Auto-Ionization in Doubly Excited Helium and the λ320.4 and 1357.5 Lines

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The probabilities of auto-ionization of the λ315, λ320.4, λ343, λ357.5 states of He are calculated with continuous wave functions which are obtained by numerical integration of the wave equations including the effect of exchange. The probabilities are 4×10^{-5}, 3×10^{-4}, 4×10^{-2} per second, respectively. For these states the theoretical energies of the doubly excited states, the identification of the two lines λ320.4 and λ357.5 observed by Compston and Boyce, and by Kruger, is discussed. The former have been reasonably definitely ascribed to the transition λ320.4 2p1s−2p3p, the state 2p3p not being subject to auto-ionization. The latter line cannot be satisfactorily accounted for with respect to both the position and the width of the line.

There have been many investigations on different aspects of the problem of doubly excited helium. Compston and Boyce, and later Kruger, observed in the extreme ultraviolet region two lines λ320.4 (ν = 312.117 cm^{-1}) and λ357.5 (ν = 270.715 cm^{-1}) which they ascribed to transitions from the doubly excited to the ordinary singly excited states of helium. Considerable interest in the energy states of doubly excited helium has been aroused by the suggestion, now abandoned, that the corona lines may be due to transitions among the doubly excited states of helium. This has led to the theoretical calculation of these energy states by many authors. Many attempts have been made to observe the spectrum of doubly excited helium under experimental conditions that would have been most favorable for their excitation according to the theoretical excitation probabilities of these states by electron impact. All these attempts have failed. Approximate calculations of the natural lifetime of the 2s2p5 state as the result of auto-ionization have been carried out by Kreiliger and by Kiang, Ma, and Wu. They have found a natural lifetime of the order 10^{-7}-10^{-8} second.

It was pointed out by Kiang, Ma, and Wu that the failure to observe the spectrum of doubly excited helium may be understood on the basis of the theoretical great natural width of these states, since the spreading of a 1 line over a spectral region of the order 100-1000 angstroms renders its observation exceedingly difficult; it was pointed out, however, by these authors that on accepting this theoretical probability of auto-ionization and on assuming the probabilities for

the other doubly excited states to be of the same order of magnitude, one would expect a width of
the order 1 angstrom for the lines X320.4 and X337.5 whereas the observed lines appear to be as
sharp as the ordinary lines of He I I. The situation
is hence an unsatisfactory one. Either the calcu-
lated probability of auto-ionization for 2s3P is
grossly in error and the assumption that all the
doubly excited states have about the same
life-
time is not justified, or an explanation of the
X320.4 and X337.5 lines must be sought elsewhere.
The purpose of the present study is to make more
calculations for a few doubly excited states of
helium and to discuss the possible identification
of the X320.4 and X337.5 lines.

PROBABILITY OF AUTO-IONIZATION

The general theory of the process of auto-ioni-
zation is a well-known one. Let $\psi_i, \psi_f$ be the wave
functions of the initial (a doubly excited atom,
for example) and the final (an ion plus an ejected
electron) state. The probability of auto-ioniza-
tion is then

$$P = \int_0^\infty |\psi_f|^2 \psi_i \, dr,$$

where the integration is taken over the coordi-
nates of all the electrons. For a triplet or a singlet
state, we have, respectively,

$$\psi_f = \psi_{2P},$$

$$\psi_f = \psi_{2S},$$

and

$$\psi_i = \psi_{2P} \left( \frac{Z}{r} \right)^{1/2},$$

$$\psi_i = \psi_{2S} \left( \frac{Z}{r} \right)^{1/2},$$

where $\psi_{2P}, \psi_{2S}$ are the discrete atomic wave
functions and $\psi_{2P}$ is the continuous wave function of the ejected electron. Kreisler employed for $\psi_{2S}$

$$\psi_{2S} = \frac{1}{\sqrt{2}} \left( \psi_1(1) \psi_2(2) + \psi_1(2) \psi_2(1) \right),$$

and $\psi_{2P}$ is the solution of

$$\left[ \Delta + \frac{Z^2}{r^2} - \frac{Z}{r} \right] \psi = 0,$$

where energy is in units of the ionization energy
of hydrogen and $\Delta$ is the effective nuclear charge. Substitution of (3) into

$$\left[ \Delta + \frac{Z^2}{r^2} - \frac{Z}{r} \right] \psi_{2P} = 0,$$

and making use of (6) give the integro-
differential equation

$$\left[ \Delta + \frac{Z^2}{r^2} - \frac{Z}{r} \right] \psi_{2P} = E \psi_{2P},$$

where $E$ is the energy of the final state.
in which
\[ V(r,s) = 2 \int_{r,s} \left( \frac{1}{r,s} - \frac{Z^2}{r,s} \right) \psi(r,s) \psi^*(r,s) dr ds \quad (8) \]
and
\[ U(r,s) = 2 \int_{r,s} \frac{1}{r,s} \psi(r,s) \psi^*(r,s) dr ds \]
\[ - (k^2 - E_0) \int \psi^2(r,s) dr ds \quad (9) \]

