Shifts of the spectral lines of He^+ produced by electron collisions

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We calculate the shifts of the Ly_α, Ly_β, and H_α lines of He^+ in a plasma, produced by electron scattering from radiating ions. Electron densities in the neighborhood of 10^{17} cm^{-3} and plasma temperatures from 1 to 6 eV are considered. The calculation is made in the impact approximation, and is based on a six-state close-coupling computation of the scattering matrices, into which an optical potential has been inserted. Small red shifts of the lines are obtained. The contribution of electron scattering to the linewidths is also considered.

I. INTRODUCTION

This paper reports the results of a calculation of the electron-impact contribution to the shift of the Ly_α, Ly_β, and H_α lines of He^+ in a plasma. The temperature of the plasma is assumed to be in the range of a few eV. We give results as a function of temperature for 1 eV $\leq k_B T \leq$ 6 eV. The theoretical expression which is the basis for our calculations predicts that the shift is approximately (linearly) proportional to the electron density. This may fail at sufficiently high densities, but is believed to hold for densities in the neighborhood of $10^{17}/cm^{-3}$.

The present calculation is based on a fully quantum-mechanical theory formulated by Baranger[1] and reviewed by Griem[2] and Peach.[3] The theory gives an expression for the width and the shift of a spectral line as the real and imaginary parts of a function which is the average of certain combinations of S matrix elements which describe scattering of electrons by the radiating system over a Maxwell distribution of electron velocities. The theory is founded on the impact approximation[1-3] in which it is assumed that there are no correlations between particles and that a radiating atom experiences only binary collisions. The calculated width and shift are approximately linear in the electron density, as is expected for a theory which is valid in a low-density limit. Previous calculations concerning lines of He^+ have been made using a semiclassical description of the collision,[4] or using close-coupling procedures in which convergence of the partial-wave expansion with respect to angular momentum was not achieved.[5,6] Other calculations determined the S matrices in the Coulomb-Born-Oppenheimer[7] and distorted-wave approximations.[8] Aspects of these calculations will be discussed subsequently. The present calculation is of the close-coupling type in which an optical potential is also included, and particular care was taken to ensure that all partial waves that contribute significantly have been included.

A particular characteristic of hydrogenic systems is the linear Stark effect. The degeneracy of atomic states of a given principal quantum number n with respect to the orbital angular momentum l is split in the presence of an external electric field by an amount linearly proportional to the field. Thus, the levels of a hydrogenic atom or ion in a plasma are split in this way by fields resulting from the local distribution of charged particles. This splitting broadens spectral lines by an amount which is large compared to that due to electron collisions as we calculate here. However the static, first-order Stark broadening is symmetric, i.e., does not lead to a shift in the position of the line. Although higher-order contributions to the Stark effect produce line asymmetries and shifts, the dominant contribution to the line shift is believed to be the effect of electron collisions.[4] Therefore, the present calculation is primarily concerned with the line shifts.

Some measurements of the shifts of lines of He^+ have previously been interpreted in terms of a "plasma polarization shift."[9] In this approach the potential energy of an electron bound to a helium nucleus is modified by Debye screening, in which some screening charge must be regarded as inserted between the nucleus and the bound electron. We consider this physical picture to be inappropriate in low-density plasmas, as the screening charge has to be quantized in the form of discrete, individual electrons. A more formal discussion of this point appears in Ref. 10. It appears, instead, to be a general characteristic of many-body physics, that for sufficiently low density, the system can be completely described in terms of two-body scattering.

II. METHOD OF CALCULATION

Consider a transition connecting an initial state 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[11-13]

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

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.

Equation (1) applies to a transition between individual levels. In fact, H_α contains three components ($3s \rightarrow 2p$, $3p \rightarrow 2s$, and $3d \rightarrow 2p$) connecting states which are exactly degenerate for an isolated atom in a nonrelativistic theory, and which are not resolvable experimentally in the conditions relevant to this paper. Although we report shifts for the components separately, an intensity weighted average is required for comparison with experiment. This is, to an excellent degree of approximation, equal to the result for the $3d \rightarrow 2p$ transition.

The scattering calculation is to be made 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',

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

are different. The S-matrix elements S_a and S_b describe the scattering. These quantities are defined with respect to Coulomb waves; i.e., they do not include any contribution from pure Coulomb scattering. Since any contribution from Coulomb scattering in the field of the ion, regarded as a point charge, would be the same in the initial and final states, it is clear that such scattering would not alter the line.

