Shift and width of the Balmer-α and Lyman-β lines of neutral hydrogen due to electron collisions

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The contribution from electron scattering to the width and shift of the H_α and Ly_β lines of neutral hydrogen is evaluated. Elements of the S matrix for electron-atom scattering calculations are obtained from close-coupling calculations including pseudostates, either of the variational or the optical potential type. The convergence of sums over angular-momentum variables is discussed. Results are compared with some other calculations and with experiment where possible.

I. INTRODUCTION

In this paper, we report the calculation of the contributions to the shift in position and to the width of the H_α and Ly_β lines of neutral hydrogen in a plasma which result from the scattering of electrons by a radiating atom. Our calculations are fully quantum mechanical. The scattering matrices are obtained from close-coupling calculations of electron-hydrogen atom scattering, as will be described below.

The present work is the third in a series: the first considered the electron-scattering contribution to the shift and width of certain lines of He^+ [1]; the second was concerned with the Ly_α line of neutral hydrogen [2]. The case of Ly_α was singled out because we were able to use the method of Seaton [3], in which analytic solutions to the three-state close-coupling scattering problem can be found for large electron-atom separations, to prove certain results about the convergence of angular-momentum sums. This topic will be discussed below in the present case. Here we consider the electron contribution to the shifts and widths of the lowest-energy Balmer line (denoted H_α henceforth), and the second line of the Lyman series (Ly_β). These lines result from the $n=3\rightarrow n=2$ and the $3p\rightarrow 1s$ transitions, respectively. We do not consider higher members of these series because our methods do not yet permit an accurate treatment of electron-hydrogen atom scattering in states of $n=4$ and higher.

The calculation of the profiles of the spectral lines of hydrogen and hydrogenic ions has been considered by many authors, with reviews by Griem [4] and Peach [5]. A recent comprehensive discussion has been given by Seaton [6], with emphasis on opacity calculations. In Seaton's work, the line profile function $\phi(\omega-\omega_0)$ [ω_0 is the center of the line] is a convolution of contributions due to electron scattering from the radiating atom and Stark broadening due to local fields of ions. The ions are treated as static; contributions to the profile due to ionic motions, which can be significant near the center of the line, are ignored. In addition, Seaton does not consider an effect we shall calculate here; the shift of the center of the spectral line away from the frequency which would be found in empty space, due to electron scattering from radiating atoms.

We shall not perform the convolution here. Our calculation is restricted to the electron-scattering contribution only, and is based on the impact approximation [7]. This leads to a profile which is Lorentzian, characterized by a width w and shift d which are given by an expression [Eq. (1), below] involving elements of the S matrices describing the scattering. Our objective is to evaluate the width and shift as precisely as possible, using the most accurate available results from scattering calculations.

Lines of hydrogen and hydrogenic ions in plasmas are typically quite broad and Seaton's method in effect allows the width parameter w to depend on frequency. It is not possible for us to include this effect, which would involve the evaluation of an integral in which multichannel wave functions involving scattering at different energies are coupled by a dipole operator, and Seaton's attack on this problem is based on the Bethe approximation which is applicable only for very large angular momenta.

We note that van Regemorter and collaborators have used an analytic solution of the three-state close-coupling equations [3] valid for large angular momenta to study the profile of Ly_α [8]. Their approach will not, however, give correct results for the line shift, which requires an accurate description of the scattering for small as well as large values of the total angular momentum.

We shall see below that the linewidth due to electron scattering is quite substantial. It is believed to dominate the profile in the line wings, owing to the fact that its contribution decays as $(\omega-\omega_0)^{-2}$ while the contributions due to local fields behave as $(\omega-\omega_0)^{-5/2}$ [6]. However, the overall profile is not Lorentzian.

The linear Stark splitting of hydrogenic lines is symmetric in energy. Consequently the random fields of static ions do not produce a shift of the position. Electron scattering is believed to make the most important contribution to the line shift, and we focus our effort on making a reliable determination of this. There are other effects which may also contribute to the shift, such as the second-order Stark effect (which also would tend to make the profile asymmetric), ion motion [9], and the interaction of a quadrupole moment on the radiating atom with a local electric field gradient [10,11]. We will not evaluate these effects here, but our discussion of the results will

consider published estimates of such contributions.

