Radiative transition rates from the 2p3p P3 and 2p3d D1,3 states of the helium isoelectronic sequence

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Radiative Transition Rates from the 2p3p 3P and 2p3d 1,3D States of the Helium Isoelectronic Sequence

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(Received 12 October 1971)

The Hylleraas-Scherr-Knight variation-perturbation method is applied to the calculation of oscillator strengths for the dominant transitions from the metastable 2p3p 3P and 2p3d 1D states of helium and the heliumlike ions. The results explain the absence of the 1s2p3P – 2p3p3P transition of He I from recent beam-foil excitation spectra.

I. INTRODUCTION

Many atoms possess rydberg series of doubly excited states which, although imbedded in the autoionizing continuum, are prevented from autoionizing by angular momentum and parity selection rules. Such states may be termed “metastable” since their lifetimes are determined by the relatively slow process of spontaneous emission of radiation, rather than autoionization. The 2p 3P metastable state of helium is the most extensively studied. A recent remeasurement of its energy has corrected an earlier error and brought the theoretical and experimental energies into good agreement. Progress in the theoretical study of multiply excited states has been reviewed by Holtsien.

In previous papers, we have applied the Hylleraas-Scherr-Knight 1/Z expansion perturbation technique to the calculation of the energies of the metastable 2p 3P, 2p 3P, 2p3p 3P, 2p3d 3D, and 2p3d 3D states of the helium isoelectronic sequence. Direct variational bounds have also been obtained for the neutral helium eigenvalues as a check on the accuracy of the perturbation expansions. In this paper, we evaluate the oscillator strengths for those transitions from the 2p3p 3P, 2p3d 3D, and 2p3d 3D states which are expected to be dominant. Results for the corresponding transitions from the 2p 3P and 2p3p 3P states have been reported previously. Transitions involving the above states have been observed in beam-foil excitation spectra and are of interest in the study of solar flares and the solar corona.

The computational method is briefly summarized in Sec. II and the results presented in Sec. III.

II. COMPUTATIONAL METHOD

The Hylleraas-Scherr-Knight variation-perturbation method used in the present work has been described previously and is only briefly summarized here. In units of Z a.u., the Hamiltonian for a two-electron atom may be written in the form $H = H_0 + Z^{-1}V$, where $H_0$ is a sum of hydrogen-atom Hamiltonians and $V = 1/r_{12}$. The above partition of $H$ leads to the following perturbation expansions for the eigenfunctions and eigenvalues:

$$\psi = \psi_0 + \sum_{n=1}^{\infty} \psi_n Z^{-n},$$

$$E = E_0 + \sum_{n=1}^{\infty} E_n Z^{-n}.$$
\( \chi_j = (1 \pm P_{12}) r_1^2 r_2^2 e^{r_1^2 + r_2^2} \),

where

\[ \psi_{L,T,\ell_1 \ell_2}^{m_1,m_2} = \sum_{m_1',m_2'} \langle m_1 | m_1' | L, M \rangle \times Y_{\ell_1 \ell_2}^{m_1,m_2} \left( \xi_1, \xi_2 \right) \]

\( H_0 \) is diagonalized in the basis set \( \phi_i \) such that

\[ \langle \phi_i | H_0 | \phi_j \rangle = \epsilon_i \delta_{ij} \]

\( P_{12} \) in (3) indicates the interchange of labels 1 and 2, with the plus sign referring to singlet states and the minus sign to triplet states. The scale factors \( \alpha \) and \( \beta \) are set equal to their hydrogenic values; for example, \( \alpha = \frac{1}{3} \) and \( \beta = \frac{1}{2} \) for the 2p3d \( 1\Delta D \) states. Then, as a consequence of the diagonalization (5), one of the \( \phi_i \), say, \( \phi_a \), is automatically the exact hydrogenic eigenfunction \( \psi_0 \) with eigenvalue \( \epsilon_a = E_0 \), and the remaining functions \( \phi_{i}(i \neq a) \) form a synthetic representation of the remaining spectrum of \( H_0 \). It can be shown from a variational principle that the \( \psi_n \) and \( E_n \) are determined by the recursion relations

\[ \psi_n = \sum_{i=0}^{n} \left( \frac{\phi_1 | \psi_{n+1} \rangle}{\epsilon_{n+1} - \epsilon_1} - \sum_{r=1}^{n} E_n \left( \frac{\phi_1 | \psi_{n+1} \rangle}{\epsilon_{n+1} - \epsilon_r} \right) \right) \phi_r \]

\[ E_n = \langle \psi_n | V | \psi_0 \rangle - \sum_{r=1}^{n} E_n \langle \psi_{n+1} | \psi_0 \rangle \]

provided that all the lower order \( \psi_i \), \( E_i \), \( i = 1, \ldots, n-1 \), are known exactly. With a finite basis set, the lower-order solutions are not known exactly, but the above equations provide useful approximations to \( \psi_n \) and \( E_n \) (but not bounds beyond \( E_0 \)) up to some finite order \( n_{\text{max}} \). The nonrelativistic perturbation expansions (1) and (2) summed up to order \( n_{\text{max}} \) increase in accuracy with increasing \( Z \) and are asymptotically correct. An advantage of the \( 1/Z \) expansion procedure over a direct variational calculation is that results for an entire isoelectronic sequence are obtained by a single diagonalization of \( H_0 \) in the finite basis set.

