ATSS-10

# OSCILLATOR STRENGTHS FOR SINGLET AND TRIPLET SERIES IN NEUTRAL HELIUM*

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* This research was supported in part by Contract Nonr 1727(00) with the Office of Naval Research, in part by Contract AT (30-1) - 2934 with the Atomic Energy Commission, and in part by Grant NsG - 287 from the National Aeronautics and Space Administration. The Office of Naval Research Contract was administered by the University of Pennsylvania. The computations were carried out at the Haverford-Bryn Mawr Computing Center on the IBM 1620 computer whose purchase was aided by Grant NSF - G19660 from the National Science Foundation to both colleges.

## ABSTRACT

33192

Oscillator strengths have been computed for all possible electric dipole transitions between the terms $n^1S$, $n^3S$, $n^1P$, $n^3P$, $n^1D$, and $n^3D$, where n goes from one to nine for S terms, two to eight for P terms, and three to eight for D terms. The computations were carried through using central field wave functions with exchange and configuration interaction. The parameters in these wave functions had previously been determined by the use of the minimum principal. The oscillator strengths as computed by the length and velocity expressions are reported. For the $1^1S - n^1P$ series, the results found with the acceleration expression are also included. The agreement between the results obtained with the length and the velocity expressions as well as that between the present work and earlier computations, where available, give confidence in the dependability of the results.

Author

## INTRODUCTION

A knowledge of the relevant oscillator strengths is essential for any relatively complete, quantitative interpretation of an astronomical spectrum. The present work gives the results of the computation of the f-values for the lines in a number of series in the spectrum of neutral helium. To obtain dependable oscillator strengths theoretically, it is necessary to employ wave functions of considerable accuracy. The wave functions used in the present computations were analytic, central field functions with exchange and configuration interaction. The reasons for the choice of wave functions of this particular kind, the procedures employed for the determination of the parameters which occur in them, and a discussion of their probable accuracy based on the computed energies and the transition probabilities in the $1^1S - n^1P$ series have been given by Green, Kolchin, and Johnson (1965 a,b). If one excludes the energy of the $1^1S$ term, the average agreement between computed and observed energies for the forty-two remaining terms was better than one part in

300,000 (Green et al. 1965 a). The agreement between the oscillator strengths as computed by the length and velocity expressions for the $1^1S - n^1P$ series was in every case to 2% or better (Green et al. 1965 b). In particular, the agreement for the $1^1S - 2^1P$ and $1^1S - 3^1P$ lines with the very extensive computations of Schiff and Pekeris (1964) was to 1%. These results suggest that a substantial degree of confidence can be placed in the dependability of oscillator strengths computed from the present set of wave functions.

The spectrum of He I was chosen for investigation for a number of reasons. The far ultra-violet spectra of the light atoms, highly ionized ions and simple molecules play an important role in the recent observations of the sun and stars from above the earth's atmosphere (Tousey, 1964, Strecher and Milligan, 1962).

These spectra are also much to the fore in the study of controlled thermonuclear reactions (Bearden, A.J., Ribe, F.L., Sawyer, G.A., and Stratton, T.F., 1961; Fawcett, B.C., Gabriel, A.H., Griffin, W.G., Jones, B.B., and Wilson, R., 1963; Fawcett, B.C., Gabriel, A.H., Jones, B.B., and Peacock, N.J., 1964; Gabriel, A.H., and Fawcett, B.C., 1965). The He I isoelectric sequence is represented in the solar spectrum by ions up through Ne IX and the Li I sequence by ions through Si XII (Tousey, 1964). Since it was unclear at the beginning of the present work whether the wave functions employed would be sufficiently accurate to yield f-values of the degree of dependability desired, it seemed wise to deal with a two electron system first. Of these systems He I was chosen because of its importance in both terrestrial and astrophysical sources. Its spectrum has been extensively investigated in the laboratory, most recently by Martin (1960). Furthermore there have been numerous theoretical investigations of He I. A comparison of the present results with this extensive material allows one to evaluate the effectiveness of the methods employed here.