The remainder of the paper is organized as follows. The procedures of our calculation are described in Sec. II. Our numerical results are presented and discussed in Sec. III. They are compared with other calculations and with experiments, where possible. A brief summary is given in Sec. IV.

II. COMPUTATION METHOD

Consider a transition connecting an initial state a of a radiating atom with a final state b. Spin-orbit coupling is neglected. The half width w of the line, and shift d, relative to the energy of the same transition in the absence of all perturbers, is given in Rydberg units by [12–14]

$$w+id=(N_e a_0^3)2\sqrt{\pi}(k_B T)^{-1/2}(2s_a+1)^{-1/2}\sum_{\substack{S,L,L',\\ l,l'}}(2S+1)(2L+1)(2L'+1)\begin{Bmatrix} L_a & L & l \\ L' & L_b & 1\end{Bmatrix}\begin{Bmatrix} L_a & L & l' \\ L' & L_b & 1\end{Bmatrix}$$
$$\times\int_0^\infty e^{-\varepsilon/k_B t}[\delta_{ll'}-S_a(E,S,L,l,l')S_b^*(E',S,L',l,l')]d(\varepsilon/k_B T)\ . \quad (1)$$

In this equation N_e is the electron density, a_0 is the Bohr radius, and T is the plasma temperature (with $k_B T$ in Rydbergs). The quantities L_a and L_b are the orbital angular momenta of the atomic states, s_a is the spin of the initial state, L and L' are the total angular momenta of the system of atom plus scattering electron in the initial and final states with l and l' the corresponding angular momenta of the free electron, while S is the total spin.

The S matrices S_a and S_b are to be calculated for fixed a kinetic energy ε of the free electron. If E_a and E_b are the energies of the atomic states, then the total energies of the system of atom plus free electron E and E' are given by

$$E=\varepsilon+E_a,\ E'=\varepsilon+E_b\ .$$

Equation (1) applies to transitions between individual levels. In fact, H_α contains three components ($3s-2p$, $3p\rightarrow 2s$, and $3d\rightarrow 2p$) which are exactly degenerate for an isolated atom in a nonrelativistic theory. The interaction with the plasma electrons breaks this degeneracy by amounts which are (at a density of 10^{17} cm^{-3} and a temperature of 1.0 eV) roughly comparable to the fine-structure splitting of the $n=3$ state. Because the spectral lines are quite broad, this splitting is not observed in experiments. Although we give splittings for the components separately, the experimentally relevant quantity would be an intensity weighted average splitting. This is, to an excellent approximation, equal to the result for the $3d\rightarrow 2p$ transition.

The S-matrix elements were obtained from the most accurate scattering information available. Three energy ranges are defined in terms of the total energy E_T(in Ry) of the system of atom plus scattering electron.

(i) $-1\le E_T<-\frac{1}{4}$. In this range only the $1s$ channel is open, and the S matrix was constructed from essentially exact phase shifts with are available in the literature [15].

(ii) $-\frac{1}{4}\le E_T\le-\frac{1}{16}$. This range extends from the $n=2$ threshold to the $n=4$ threshold. It is an extremely important range for the calculations, which consider relatively low plasma temperatures, both because of the Maxwell distribution of electron energies, and because the scattering is strong and energy dependent. In this range, we used results of variational calculations with a large basis of atomic states and pseudostates (all exact atomic states through $n=4$, plus eighteen pseudostates) [16]. However, resonance structure in this region was not included because an extremely fine grid of energies would be required. Scattering matrices for total angular momenta in the range $4\le L\le 14$ were obtained using six-state close coupling.