\( k^2 \) is the kinetic energy of the ejected electron so that \( E = E_0 + k^2 \), \( V \) is the energy of the ejected electron in the atomic field and \( U(r,s) \) represents the effect of exchange. The subscript \( j \) is the azimuthal quantum number of the ejected electron. For a given initial state \( \psi_j (n_j, l_j, m_j, l, s) \) and a given \( \psi_j (n_j, l_j, m_j, l, s) \), the value of \( U \) is determined by the following rule for the non-vanishing of the matrix element \( \psi_j \) and is the presence of auto-ionization: (i) the states \( J \) and \( L \) must be of the same parity, (ii) have the same value of \( J \), and in the case of \( L,S \) coupling. (iii) have the same values of \( L, \Sigma, S \). To obtain the solution of (7), since the effect of exchange is expected to be small, we shall, as an initial approximation, obtain the solution of the homogeneous equation
\[ [\Delta + k^2 - V(r)] \psi_{(0)} = 0 \quad (10) \]
by numerical integration. The solution \( \psi_{(0)} \), so obtained is substituted into (9) and Eq. (7) is solved again by numerical integration. If the solution \( \psi_{(0)} \), so obtained differs considerably from the initial \( \psi_{(0)} \), Eq. (7) is solved again by using \( \psi_{(0)} \) in \( U(r,s) \). The process is repeated until the ith solution \( \psi_{(i)} \) of (7) gives a value for \( V_{ij} \) differing by less than 20 percent from the one obtained with the previous solution \( \psi_{(i-1)} \). It is found that the successive approximations oscillate about and converge upon the final solution very rapidly.

For the discrete wave functions, the simple variational wave functions of the earlier work are employed. The continuous wave function is normalized according to (4) where \( \cos (\lambda \theta - \alpha) \) is the asymptotic form of \( \psi_{(0)} \).

As an example, the equation for the radial part of the continuous wave function for the auto-ionization of \( 2s2p^3P \) is
\[ \frac{d^2}{dr^2} \psi_{(0)} + \left[ 2 - 4/4 - 1/4 \right] \psi_{(0)} = 0 \]
and
\[ U_{(0)} = \frac{1}{r^2} \int \psi_{(0)} \psi_{(0)}^* dr ds \]
\[ - (k^2 - E_0) \int \psi_{(0)}^2 dr ds \]

The probabilities of auto-ionization of a few states of doubly excited helium calculated in this manner are given in Table I.

Concerning the magnitude of the probability of auto-ionization in general, we may set the magnitude of the probability of auto-ionization of \( 3sP^3P \) given in Table I.

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tion of the variational principle to the determination of the parameter c leads to the secular equation for the energy of the system. For our purpose, we shall evaluate the integrals involved in the theory by means of the variational wave functions of \( \psi_u \) and \( \psi_v \) instead of Wilson's self-consistent field solutions. Since the energy correction given by Stevenson's method is small in an \( \alpha \) case, this procedure is completely justified.

Using the notation of Stevenson, and with \( \psi_3 \sim e^{-\gamma r} \) where \( \gamma = 0.836 \), we find

\[
H_{01} = \gamma \psi_3^2 \quad H_{11} = 4\gamma \psi_3 \quad \Delta E = -0.0091 \text{ Rh.}
\]

Thus the corrected energy of \( 2p^2 {^2}P \) is \(-1.4018 \) -0.0091 \text{ Rh.} With this value, the calculated frequency of the line \( 1s2p^2 {^2}P \rightarrow 2p^2 {^2}P \) is 313.348 cm\(^{-1}\) which differs by 0.4 percent from the observed 312.348 cm\(^{-1}\) for the line \( X^1 \Sigma^+ \rightarrow X^1 \Pi \). Hence it appears that, unless the calculated energies of the doubly excited states and the probabilities of auto-ionization are seriously in error, the line \( \lambda 357.5 \) cannot be satisfactorily explained.

**Satellite Lines in C V and C VI Observed by Edlen**

Edlen and Tyrén observed groups of weak lines on the long wave-length side of the lines \( 1s^2 \Sigma \rightarrow 1s2p^2 {^2}P, 1s^2 \Sigma \rightarrow 2p^2 {^2}P \) in C V and C VI, respectively. They found that these transitions are accompanied by satellite lines with such transitions on the basis of the energies of such doubly excited states calculated by the variational method. Most of these doubly excited states are capable of auto-ionization and accordingly the satellite lines should show some broadening. If, however, the probabilities of auto-ionization of such states as \( 1p^2 {^4}P \rightarrow 2p^2 {^2}D \) are of the same general order of magnitude as in He, namely, \( 10^{-4} - 10^{-5} \) per second, the width of these lines in the region of 40 \text{ A} would be 0.001 - 0.01 \text{ A}, which is not hopelessly inconsistent with observation, in distinction to the case of the \( \lambda 357.5 \) line of He.

**References**


T. Y. Wu, Phys. Rev. 58, 1114 (1940).