## THE WAVE FUNCTIONS

The trial variational wave functions were given the form

$$\Psi_n = \sum_{k=L+1}^{n} c_k \Phi_k \qquad (1)$$

Here n is the value of the principal quantum number of the running electron in whichever series of terms is being considered. $L$ is the total orbital angular momentum quantum number for the series and the $\Phi_k$'s are defined by the equation,

$$\Phi_k = \sum_i c_{ki} \Psi_i$$

where the $\Psi_i$'s are linear combinations of normalized antisymmetrized products of Slater orbitals. The orbitals are chosen so that $M_S=0$ and $M_L=0$ for each product. Clebsch-Gordan coefficients are employed to assign weights to these products such that their linear combinations have the correct spin and angular dependence for eigenfunction in LS-coupling. The $\Psi_i$'s therefore have the form

$$\Psi_i = \sum_{m_s} \Big\{ C\left(\tfrac{1}{2}, \tfrac{1}{2}, S, m_s\right) \sum_{m_i=-\ell_i}^{\ell_i} \Big[ C(\ell_i, \lambda_i, L, m_i) \cdot N\mathcal{A}\Big\{ r_1^{a_i} \exp\left(-Z\frac{\alpha_i}{n_{\alpha i}} r_1\right) Y(\ell_i, m_i; \theta_1, \varphi_1)\, \delta(m_s; \sigma_1) \cdot r_2^{b_i} \exp\left(-Z\frac{\beta_i}{n_{\beta i}} r_2\right) Y(\lambda_i, -m_i; \theta_2, \varphi_2)\, \delta(-m_s; \sigma_2) \Big\} \Big] \Big\} \qquad (3)$$

Here $\ell_i$ and $\lambda_i$ are the orbital angular momentum quantum numbers of the two electrons with $\ell_i \leq \lambda_i$, the C's are the Clebsch-Gordan coefficients, N is the normalization constant for the spacial part of the antisymmetrized product which follows, $\mathcal{A}$ is the antisymmetrizer operator, the Y's are surface spherical harmonics and the $\delta$'s are Kroeneker deltas, employed here as spin functions. The $a_i$'s and $b_i$'s are integers, Z is set equal to the nuclear charge, the $n_{\alpha i}$'s and the $n_{\beta i}$'s are the principal quantum numbers of the two electrons, the $\alpha_i$'s and the $\beta_i$'s measure the strength of the "effective nuclear charge" for each electron.

The procedures by which the adjustable parameters were chosen have been described elsewhere (Green et al., 1965 a,b). Both the linear ones, the $c_k$'s and the $c_{ki}$'s, and the nonlinear ones, the $\alpha_i$'s and $\beta_i$'s were chosen by the variational principle. When sets of parameters in the $\psi_i$'s of Eq. (2) have been found which give an energy sufficiently close to the experimental value for the lowest member of any series, the values of these parameters are fixed and $\Psi_{L+1}$ is set equal to $\phi_{L+1}$. For $\Psi_{L+2}$,

one writes

$$\psi_{L+2} = c_{L+1}\phi_{L+1} + c_{L+2}\left(\sum_i c_{L+2,i}\,\psi_i\right) \qquad (4)$$

A set of parameters is now chosen to give an energy close to that of the second member of the series. The values of these parameters in $\phi_{L+2}$ are now fixed, and the process repeated for $\psi_{L+3}$. If N is the value of n for the highest series member of interest, one may write instead of Eq. (2),

$$\psi_n = \sum_{k=L+1}^{N} c_k \phi_k \qquad (5)$$

For the present wave functions, the energies as calculated with the wave functions of Eqs. (1) and (5) did not differ by as much $1 \cdot 10^{-6}$ rydbergs.

## CALCULATION OF THE OSCILLATOR STRENGTHS

For two-electron systems, the length, velocity and acceleration expressions for the oscillator strength or f-value for an electric dipole transition take the form (Schiff and Pekeris, 1964):

$$f_\ell = 2(E_{n'} - E_n) \left| \int \Psi^*_{n'} (z_1 + z_2) \Psi_n \, d\tau \right|^2 \qquad (6.1)$$

$$f_v = \frac{2}{E_{n'} - E_n} \left| \int \Psi^*_{n'} \left( \frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2} \right) \Psi_n \, d\tau \right|^2 \qquad (6.2)$$

$$f_a = \frac{2}{(E_{n'} - E_n)^3} \left| \int \Psi^*_{n'} \left( \frac{z_1}{r_1^3} + \frac{z_2}{r_2^3} \right) \Psi_n \, d\tau \right|^2 \qquad (6.3)$$

Where atomic units are used throughout and $Z$ is the atomic number. If the $\Psi_n$'s are exact solutions of a Schrödinger equation, the three f-values will be the same. If the solutions are only approximate, the difference between the computed results should decrease as the accuracy of the wave functions increases, but the physical significance of the results is assured only if the functions are exact or approximate solutions of a Schrödinger equation which adequately represents the physical problem.