(iii) $E_T>-\frac{1}{4}$. Results in this region were primarily obtained from a close-coupling plus optical potential calculation using methods described previously [17,18]. The calculations involve an 18-state basis, the lowest six of which ($1s,2s,3s,2p,3p,3d$) are explicitly included in the close-coupling calculation, while the remaining 12 states are used to construct a complex, energy-dependent, nonlocal optical potential. However, for total energies close to the ionization threshold ($E_T=-0.03$ and 0.03) the optical potential was not included because of apparent numerical instabilities. Calculations were carried out through $L=14$ close to threshold, and out to increasingly larger values of L ($L=48$ generally) for higher energies. An extrapolation procedure used for still higher L is discussed below.

There are two computational problems in this calculation. The easier one results from the thermal average in Eq. (1). One has to evaluate the scattering matrices at enough energies to permit a reasonably accurate evaluation of the integral. The integral involves electron kinetic energies. Relatively low plasma temperatures imply low kinetic energies. We calculated scattering matrices for incident energies relative to the $1s$ state of 0.77, 0.81, 0.85, 0,91, 0.97, 1.03, 1.10, 1.44, 1.96 2.25, 2.57, and 4.00 Ry. Phase shifts for lower incident energies were obtained from the literature as mentioned above. The S-matrix elements were fitted by two polynomials in momentum, one at low energies and the other at high energies.

The most serious problem concerns the convergence of the angular-momentum sums in Eq. (1). We reported a detailed analysis of this problem for the $2p-1s$ (Ly_α)

transition in Ref. [2].

Let us denote the contributions of a partial wave of angular momentum L in Eq. (1) be w_L and d_L, i.e.,

$$w+id=\sum_L (w_L+id_L) \ . \tag{2a}$$

Then we showed for Ly_α that for L sufficiently large

$$w_L \approx c_1/L \ , \tag{2b}$$

$$d_L \approx c_2/L^2 \ , \tag{2c}$$

where c_1 and c_2 are independent of L but depend on electron temperature. The L^{-1} dependence of W_L indicates that the sum over L must be cut off at some $L_{\max}$. The resulting w will depend logarithmically on $L_{\max}$. We have taken for $L_{\max}$ a value obtained from Debye screening:

$$L_{\max}=m^{1/2}k_BT/(2\pi\hbar^2N_e e^2)^{1/2} \ . \tag{3}$$

The value of $L_{\max}$ relevant to these calculations ranges from $L_{\max}\approx 19$ at a density of 10^{18} cm^{-3} and a temperature of 0.5 eV to 1520 for a density of 10^{16} cm^{-3} and a temperature of 4.0 eV.

An analysis of the angular-momentum dependence of S-matrix elements relating to lines originating from $n=3$ levels has not been reported. Here, we simply assume that Eqs. (2b) and (2c) are applicable. Then the shifts are only weakly dependent on $L_{\max}$, and from Eq. (1)

$$d \approx N_e d_0(T) \ , \tag{4}$$

where d_0 depends on electron temperature only. Converged values of d_0 are readily evaluated by the techniques described above. The shift d is given for $N_3=10^{17}$ cm^{-3} in Table I.

In contrast, the calculation of w frequently requires consideration of angular momenta much larger than those for which it is convenient to perform close-coupling calculations. In the case of Ly_α, our analysis yielded an explicit result for the coefficient c_1 in Eq. (2b). That is not available in the present case, and a numerical extrapolation procedure is needed. We fit the S-matrix elements $S_{ll'}$ which contribute according to

$$L^2(S_{ll'}-\delta_{ll'})=A_{ll'}+B_{ll'}/L \ , \tag{5}$$

TABLE I. Line shifts d (in Å) are given as functions of plasma temperature (in eV) for an electron density of $N_e=10^{17}$ cm^{-3}.

	d (Å)			
T (eV)	$3s$-$2p$	$3d$-$2p$	$3p$-$2s$	$3p$-$1s$
0.5	0.540	0.692	0.584	0.0143
1.0	0.522	0.414	0.476	0.0116
2.0	0.497	0.262	0.398	0.0097
3.0	0.486	0.228	0.375	0.0091
4.0	0.480	0.221	0.370	0.0090

in which L is the total angular momentum. The quantities $A_{ll'}$ and $B_{ll'}$ are complex and depend on energy. Terms of higher order in L^{-1} are ignored. However, for scattering from the $1s$ state, $A_{ll'}=0$.

