Shift and width of the Lyman-α line of neutral hydrogen due to electron collisions

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The convergence of the quantum-mechanical (impact-theory) partial-wave series for the shift d and width w of the Lyman-α line due to electron collisions in a plasma is studied. Asymptotically exact expressions for the relevant S-matrix elements are derived, and it is shown that the series for d converges, whereas w diverges logarithmically as in semiclassical theories. The conclusions are verified by numerical calculations. Some numerical results are reported for plasmas with temperatures in the range 1–5 eV and densities 2×10^{17} and 4×10^{17} cm^{-3}.

I. INTRODUCTION

This paper is concerned with the shift and width of the Ly_α line ($2p\rightarrow1s$) of neutral hydrogen in a plasma produced by electron collisions with radiating atoms. It must be said at the outset that electron collisions are only one of many possible contributions to the shift and width: in the case of the shift, their contribution is probably the dominant one; but not so for the width, for which the electron collision contribution is not the largest (local electron fields are more important). However, we will not consider other contributions here. Our discussion of electron collisions is based on the so-called impact theory[1–3] which leads to a specific formula for the shift and width (below, Sec. II) which is quite difficult to evaluate correctly. We will not be concerned here with questions as to whether there are, in nature, important contributions to the shift that are not described by the impact theory. Our interest is directed toward the question of the convergence of the required sums over angular momentum variables.

We became aware of this problem in the course of a calculation of the shifts and widths of the Ly_α, Ly_β, and H_α lines of He^+, in which it became apparent that the S-matrix elements describing scattering on the excited (upper) states were required for large angular momenta, beyond the range for which results are normally available from existing programs for close-coupling scattering calculations. We developed an extrapolation procedure to determine these contributions. Persistent questions prompted us to look closely at the question of convergence of these sums. In the course of this, we observed that the expression for the shift and width of $p\rightarrow s$ transitions could be simplified into a form that was fairly easy to understand. In addition, we were able to obtain the relevant S-matrix elements analytically for large angular momenta including all coupling effects for the case of Ly_α in neutral hydrogen. This analysis is of some interest as one of the few analytically solvable problems in multichannel scattering theory, and is reported below. We show in this case that the electron-scattering contribution to the width is logarithmically "divergent," while the shift converges. We think it is plausible, primarily on the basis of numerical evidence, that this is also the result for the transitions other than Ly_α in He^+ (and for their counterparts in neutral hydrogen) that prompted this study, but we do not have formal proof.

The use of the words "divergent" and "convergent" in the present context requires some elaboration. We mean, explicitly, that the expression for the width involves a sum over angular momenta of the form $\sum_L 1/L$ that would be infinite if extended to infinite L and, if cut off at some finite upper limit, would depend logarithmically on the cutoff. No such term is present in the expression for the shift. The leading large-L contributions fall off at least as rapidly as L^{-2}. In nature, an infinite width does not occur. Contributions from very large angular momenta are cut off by properties of the plasma environment; one particular source of such a cutoff is the Debye screening of long-range potentials in the plasma. We report below numerical values for the shift and width when this effect is used to define a maximum angular momentum. Related problems occur in the more commonly employed semiclassical theory.

This paper is organized as follows. In Sec. II we specialize the general formula for the shift and width to the case of p-to-s transitions and then describe the calculation of the S matrices for large angular momenta. Section III contains numerical results for a few temperatures and densities, plus some discussion of the results and comparison with other theoretical approaches.

II. THEORY

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[4–6]

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

In this equation N_e is the electron density, a_0 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 intial 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 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

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

Equation (1) is quite complicated. If, however, one of the atomic states involved (we choose it to be the final one) is an S state ($L_b=0$), and the initial state is P ($L_a=1$) a simple expression for the $6-j$ symbols enables us to reduce Eq. (1) to

$$w+id=\frac{1}{3}\left[\frac{\pi}{k_B T}\right]^{1/2}(N_e a_0^3)\int_0^\infty e^{-\varepsilon/k_B T}\sum_S\sum_L\left[(2L+1)\sum_l[1-S_a(E,S,L,l,l)S_b^*(E',S,L,l,l)]\right]d(\varepsilon/k_B T)\ . \quad (2)$$

Furthermore, for a given value of L, ($L>0$) l can only take the values $L-1$, L, and $L+1$.

It is apparent from Eq. (2) that in order for the sum over L to yield a finite result in the absence of a cutoff, the quantity in large parentheses must decrease with L, when L is large, faster than $1/L$. We therefore begin by investigating the large-L behavior of the S-matrix elements.