The oscillator strengths can be computed by substituting the wave functions obtained from either Eqs. (1)

or (5) into Eqs. (6) and proceeding with the direct evaluation of the resulting integrals. An alternative and more rapid procedure is to use one of the expressions given in the literature such as that of Slater (1960) in which the summations over the possible values of the magnetic quantum numbers and the corresponding weighting by the Clebsch-Gordan coefficients have already been carried out for transitions between two sets of Slater orbitals, one set associated with the contribution of one configuration to the lower term and the other with the contribution of another configuration to the upper term. The matrix elements for the transitions between pairs of contributing configurations are then summed with the weights as given by the $c_k$'s and $c_{ki}$'s. The square of the dipole matrix elements are found from Eq. (25-30) of Slater's treatment (1960). The f-values were computed both by the direct procedure and by the expressions given by Slater. In the absence of a gross error, the two methods should agree exactly and in fact, this was the case.

## RESULTS AND DISCUSSION

Tables 1, 2, 3 and 4 give the f-values found for the series $n^1S - n'^1P$, $n^3S - n'^3P$, $n^1P - n'^1D$ and $n^3P - n'^3D$ respectively. To obtain the f-values for $n^1P - n'^1S$, $n^3P - n'^3S$, $n^1D - n'^1P$, and $n^3D - n'^3P$, one should multiply the values given in Tables 1, 2, 3, and 4 respectively by $-(2L + 1) / (2L + 3)$ where L has the value associated with the term of lower total orbital angular momentum. For all series, the values of the oscillator strengths are given both as computed from the length and the velocity expressions. For the $1^1S - n'^1P$ series, the value as computed from the acceleration expression is also given. As was pointed out long ago by Chandrasekhar (1945), the largest contribution to the f-value as computed from Eqs. (6.1), (6.2), and (6.3) comes from regions far from the nucleus, at intermediate distances, and close to the nucleus respectively. On the other hand the minimum principle determines the wave function most strongly at intermediate distances. One would thus expect that f-values computed from the dipole velocity formula will be more dependable than those computed from the other two expressions. Experience shows that the

length and velocity formulae results are usually in much better accord with one another than with the values obtained from the acceleration. In the present case the acceleration value was found for every line, but the difference between it and the other two was often substantial, so that only for the $1^1S - n'^1P$ series did it seem desirable to include the acceleration results.

All f-values were also computed using both the wave functions of Eq. (1) and those of Eq. (5). In all cases, with the single exception of the $5^3S$ - $n'^3P$ series, the agreement of the results from the length, velocity and acceleration expressions was closer when wave functions from Eq. (5) were employed. For this single series therefore, the values given in Table 2 are computed with wave functions derived from Eq. (1).

A comparison of the f-values reported by Green et al. (1965 b) for the $1^1S$ - $n'^1P$ series, which were obtained with wave functions from Eq. (1), with those given here shows the typical slightly narrower spread in results from the three dipole expressions when wave functions from Eq. (5) are employed.

The wave functions used for the $^1S$, $^3S$, $^1P$, $^3P$, and $^1D$ terms were those described by Green et al. (1965 a). In the case of the $^3D$ terms, closer agreement between the various f-value expressions were obtained using an older set of wave functions with less configuration interaction which gave slightly poorer energies.[1]

1. Complete tables of the values of $a_i$, $\alpha_i$, $k_i$, $b_i$, $\beta_i$ $\lambda_i$, $c_{ni}$, and $c_k$ as determined both from Eq. (1) and from Eq. (5) have been deposited as Document No. with the American Documentation Institute, Auxiliary Publications Project, Photoduplication Service, Library

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Examination of the more recent wave functions for the $^3D$ series suggests that these functions can be improved. It seemed best to publish the results from the old functions at this time.

Comparison of the present results with those of Trefftz, Schlüter, Dettmar, and Jörgens (1957) shows that the average difference without regard to sign between the f-values as determined from the velocity expression is 4.5% in the 27 common cases.

The rather large amount of material available, from which Tables 1 to 4 show only selected values, demonstrates certain regularities. It seems to the authors that a further examination of these regularities will allow us to compute appreciably more dependable f-values and the recomputation of the $^3D$ series will await this work.