Figure 1 shows the cumulative contributions to d and w for the $3d$-$2p$ component of H_α as a function of the maximum value of the total angular momentum included in the sum L_M. The graph refers to a density of 10^{17} cm^{-3} and a plasma temperature of 1 eV. In this case $L_{\max}$ [Eq. (3)] is 120 (off scale). We see that d converges with increasing L, as it should. A substantial portion of d comes from small and moderate values of L; the contribution from $L\leq 10$ is 50% of the final value and that from $L\leq 20$ is 77% of this total. In contrast, w continues to increase. The portion coming from $L\leq 10$ is 30% of that of $L_{\max}$, and for $L\leq 20$ the fraction is 49%, so that the small L contribution, while significant, is not as important for w as for d. It should be pointed out that these results are consistent with those obtained for He^+ in Ref. [1].

The discussion above concerning Eqs. (2) and (3) suggests that w can be expressed with reasonable accuracy as

$$w=N_e w_0(N_e,T) \ , \tag{6a}$$

where

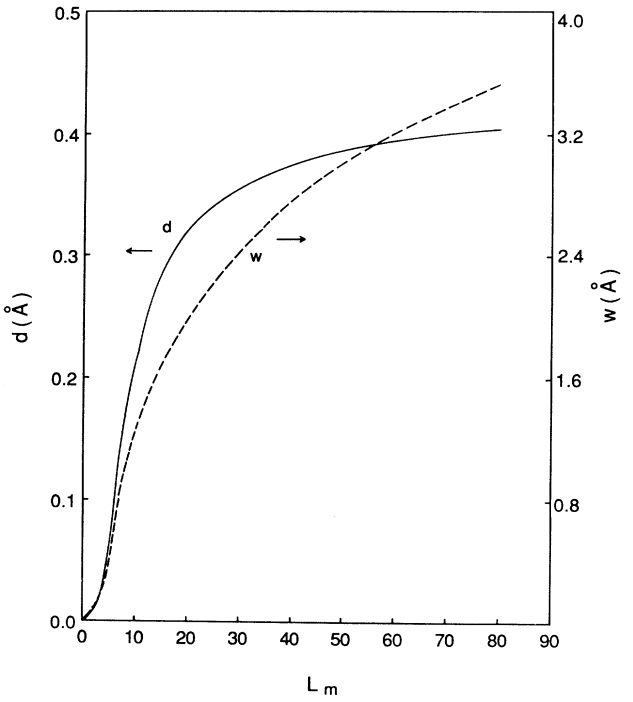

FIG. 1. The shift (left scale) and width (right scale) of the $3d$-$2p$ component of H_α is shown as a function of the maximum value of L included in the sum. The calculation refers to an electron density of 10^{17} cm^{-3} and a plasma temperature of 1 eV.

TABLE II. Parameters a and b appearing in the least-squares fit to the linewidth w [see Eqs. (6a) and (6b)]. Units are angstroms.

	$3s$-$2p$		$3d$-$2p$		$3p \rightarrow 2s$		$3p \rightarrow 1s$	
T (eV)	a	b	a	b	a	b	a	b
0.5	12.09	−6.63	4.65	−1.89	9.18	−4.68	0.224	−0.1146
1.0	11.48	−4.93	4.04	−1.34	8.55	−3.44	0.208	−0.0838
2.0	10.22	−3.55	3.38	−0.905	7.42	−2.40	0.181	−0.0585
3.0	9.31	−2.89	3.00	−0.713	6.63	−1.90	0.162	−0.0466
4.0	8.65	−2.49	2.75	−0.599	6.09	−1.62	0.149	−0.0394

$$N_0 w_0(N_e T) = a(T) + b(T)\log_{10}\left[\frac{N_e}{N_0}\right], \tag{6b}$$

in which the coefficients $a(T)$ and $b(T)$ depend only weakly on density, and the reference density N_0 is taken as 10^{17} cm^{-3}. We have used Eqs. (6a) and (6b) to make a least-squares fit to our calculated values of w in which the possible density dependence of a and b is ignored. These coefficients are assumed to be independent of temperature. Their values are listed in Table II. The fit was made to calculated values covering the range of densities from 10^{16} to 10^{18} cm^{-3}. The fit is reasonably good, with errors of 1% or less for $T \geq 1.0$ eV. At $T=0.5$ eV, the maximum error which occurs for $N_e = 10^{18}$ cm^{-3} is about 5%, apparently due to the low value of $L_{\max}(\sim 19)$ for this temperature and density.

