_{1} r_{2}^{-1}+r_{1}^{-1} r_{2}-r_{1}^{-1} r_{2}^{-1} r_{12}^{2}\right) / 2 \tag{A13}
\end{equation*}
$$

into Eqs. (A9)-(A12) and noting that $P_{l}$ is a polynomial of the $l$ th degree, we find that $F_{0 ; i j l}$ is given as a sum of a finite number of $f_{0 ; i j k}$ terms, $F_{1 ; i j l}$ and $\widetilde{F}_{1 ; i j l}$ as a sum of a finite number of $f_{1 ; i j k}$ and $\widetilde{f}_{1 ; i j k}$ terms, and $F_{2 ; i j l}, \widetilde{F}_{2 ; i j l}$, and $G_{i j l}$ as a sum of finite number of $f_{2 ; i j k}, \widetilde{f}_{2 ; i j k}$, and $g_{i j k}$ terms. This proves the completeness of the expansions using $f_{L ; i j k}, \widetilde{f}_{L ; i j k l}$, and $g_{i j k}$, and hence $v_{i j k}$ and $w_{i j k}$, in the subspace of the functions of a given symmetry [the terms with even $k$ are sufficient for the completeness of the expansion, since Eq. (A13) involves $r_{12}$ only in the second power].
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[^0]:    ${ }^{\text {a }}$ Calculated (nonrelativistic) ionization energies are estimated to be accurate to within one, or occasionally two, in the last digits quoted, unless these are underlined.
    ${ }^{\text {b }}$ Pekeris (Ref. 5); Accad, Pekeris, and Schiff (Ref. 6).
    ${ }^{\mathrm{d}} \mathbf{A}$ few $v_{i j k}$ terms were omitted to limit the expansion length to 140 .