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TABLE 1

OSCILLATOR STRENGTHS FOR THE SERIES $n^1S - n'^1P$ OF He I

| | n / n' | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|---|
| Len. | | 0.27537 | 0.3773 | -0.1457 | -0.0260 | -0.00967 | -0.00476 | -0.00273 | -0.00169 | -0.00141 |
| Vel. | 2 | 0.27586 | 0.3950 | -0.1446 | -0.0256 | -0.00951 | -0.00471 | -0.00272 | -0.00171 | -0.00115 |
| Acc. | | 0.26908 | | | | | | | | |
| Len. | | 0.07292 | 0.1513 | 0.6279 | -0.3081 | -0.0554 | -0.0210 | -0.0105 | -0.00602 | -0.00475 |
| Vel. | 3 | 0.07296 | 0.1540 | 0.6448 | -0.3092 | -0.0556 | -0.0212 | -0.0107 | -0.00626 | -0.00401 |
| Acc. | | 0.07047 | | | | | | | | |
| Len. | | 0.02957 | 0.0493 | 0.1429 | 0.8603 | -0.4767 | -0.0860 | -0.0329 | -0.0165 | -0.0115 |
| Vel. | 4 | 0.02960 | 0.0506 | 0.1433 | 0.8754 | -0.4780 | -0.0864 | -0.0329 | -0.0169 | -0.0099 |
| Acc. | | 0.02835 | | | | | | | | |
| Len. | | 0.01481 | 0.0224 | 0.0499 | 0.1455 | 1.0869 | -0.6476 | -0.1170 | -0.0446 | -0.0258 |
| Vel. | 5 | 0.01487 | 0.0231 | 0.0506 | 0.1445 | 1.0901 | -0.6526 | -0.1185 | -0.0456 | -0.0232 |
| Acc. | | 0.01419 | | | | | | | | |
| Len. | | 0.00841 | 0.0121 | 0.0236 | 0.0525 | 0.1513 | 1.3094 | -0.8212 | -0.1486 | -0.0563 |
| Vel. | 6 | 0.00851 | 0.0125 | 0.0243 | 0.0521 | 0.1513 | 1.3170 | -0.8246 | -0.1495 | -0.0575 |
| Acc. | | 0.00814 | | | | | | | | |
| Len. | | 0.00518 | 0.00741 | 0.0130 | 0.0257 | 0.0549 | 0.1592 | 1.5300 | -0.9959 | -0.1789 |
| Vel. | 7 | 0.00531 | 0.00763 | 0.0138 | 0.0257 | 0.0554 | 0.1598 | 1.5373 | -0.9986 | -0.1799 |
| Acc. | | 0.00508 | | | | | | | | |
| Len. | | 0.00340 | 0.00473 | 0.00775 | 0.0148 | 0.0269 | 0.0573 | 0.1690 | 1.7489 | -1.1638 |
| Vel. | 8 | 0.00356 | 0.00498 | 0.00865 | 0.0148 | 0.0275 | 0.0586 | 0.1686 | 1.7626 | -1.1669 |
| Acc. | | 0.00341 | | | | | | | | |

TABLE 2

OSCILLATOR STRENGTHS FOR THE SERIES $n^3S - n'^3P$ of He I

| | n / n' | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|
| Len. | 2 | 0.5398 | -0.2087 | -0.0318 | -0.0113* | -0.00552 | -0.00314 | -0.00196 | -0.00125 |
| Vel. | | 0.5487 | -0.2055 | -0.0312 | -0.0111* | -0.00539 | -0.00306 | -0.00190 | -0.00128 |
| Len. | 3 | 0.0644 | 0.8922 | -0.4363 | -0.0693* | -0.0248 | -0.0122 | -0.00705 | -0.00471 |
| Vel. | | 0.0668 | 0.9110 | -0.4384 | -0.0679* | -0.0248 | -0.0123 | -0.00707 | -0.00450 |
| Len. | 4 | 0.0259 | 0.0499 | 1.2164 | -0.6605* | -0.1041 | -0.0383 | -0.0189 | -0.0132 |
| Vel. | | 0.0271 | 0.0491 | 1.2305 | -0.6742* | -0.1043 | -0.0383 | -0.0192 | -0.0112 |
| Len. | 5 | 0.0125 | 0.0228 | 0.0439 | 1.5369* | -0.9045 | -0.1402 | -0.0514 | -0.0305 |
| Vel. | | 0.0132 | 0.0226 | 0.0430 | 1.5383* | -0.9066 | -0.1406 | -0.0519 | -0.0259 |
| Len. | 6 | 0.00691 | 0.0118 | 0.0214 | 0.0528* | 1.8436 | -1.1407 | -0.1766 | -0.0644 |
| Vel. | | 0.00733 | 0.0118 | 0.0210 | 0.0398* | 1.8534 | -1.1430 | -0.1767 | -0.0651 |
| Len. | 7 | 0.00421 | 0.00690 | 0.0116 | 0.0173* | 0.0402 | 2.1525 | -1.3779 | -0.2137 |
| Vel. | | 0.00452 | 0.00698 | 0.0115 | 0.0195* | 0.0395 | 2.1573 | -1.3791 | -0.2120 |
| Len. | 8 | 0.00271 | 0.00434 | 0.00686 | 0.0094* | 0.0211 | 0.0393 | 2.4614 | -1.6176 |
| Vel. | | 0.00298 | 0.00449 | 0.00699 | 0.0110* | 0.0206 | 0.0394 | 2.4700 | -1.6150 |