For low densities or high temperatures, the extrapolated d sometimes decreases with increasing L when L is very large. We believe this is an artifact of the numerical extrapolation. The values of d we quote below ignore this behavior.

III. DISCUSSION OF RESULTS

Figure 2 shows the calculated line shifts for the components of H_α at a density of 10^{17} cm^{-3} and temperatures from 0.5 to 4 eV. Numerical values are contained in Table I. The shifts decrease rapidly with increasing temperature in the lower part of the range, but are nearly constant in the upper part. The width parameter for the same transition is shown in Fig. 3. Numerical values for the fitting parameters a and b in Eq. (6b) are given in Table II. It should be noted that the quantity a is the electron contribution to the width at the reference density of 10^{17} cm^{-3}.

It will be immediately observed that the widths are roughly 10–20 times larger than the shifts. This fact, combined with the existence of large contributions from local electric fields to the line profile, makes the shifts difficult to measure experimentally. Corresponding results for the $3p \rightarrow 1s$ transition (Ly_β) are shown in Figs. 4 and 5. Again, the ratio of width to shift is in the range 15–20. Although the numerical values of the widths and shifts for H_α and Ly_β are very different when expressed in angstroms, they are quite comparable (especially $3p$-$2s$ with Ly_β) in energy units. This occurs because the dominant scattering is in the initial ($n=3$) state.

As pointed out previously, our calculated widths are not to be compared directly with experiment except in regard to orders of magnitude. The following discussion concerns line shifts.

First it must be emphasized that all calculated shifts are to the red. Second, the shifts are linear functions of density in the range of interest (this agrees with experiment [19]). Third, the shifts depend significantly on electron temperature, with the most rapid variation occurring at lower temperatures. It is not possible to make a meaningful comparison with experiment unless the electron temperature is specified. Unfortunately, many experimental papers do not report the temperature. The strong temperature dependence of the shifts is a consequence of the energy dependence of electron-atom scattering in hydrogen. This is a more significant effect in hydrogen than in He^+, and probably can be attributed to the large, energy-dependent polarizability of the $n=3$ atomic states.

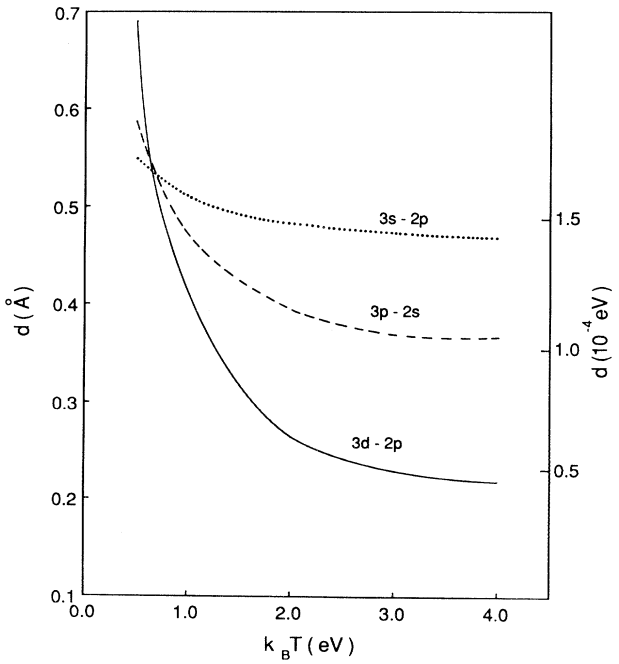

FIG. 2. Line shift d for the components of H_α. The left scale gives the shift in Å; the right, in units of 10^{-4} eV. The electron density is 10^{17} cm^{-3}.