### III. CALCULATED OSCILLATOR STRENGTHS

We are concerned with the calculation of oscillator strengths for the dominant transitions from the 2p3d \( ^5P \), 2p3d \( ^3D \), and 2p3d \( ^1D \) states. The transitions considered are

\[ 2p3d \times 1s2p3p, \quad 2p3d \times 1s4p3p, \quad 2p3d \times 1s3d3d, \quad 2p3d \times 1s3d3p, \quad 2p3d \times 2p3p, \quad 2p3d \times 2p3d, \quad 2p3d \times 2p3p. \]

In addition, there are one-electron transitions to doubly excited autoionizing states, but these should be less important than transitions to singly excited states since the energy separations are much smaller in the former case.

The "length" form of the oscillator strength for a transition between two atomic states labeled by angular momentum quantum numbers \( LM \) and \( L'M' \) and having energies \( E \) and \( E' \) is defined as

\[ f_i(E') = \frac{1}{3} \left( E' - E \right) \left( \psi_{L'M'} \sum_{i} \langle \psi_i | \gamma LM \rangle \right)^2 \]

in atomic units. The sum runs over all the electrons in the atom. An averaged oscillator strength \( \bar{f} \) which is independent of magnetic quantum number is obtained by averaging over the initial-state orientation degeneracy and summing over the final-state degeneracy. It is first convenient to introduce reduced matrix elements through the relation involving the 3-j symbol

\[ \langle \psi_{L'M'} | \sum_{i} \gamma \rangle \]

The results are presented in terms of the above reduced matrix elements and averaged oscillator strengths.

For exact initial- and final-state wave functions, the length form given by Eq. (10) is formally identical to the velocity form

\[ \bar{f}_v(E') = \frac{2}{3(2L+1)} \left( \langle \gamma \gamma' \rangle \sum_{i} \hat{P}_i \right) \left( \gamma \gamma' \right)^2, \]

where \( \hat{P}_i = \langle \gamma \rangle \). The length and velocity transition integrals \( R = \langle \gamma \gamma' \rangle \sum_{i} \hat{P}_i \left( \gamma \gamma' \right) \) and \( P = \langle \gamma' \gamma' \rangle \sum_{i} \hat{P}_i \left( \gamma \gamma' \right) \) have the \( Z^2 \) expansions

\[ R = Z^2 \sum_{n=0}^{n_{\text{max}}} R_n Z^n, \]

\[ P = Z^2 \sum_{n=0}^{n_{\text{max}}} P_n Z^n, \]

with the exact expansion coefficients being related through

\[ P_n = \frac{i}{E} \sum_{m=0}^{n} R_{n-m} \Delta E_m \]

as a consequence of the equivalence of Eqs. (10) and (11). \( \Delta E_m \) in (14) is the \( m \)th coefficient in the \( Z^2 \) expansion of \( E' - E \). With the approximate perturbed eigenfunctions obtained by expansion in
a finite basis set, (14) is not satisfied exactly (except in lowest nonvanishing order) and thus provides a check on the accuracy of the calculation. We denote by $R^{(1)}_{nl}$ the $R$ expansion coefficients calculated directly from the matrix elements of $\mathfrak{T}_1$, and by $R^{(a)}_{nl}$ the coefficients calculated indirectly from the matrix elements of $\mathfrak{T}_1$ and the use of Eq. (14). Similarly, $P^{(a)}_{nl}$ denotes the $P$ expansion coefficients calculated directly from the matrix elements of $\mathfrak{T}_1$ and $P^{(b)}_{nl}$ those calculated indirectly from the $R^{(a)}_{nl}$ and Eq. (14). The above four sets of expansion coefficients each yield slightly different results for the oscillator strengths.

One could also eliminate the energy difference between (10) and (11) to obtain the intermediate form for the oscillator strength

$$\bar{f}(\gamma L - \gamma' L') = \frac{2}{3(2L + 1)} |RP|,$$

(15)

thus generating several more possible procedures.

It is not clear which of the above procedures is the most accurate. Starace\textsuperscript{12} argues that the length formulation is preferable if the wave functions are exact eigenfunctions of an approximate nonlocal Hamiltonian, but he specifically excludes correlated variational wave functions. In the latter case, Dalgarno and Lewis\textsuperscript{13} and Crossley\textsuperscript{14} argue that for large excitation energies the velocity form is preferable, while Stewart\textsuperscript{15} has shown that for transitions between adjacent states involving no change in principal quantum number, the length form is preferable. We have adopted the procedure of calculating the oscillator strengths in the length formulation, with the transition integrals $R$ obtained by summing the $R^{(ab)}_{nl}$ for transitions in which the principal quantum number changes and by summing the $R^{(a)}_{nl}$ for transitions in which the principal quantum number does not change.