A. Asymptotic S-matrix elements

To study the convergence of the series in Eq. (2) it is only necessary to evaluate the sum in square brackets through order $1/L^2$ for large L. For elastic scattering from $1s$, the polarization potential dominates at large L, so that

$$S_b\sim 1+O(L^{-3})\ , \quad (3)$$

and therefore we only need the aymptotic form of S_a. This is essentially governed by the strong coupling between the degenerate $2s$ and $2p$ states, which can be dealt with by an extension of Seaton's method.[7] This approach has previously been applied to calculations of the profile of Ly_α by van Regemorter and collaborators[8] and by Baryshnikov and Lisitsa.[9] There are three channels of parity $(-1)^L$, and one with parity $(-1)^{L+1}$, which is not coupled to the others and may be considered independently. Following Seaton,[7] we label the three coupled channels by $\nu=1,2,3$ corresponding to the atomic state and projectile angular momentum combinations $(2s,L)$, $(2p,L-1)$, and $(2p,L+1)$, respectively. Keeping all the long-range potentials[7] and neglecting exchange, the coupled differential equations for the radial functions may be written as

$$r^2\left[\frac{d^2}{dr^2}+k^2\right]\mathbf{F}=(\mathbf{A}+\mathbf{B}/r)\mathbf{F}\ , \quad (4)$$

where k^2 is the incident energy (Ry) with respect to $n=2$, and the matrices $\mathbf{A}$ and $\mathbf{B}$ are given by

$$\mathbf{A}=\begin{bmatrix} L(L+1) & L^{1/2}\beta & -(L+1)^{1/2}\beta \\ L^{1/2}\beta & L(L-1) & 0 \\ -(L+1)^{1/2}\beta & 0 & (L+1)(L+2)\end{bmatrix}, \quad (5)$$

$$\mathbf{B}=\begin{bmatrix} 0 & 0 & 0 \\ 0 & \dfrac{12(L-1)}{2L+1} & -[L(L+1)]^{1/2}\beta^2 \\ 0 & -[L(L+1)]^{1/2}\beta^2 & \dfrac{12(L+2)}{2L+1}\end{bmatrix}, \quad (6)$$

with $\beta=6/(2L+1)$. As in Seaton,[7] we first diagonalize $\mathbf{A}$. Let $\mathbf{A}\,\mathbf{X}=\mathbf{X}\,\mathbf{a}$, where $\mathbf{X}$ is unitary and $\mathbf{a}$ diagonal. Equation (4) may then be written as

$$\left[\frac{d^2}{dr^2}+k^2-\frac{\mathbf{a}}{r^2}\right]\mathbf{G}=\frac{\mathbf{X}^\dagger\mathbf{B}\,\mathbf{X}}{r^3}\mathbf{G}\ , \quad (7)$$

where $\mathbf{G}=\mathbf{X}^\dagger\mathbf{F}$. Neglecting the right-hand side, we get the solutions of Seaton,[7]

$$G_i^0=(-2i)e^{-(i/2)\pi\mu_i}krj_{\mu_i}(kr)\ , \quad (8)$$

with the constants $\mu_i, i=1,2,3$ as given in Seaton.[7] The functions G_i^0 have the asymptotic behavior

$$\mathbf{G}_i^0 \underset{r\to\infty}{\sim} e^{-ikr}\mathbb{1}-e^{ikr}\boldsymbol{\sigma} , \tag{9}$$

where $\sigma=e^{-i\pi\mu}$. The modification induced by the term on the right-hand side of Eq. (7) can be determined, to leading order in L, by using the Born approximation. Defining

$$K_{ij}=-k\int_0^\infty j_{\mu_i}(kr)(X^\dagger BX)_{ij}j_{\mu_j}(kr)\frac{dr}{r} , \tag{10}$$

we may express the modified asymptotic form as

$$\mathbf{G}_i\sim e^{-ikr}\mathbb{1}-e^{ikr}\boldsymbol{\sigma}\boldsymbol{\tau} , \tag{11}$$

where

$$\boldsymbol{\tau}=\frac{1+i\mathbf{K}}{1-i\mathbf{K}} . \tag{12}$$

The required calculations are greatly simplified since, to leading order in L^{-1},

$$\mathbf{X}\sim\begin{bmatrix} 1-\frac{9}{2L^2} & -\frac{3}{\sqrt{2L}}\left[1-\frac{1}{4L}\right] & \frac{-3}{\sqrt{2L}}\left[1-\frac{3}{4L}\right] \\ -\frac{3}{\sqrt{2L}}\left[1-\frac{1}{4L}\right] & -\left[1-\frac{9}{4L^2}\right] & \frac{9}{4L^2} \\ \frac{-3}{\sqrt{2L}}\left[1-\frac{3}{4L}\right] & \frac{9}{4L^2} & -\left[1-\frac{9}{4L^2}\right] \end{bmatrix}=\mathbf{X}^\dagger . \tag{13}$$