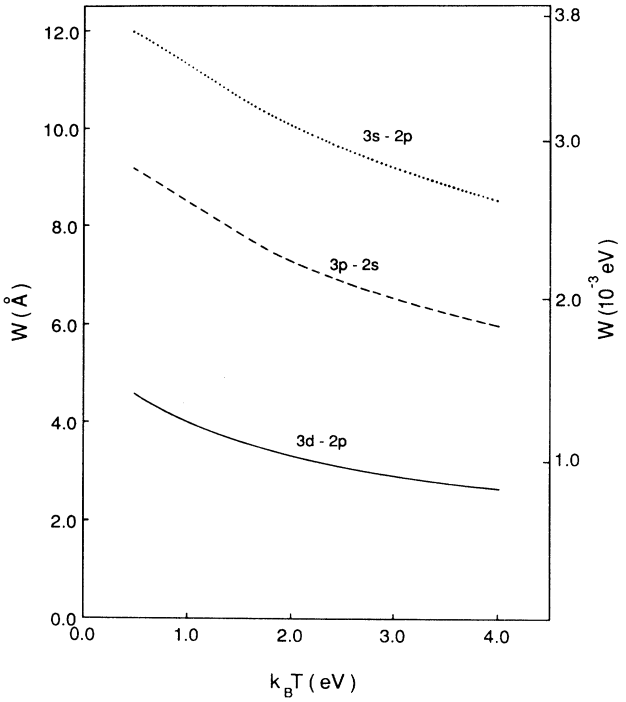

FIG. 3. Electron contribution to the linewidth for the components of H_α. The electron density is 10^{17} cm^{-3}.

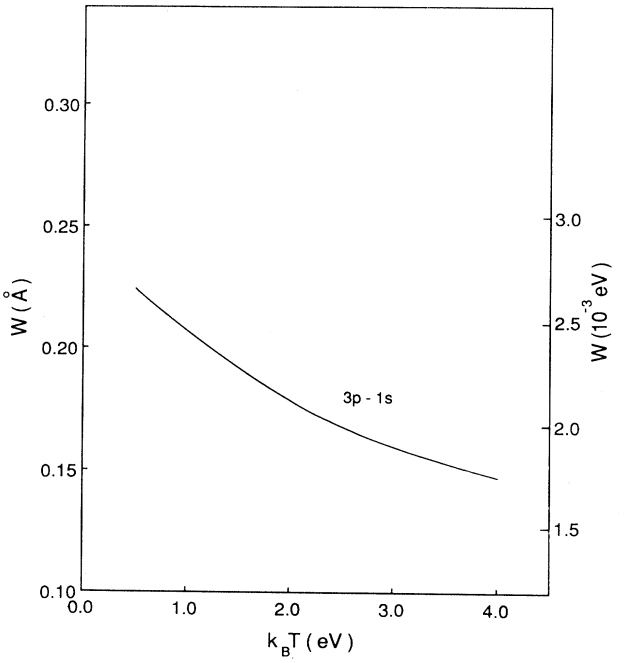

FIG. 5. Electron contribution to the linewidth of Ly$_\beta$ for a plasma density of 10^{17} cm^{-3}. Note that the vertical scale does not start at zero.