The S-matrix elements were obtained by the close-coupling plus optical potential approach we have described previously.[14,15] The same 18-state basis used in calculations[14,15] for electron hydrogen scattering was used in this case (after appropriate scaling to allow for the different nuclear charge). The lowest six states ($1s, 2s, 2p, 3s, 3p, 3d$) are included in a close-coupling calculation. All interactions between states in this group produced by the impact of the incoming electron are incorporated in this calculation. The remaining states ($4f$ plus eleven pseudostates) are used to define a second-order optical potential. The optical potential includes interaction with both higher bound and continuum states in an approximate way. This approach was used for kinetic energies in the range 3.1 to 6.0 Ry. This is sufficient to cover the range of incident electron energies of interest as far as scattering from the $n=2$ and 3 states was concerned. However, we also require ground-state scattering S matrices for incident energies below the $n=2$ threshold. These were taken from the variational calculations of Oza.[16]

Because the $n=3$ levels are strongly coupled to the $n=4$ levels, it would have been better to include those states in the close-coupling calculation explicitly, rather than only implicitly, through the optical potential. However, such a calculation would have been prohibitively difficult for us.

The convergence of these calculations with respect to the angular momentum variables of Eq. (1) is a very delicate matter. The sum over L requires, in regard to the width and for hydrogenic systems, a finite upper limit ($L_{\max}$). There are different ways of estimating $L_{\max}$, but we will consider here only the limit imposed by Debye screening. Then the maximum angular momentum to be considered in a collision is approximately given by

$$L_{\max}=m^{1/2}k_B T/(2\pi\hbar^2 N_e e^2)^{1/2} \ . \quad (2)$$

This is a large number for temperatures and densities of interest to us. For example, if $N_e=2\times10^{17}$ cm^{-3} and $T=4$ eV, $L_{\max}=340$.

We have included contributions from all angular momenta $L \leq L_{\max}$. This was done in the following manner. Full calculations, including exchange and the optical potential, were carried out through $L=13$. The optical potential was dropped for $L=14$, 15, and 16. Higher L contributions were included by extrapolation from $L=14$–16. The S-matrix elements which contribute to Eq. (1) connect different angular momentum channels associated with the same atomic state. For hydrogenic atoms and ions, these elements depend on the total angular momentum L according to

$$L^2(S_{ll'}-\delta_{ll'})=A_{ll'}+B_{ll'}/L \ , \quad (3)$$

where the quantities $A_{ll'}$ and $B_{ll'}$ may be complex and depend on energy. We ignore terms of higher order in L^{-1}. However, for scattering from the $1s$ state, $A_{ll'}=0$.

Equation (3) can be obtained analytically, and is confirmed numerically. We hope to discuss the origin of Eq. (3) and its consequences in more detail in a subsequent note. It suffices to point out here that Eq. (3) appears to imply that both the width and the shift according to Eq. (1) will depend logarithmically on $L_{\max}$. However, as a result of cancellations between terms, it appears that the shift converges to a finite value even if $L_{\max}$ is made infinite. We have used Eq. (3) to extrapolate the S-matrix elements out to $L_{\max}$, where $L_{\max}$ is given by Eq. (2). Because the dependence on $L_{\max}$ is only logarithmic,

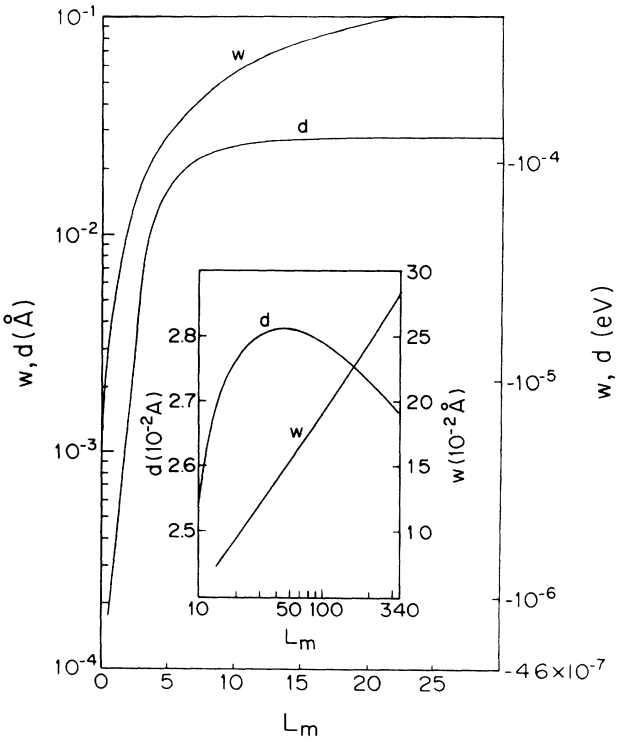

FIG. 1. The shift and width of the $3s \rightarrow 2p$ transition in He^+ at an electron density of 2×10^{17} cm^{-3} and a temperature of 4 eV are shown as a function of the maximum (total) angular momentum included in the calculation. The left scale is in angstroms, the right in eV. The inset shows, on a different scale, the large L dependence of these quantities, up to $L_{max}=340$

the results are not sensitive to the precise value of L_{max}. It should be noted that the semiclassical approach gives an apparently related logarithmic dependence on an upper cutoff impact parameter which is estimated by the Debye length.[2]

In order to be able to do the energy integration in Eq. (1) analytically, the S-matrix elements were fitted by least squares to two third-order polynomials; one for low energies ($\varepsilon<1.8$) and one for high ($\varepsilon>1.8$) except for $1s$, where the cut was made at $\varepsilon=3.0$. We further verified that the final result was not sensitive to any reasonable choice of these energy ranges.