The final form of τ to the required order in L^{-1} is

$$\tau\sim\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1-\frac{12ik}{L(2L+1)} & \frac{6ik}{L^2} \\ 0 & \frac{6ik}{L^2} & 1-\frac{12ik}{(L+1)(2L+1)} \end{bmatrix} . \tag{14}$$

Now, the asymptotic form of $\mathbf{F}=\mathbf{X}\,\mathbf{G}$ is, from Eq. (11),

$$\mathbf{F}\sim e^{-ikr}\mathbb{1}-e^{ikr}\mathbf{S}' , \tag{15}$$

where $\mathbf{S}'=\mathbf{X}\boldsymbol{\sigma}\boldsymbol{\tau}\mathbf{X}^\dagger$. The S-matrix elements, defined with respect to $\exp[\pm i(kr-l\pi/2)]$, may be calculated by multiplying $\mathbf{S}'$ with appropriate phase factors. The elements of $\mathbf{T}=\mathbb{1}-\mathbf{X}\boldsymbol{\sigma}\mathbf{X}^\dagger$ are given in Seaton,[7] and have the asymptotic form

$$\mathbf{T}\sim\begin{bmatrix} \frac{18}{L^2} & -\frac{3i\sqrt{2}}{L} & \frac{3i\sqrt{2}}{L} \\ -\frac{3i\sqrt{2}}{L} & \frac{9}{L^2}-\frac{i9\pi}{2L^2} & -\frac{9}{L^2} \\ \frac{3i\sqrt{2}}{L} & -\frac{9}{L^2} & \frac{9}{L^2}+\frac{i9\pi}{2L^2} \end{bmatrix} . \tag{16}$$

The $\mathbf{S}$ matrix in the present case can be calculated from Eqs. (12), (13), and (15), since

$$\mathbf{S}=(\mathbb{1}-\mathbf{T})\mathbf{X}\boldsymbol{\tau}\mathbf{X}^\dagger . \tag{17}$$

From Eqs. (13), (14), (16), and (17), we obtain

$$\mathbf{S}\sim\begin{bmatrix} 1-\frac{18}{L^2} & \frac{3i\sqrt{2}}{L} & \frac{-3i\sqrt{2}}{L} \\ \frac{3i\sqrt{2}}{L} & 1-\frac{9}{L^2}-i\left[\frac{12k}{(2L+1)(L+1)}-\frac{9\pi}{2L^2}\right] & \frac{9}{L^2}+\frac{6ik}{L^2} \\ \frac{-3i\sqrt{2}}{L} & \frac{9}{L^2}+\frac{6ik}{L^2} & 1-\frac{9}{L^2}-i\left[\frac{12k}{(2L+1)L}+\frac{9\pi}{2L^2}\right] \end{bmatrix} . \tag{18}$$

There remains the channel of parity $(-1)^{L+1}$. The long-range potential here is[10] $(-12/r^3)$ and this leads to

$$1-S_{2p}(l=L)\sim-\frac{12ik}{L(L+1)} . \tag{19}$$

B. Contribution to w and d from high partial waves

For large L, the Lth term in Eq. (2) becomes, in view of Eq. (3),

$$w_L+id_L\sim\frac{4}{3}\left[\frac{\pi}{k_BT}\right]^{1/2}(N_ea_0^3)(2L+1) \times\sum_{l=L-1}^{L+1}\int_0^\infty e^{-k^2/k_BT}[1-S_{2p}(l)]d(k^2/k_BT) . \tag{20}$$

On using Eqs. (17)–(19) in Eq. (20), we find

$$w_L\sim48\left[\frac{\pi}{k_BT}\right]^{1/2}(N_ea_0^3)\frac{1}{L} \tag{21}$$

and

$$d_L\sim O(1/L^2) . \tag{22}$$

The convergence of the series for d and the logarithmic divergence of w therefore follow. A more careful calculation retaining higher orders of $(1/L)$ shows that actually $d_L\sim O(1/L^3)$. However, we have neglected the polarization potentials which fall off as r^{-4} in the analytic calculation, and these can lead to an asymptotic form of the same order as Eq. (22).

It is interesting to compare these results with those obtained on the basis of a Born approximation (for the dipole potentials also) calculation of the S matrix. Since the Born K-matrix elements which are given in Ref. 11 are real, the Born approximation for $1-\mathbf{S},-2i\mathbf{K}$, is purely imaginary and therefore contributes nothing to the width. The unitarized Born approximation, obtained from $\mathbf{S}=(1+i\mathbf{K})/(1-i\mathbf{K})$, supplies the missing real parts correctly along the diagonal, but still does not provide the terms $\pm9\pi i/2L^2$ present in Eq. (18). However, since the latter cancel each other in Eq. (20), the unitarized Born approximation does yield the right asymptotic behavior.