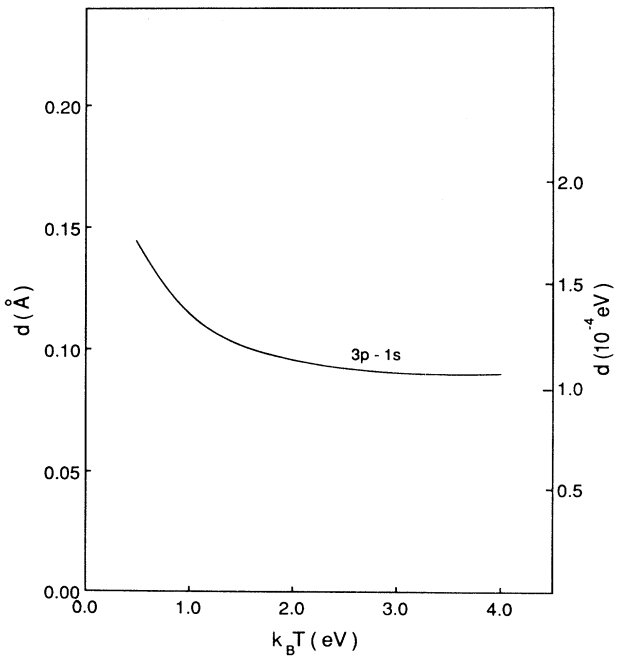

FIG. 4. Line shift d for the $3p \rightarrow 1s$ transition (Ly$_\beta$) for a plasma density of 10^{17} cm^{-3}.

The shifts of Ly$_\beta$ and H_α (also many other lines) have been calculated recently by Griem [11]. He considers the total (observable) line shift to be primarily the sum of a positive (red) contribution due to electron scattering and a considerably smaller negative (blue) shift due to interactions of the radiating atom with quadrupole fields of neighboring atoms. This correction leads to about a 15% reduction of the electron contribution in the case of H_α. He finds smaller blue-shift contributions due to the quadratic Stark effect and other causes at the 5% level for H_α. We have not included quadrupole interactions and the other effects in our calculations.

Our calculated electron contribution tends to be somewhat smaller than that obtained by Griem. Our value, obtained for the $3d$-$2p$ transition which dominates the H_α line, is about 72% of his result at a temperature of 1.3×10^4 K. Further, our calculated shift is a decreasing function of temperature, whereas his increases. Our result for a temperature of 1.9×10^4 K is only about 50% of his value.

The experimental situation in regard to the shift of H_α is complicated, with conflicting results being reported by different groups. Griem [11] has tabulated results from several measurements. We will discuss only two of these here. Kelleher, Konjevic, and Wiese [20] obtained for H_α

$$d\ (\text{Å}) = (0.43 \pm 0.05) \times 10^{-17} N_e\ ,$$

where N_e is in units of cm^{-3}.

The temperature is not specified in Griem's paper.

Griem gives the temperature of the measurement as 1.3×10^4 K. Our result (electron contribution only) at this temperature is $0.39\times10^{-17}N_e$. Vitel [19] obtained

$$d\ (\text{Å})=0.31\times10^{-17}N_e$$

(uncertainty not specified) at a temperature of 1.9×10^4 K. Our result at this temperature is $0.29\times10^{-17}N_e$.

It is to be noted that our results are in rather good agreement with these experiments without the inclusion of ion quadrupole interactions or other contributions. If those corrections are included (using the values given by Griem) our calculated shifts are reduced to 0.27 and $0.17\times10^{-17}N_e$, respectively. Such results would be substantially below experiment.

Clearly, further investigation is required. From the point of view of our calculations, the most important improvement would be the inclusion of $n=4$ states explicitly in the close-coupling basis. This is expected to increase the phase shifts for elastic scattering in the $n=3$ states, and so probably would increase the magnitude of the shift.

Considerably less experimental information is available for Ly_β than for H_α. Griem [11] quotes a value obtained from the work of Grützmacher and Wende [21],

$$d=0.005\ \text{Å}\ ,$$

normalized to $N_e=10^{17}$ cm^{-3}, at a temperature of 1.6×10^4 K. Our result for this density and temperature is $d=0.010$ Å. Inclusion of the quadrupole and other effects as calculated by Griem would reduce this to about 0.007 Å, larger than the value reported above. Griem obtains a value of 0.013 Å for this width [11].

IV. CONCLUSIONS

We have calculated the electron-scattering contribution to the shift and width of the H_α and Ly_β lines of neutral hydrogen. The calculation was made using the most accurate information available concerning electron scattering by neutral hydrogen. We cover a range of electron densities $10^{16}<N_e<10^{18}$ (in cm^{-3}) and temperatures $0.5<T<4.0$ (in eV). The widths cannot be compared directly with experiment because we have not included other important contributions to the line profile; but the shift (of H_α) appears to be in fairly good agreement with experiment. However, other contributions we do not include might act to reduce the shift below the experimental values.

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