*Matrix elements computed with wave functions from Eq. (1)

TABLE 3

OSCILLATOR STRENGTHS FOR THE SERIES $n^1P - n'^1D$ OF He I

| | n / n' | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| Len. | 3 | 0.71059 | -0.0218 | -0.0152 | -0.00309 | -0.00118 | -0.000578 | -0.000345 |
| Vel. | | 0.70949 | -0.0209 | -0.0152 | -0.00304 | -0.00118 | -0.000612 | -0.000345 |
| Len. | 4 | 0.12028 | 0.6490 | -0.0415 | -0.0390 | -0.00834 | -0.00326 | -0.00169 |
| Vel. | | 0.12018 | 0.6486 | -0.0403 | -0.0399 | -0.00841 | -0.00332 | -0.00168 |
| Len. | 5 | 0.04325 | 0.1413 | 0.6490 | -0.0597 | -0.0680 | -0.0149 | -0.00591 |
| Vel. | | 0.04324 | 0.1412 | 0.6490 | -0.0653 | -0.0673 | -0.0148 | -0.00584 |
| Len. | 6 | 0.02093 | 0.0562 | 0.1528 | 0.6714 | -0.0765 | -0.1002 | -0.0223 |
| Vel. | | 0.02095 | 0.0563 | 0.1530 | 0.6728 | -0.0862 | -0.0994 | -0.0221 |
| Len. | 7 | 0.01185 | 0.0287 | 0.0634 | 0.1629 | 0.7048 | -0.0929 | -0.1346 |
| Vel. | | 0.01190 | 0.0289 | 0.0637 | 0.1636 | 0.7067 | -0.0985 | -0.1337 |
| Len. | 8 | 0.00735 | 0.0167 | 0.0331 | 0.0686 | 0.1736 | 0.7440 | -0.1088 |
| Vel. | | 0.00747 | 0.0171 | 0.0337 | 0.0696 | 0.1741 | 0.7453 | -0.1143 |

## TABLE 4

OSCILLATOR STRENGTHS FOR THE SERIES $n^3P - n'^3D$ OF He I

| | n / n' | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| Len. | 3 | 0.6105 | 0.1130 | -0.0371 | -0.00695 | -0.00261 | -0.00131 | -0.000779 |
| Vel. | | 0.6269 | 0.1216 | -0.0378 | -0.00690 | -0.00263 | -0.00131 | -0.000760 |
| Len. | 4 | 0.1232 | 0.4766 | 0.2023 | -0.0886 | -0.0171 | -0.00654 | -0.00332 |
| Vel. | | 0.1275 | 0.4790 | 0.2119 | -0.0910 | -0.0175 | -0.00668 | -0.00338 |
| Len. | 5 | 0.0472 | 0.1245 | 0.4374 | 0.2815 | -0.1475 | -0.0290 | -0.0112 |
| Vel. | | 0.0490 | 0.1254 | 0.4363 | 0.2884 | -0.1479 | -0.0291 | -0.0112 |
| Len. | 6 | 0.0236 | 0.0530 | 0.1237 | 0.4281 | 0.3564 | -0.2106 | -0.0419 |
| Vel. | | 0.0245 | 0.0535 | 0.1237 | 0.4276 | 0.3562 | -0.2106 | -0.0419 |
| Len. | 7 | 0.0137 | 0.0281 | 0.0549 | 0.1243 | 0.4327 | 0.4282 | -0.2767 |
| Vel. | | 0.0142 | 0.0285 | 0.0552 | 0.1249 | 0.4328 | 0.4279 | -0.2762 |
| Len. | 8 | 0.00870 | 0.0169 | 0.0295 | 0.0556 | 0.1280 | 0.4443 | 0.4985 |
| Vel. | | 0.00901 | 0.0172 | 0.0303 | 0.0570 | 0.1279 | 0.4442 | 0.4966 |