III. NUMERICAL RESULTS

Numerical calculations presented in this section closely followed those reported earlier[12] for He^+. The S-matrix elements for energies above the $n=3$ threshold were calculated using a close-coupling plus optical potential approach.[13] The lowest six states $(1s,2s,2p,3s,3p,3d)$ were explicitly included in the close-coupling calculation. A second-order optical potential was constructed on the basis of 12 ($4f$ plus 11 pseudostates) states representing higher bound and continuum states. Between the $n=2$ and 4 thresholds accurate calculations could be carried out for $L\leq3$ using a variational method.[14] Below $k^2=0.75$ Ry, essentially exact phase-shift data available in the literature[15] were used. In view of Eqs. (17)–(19), the integration in Eq. (2) was carried out over k rather k^2 by fitting the S-matrix elements to polynomials in k. At most energies, calculations were carried out up to $L=48$, beyond which the S-matrix elements were extrapolated using a polynomial in $1/L$. More details will be given in a later paper where we hope to present results for all transitions between the $n=1$, 2, and 3 states of hydrogen.

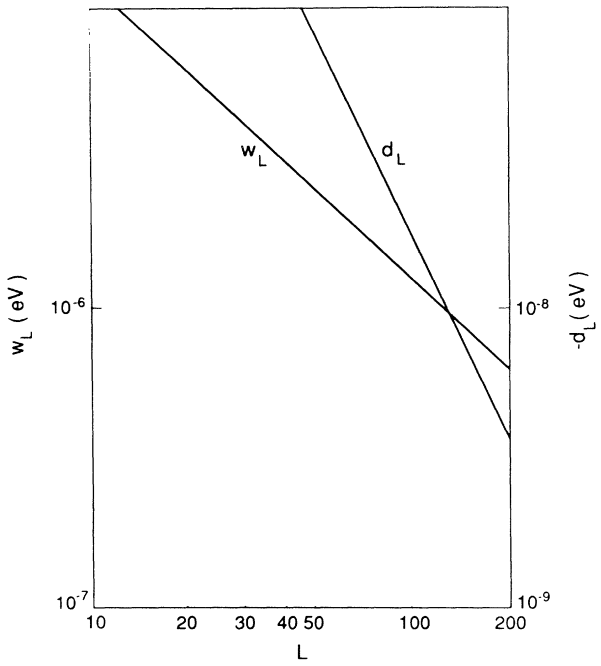

FIG. 1. Partial shift d_L and width w_L of the $2p-1s$ transition in hydrogen due to electron collisions for density $N_e=2\times10^{17}$ cm^{-3} and temperature $k_BT=1$ eV.

In Fig. 1 are presented the variations of d_L and w_L (eV) with L at $k_BT=1$ eV and $N_e=2\times10^{17}$ cm^{-3}. It is seen that w_L follows Eq. (21) for $L\gtrsim12$ and therefore the contribution due to all higher partial waves up to the cutoff limit can be calculated simply by summing a harmonic series. This is significant, since nearly half the contribution to the total width comes from $L\geq12$. In fact, use of Eq. (12) for all L (1 through $L_{\max}$) actually gives a reasonable estimate of w. For example, at $k_BT=1$ eV and $N_e=2\times10^{17}$ cm^{-3}, w calculated in this manner is 0.075

TABLE I. Shift d (Å) and width w (Å) of hydrogen Lyman α spectral line at temperature k_BT (eV) and electron density N_e (cm^{-3}).

	d		w	
k_BT	$N_e=2\times10^{17}$	4×10^{17}	2×10^{17}	4×10^{17}
1	0.0087	0.017	0.064	0.117
2	0.011	0.021	0.053	0.099
3	0.011	0.021	0.048	0.089
4	0.011	0.022	0.044	0.083
5	0.011	0.022	0.042	0.079

Å, whereas the correct value (see Table I) is 0.064 Å.

A few remarks are in order regarding the numerical evaluation of d_L for large L. First of all, owing to the L^{-2} behavior, this contribution is quite small. In the present case, the contribution from $L > 48$ is about 2%. To determine this correctly, the numerical scheme should account for the asymptotic polarization potentials in all channels at all energies.[16] In the optical potential model we have employed,[13] this would mean using a different pseudostate basis at each energy. However, since the major contribution to d comes from low partial waves, the large-L ($L > 48$) contributions actually can be neglected without incurring any appreciable error and therefore no effort has been made to determine d_L for large L accurately. The data presented in Fig. 1 are only intended to serve the purpose of confirming the L^{-2} dependence of d_L, for large L.

Finally, some representative values of w and d are presented in Table I. No comparison with corresponding experimental data has been made, since we are not aware of any. In calculating these, the maximum value of the angular momentum, $L_{\max}$, was estimated on the basis of Debye screening as (using atomic units) $L_{\max} = k_B T/(2\pi N_e)^{1/2}$. As is clear from the table, the departure from a linear dependence of w and d on N_e on this account is quite small.

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