The reduced $R^{(1)}_{nl}$ and $R^{(a)}_{nl}$ transition integral expansion coefficients calculated from 50-term basis sets, as discussed in Sec. II, are given in Table I. The relative phases are internally consistent and correspond to radial wave functions which are positive near the origin. The zero-order coefficients are related to the one-electron hydrogenic reduced transition integrals by\textsuperscript{11}

$$\langle \gamma' L' I_2' I_2' \| \mathfrak{T}_1 \| \gamma L I_1 I_2 \rangle = (-1)^{I_1' + I_2' + 1} \left( \frac{2}{3(2L + 1)} \right)^{1/2} \times \begin{cases} I_1' & L' I_2' I_2' \langle \gamma' L' \| \mathfrak{T}_1 \| \gamma L I_1 I_2 \rangle. 
\end{cases}$$

(16)

A comparison of the $R^{(1)}_{nl}$ and $R^{(a)}_{nl}$ in Table I indicates that the accuracy varies considerably from transition to transition. The neutral helium oscillator strengths calculated from the truncated expansions

$$\bar{f}_1 = \frac{2\Delta E}{3(2L + 1)} \sum_{n=0}^{\text{max}} R^{(1)}_{nl} Z^{(nl)} \left( \frac{2\Delta E}{3(2L + 1)} \sum_{n=0}^{\text{max}} R^{(a)}_{nl} Z^{(nl-a)} \right) \left( \frac{2\Delta E}{3(2L + 1)} \sum_{n=0}^{\text{max}} R^{(a)}_{nl} Z^{(nl-a)} \right)^2$$

(17)

and

$$\bar{f}_e = \frac{2\Delta E}{3(2L + 1)} \sum_{n=0}^{\text{max}} R^{(1)}_{nl} Z^{(nl)} \left( \frac{2\Delta E}{3(2L + 1)} \sum_{n=0}^{\text{max}} R^{(a)}_{nl} Z^{(nl-a)} \right)^2$$

(18)

are compared in Table II. Although the above two
The predicted correlation in Table II is compared with the single and double-electron calculations discussed earlier, the comparison in Table II probably overestimates the accuracy by about an order of magnitude. The agreement for the $1s3d^{1}D - 2p3d^{1}P$ transitions is particularly good.

The energy differences, absorption oscillator strengths, and emission Einstein $A$ coefficients are given in Table III for the isoelectronic sequences up to $Z = 18$. Although the nonrelativistic results become increasing accurate with increasing $Z$, it is important to consider relativistic corrections to the energy differences for large $Z$, particularly for transitions between adjacent states. The effect is to increase the decay rate through the $\Delta E^3$ dependence of the $A$ coefficient. Relativistic and retardation contributions to the transition integral itself are probably not important for $Z \leq 25$.

### IV. DISCUSSION OF RESULTS

Berry et al. have observed several transitions from the doubly excited states of He I, including the $1s2p^{3}P - 2p3p^{3}P$ and $1s3p^{3}P - 2p3p^{3}P$ transitions at 295.2 and 308.0 Å, respectively. For the corresponding triplet transitions, they observe only a single line at 306.1 Å which they tentatively identify as the $1s3p^{3}P - 2p3p^{3}P$ transition predicted to be at 305.7 Å. The unexpected absence of the $1s2p^{3}P - 2p3p^{3}P$ transition at 291.1 Å from their spectra is understandable from our calculated oscillator strengths. The transition integral is anomalously small (and inaccurate) due to severe numerical cancellation in the summation of the $Z^3$ expansion series given in Table I. The oscillator strength in Table II is nearly an order of magnitude smaller than that for the two-electron jump $1s4p^{3}P - 2p3p^{3}P$, even though the latter is forbidden for simple product-type eigenfunctions and proceeds only through correlation effects. The lifetime of the $2p3p^{3}P$ state is then determined primarily by the $1s3p^{3}P - 2p3p^{3}P$ transition. In contrast,
The oscillator strengths for both the 1s2p^1P - 2p3p^1P and 1s3p^1P - 2p3p^1P transitions are large and of roughly equal magnitude.\(^5\)

The line\(^7\) observed at 306 ± 1 Å may also contain a contribution from the 1s3d^1D - 2p3d^1D transition\(^5\) at 305.4 Å since the experimental resolution is not sufficient to separate the two possible contributions. One would further expect the 1s3d^3D - 2p3d^3D transition\(^5\) at 304.5 Å to be present since the companion 2p^3P - 2p3d^3D transition predicted to be at 3014 Å has been observed in unpublished work by Berry. Higher-resolution wavelength and lifetime measurements would make possible a positive identification of these transitions.

The selection rule preventing autoionization ap-
plies rigorously only in the limit of exact $LS$ coupling. Holšien\(^6\) has pointed out that some of the fine-structure levels of the doubly excited metastable states are coupled directly with the continuum by the spin-orbit, spin-other-orbit, and spin-spin interactions, thereby making autoionization possible. Although the autoionization rate for the He\(i\) states is small compared to radiative decay, the rate increases rapidly with increasing nuclear charge and eventually leads to the selective depopulation of some of the triplet fine-structure levels.

\*Research supported by the National Research Council of Canada.