Most of the contributions to the line shift for the ranges of temperature and density of interest here occur for fairly small angular momenta. This is illustrated in Fig. 1, where we show for the $3s \rightarrow 2p$ transition (plasma temperature of 4 eV and density $N_e=2\times10^{17}$ cm^{-3}) the variation of w and d as the maximum value of L in Eq. (1) is increased toward L_{max}. Both w and d increase rapidly for small L. The shift passes through a maximum and then decreases; the width continues to increase.

The relative importance of small and large angular momenta is of some interest in the assessment of the validity of the simpler and more frequently employed semiclassical treatment of the scattering. We find that around $k_BT=4$ eV (as shown in Fig. 1), about 60% of d comes from partial waves of $L\leq5$, while for w the corresponding contribution is less than 10%. For $T=4$ eV, the largest contributions to w and d occur in the range $3\leq L\leq7$ even though the contributions from large angular momenta are significant. These considerations suggest to us that a full quantum treatment of scattering is probably necessary to determine d reliably.

Results for the other transitions are qualitatively similar in that d is determined mainly by contributions from small angular momenta. In the case of the $3d \rightarrow 2p$ transition (only) the large L contributions lead to a slow increase with the maximum value of $L(\leq L_{max})$, rather than a decrease.

III. RESULTS

Our specific results were calculated for a plasma density of 2×10^{17} cm^{-3}. Tables I, and II give the shift d and the width w for the $2p \rightarrow 1s$, $3p \rightarrow 1s$, $3p \rightarrow 2s$, $3s \rightarrow 2p$, and $3d \rightarrow 2p$ transitions for plasma temperatures from 1 to 6 eV. These results are shown graphically in Figs. 2–5. When the contributions to H_α are weighted according to the intensity of the transition, the results are essentially identical with those given for the $3d \rightarrow 2p$ transition. It should be understood that electron impact gives only one of many contributions, and ordinarily not the largest one, to the width, while it almost certainly makes the dominant contribution to the shift.

It will be observed from the figures and tables that the widths and shifts are decreasing functions of the plasma temperature in this range. Apparently, most of this variation results from the multiplicative factor $T^{-1/2}$ in Eq. (1). The shifts are always to the red, corresponding to a small reduction in the energy of the transition which, under the conditions for which we give results, is up to one order of magnitude smaller than the fine-structure split-

TABLE I. Shifts (Å) of various He II spectral lines at an electron density of 2×10^{17} cm^{-3}. Numbers in brackets indicate powers of 10.

Transition \ k_BT (eV)	1	2	3	4	5	6
$2p \rightarrow 1s$	3.3[−4]	2.3[−4]	2.0[−4]	1.8[−4]	1.8[−4]	1.8[−4]
$3p \rightarrow 1s$	7.7[−4]	6.8[−4]	6.2[−4]	5.7[−4]	5.2[−4]	4.7[−4]
$3p \rightarrow 2s$	3.1[−2]	2.8[−2]	2.5[−2]	2.3[−2]	2.1[−2]	1.9[−2]
$3s \rightarrow 2p$	3.8[−2]	3.2[−2]	2.9[−2]	2.7[−2]	2.4[−2]	2.2[−2]
$3d \rightarrow 2p$	3.3[−2]	2.9[−2]	2.6[−2]	2.4[−2]	2.2[−2]	2.1[−2]

TABLE II. Electron scattering contribution to the widths (Å) of various He II spectral lines at an electron density of 2×10^{17} cm^{-3} Numbers in brackets indicates powers of 10.

Transition \ k_BT (eV)	1	2	3	4	5	6
$2p\rightarrow1s$	1.4[−3]	1.1[−3]	9.0[−4]	8.0[−4]	7.3[−4]	6.9[−4]
$3p\rightarrow1s$	6.7[−3]	6.0[−3]	5.5[−3]	5.2[−3]	4.9[−3]	4.7[−3]
$3p\rightarrow2s$	2.7[−1]	2.5[−1]	2.3[−1]	2.1[−1]	2.0[−1]	1.9[−1]
$3s\rightarrow2p$	3.7[−1]	3.3[−1]	3.1[−1]	2.8[−1]	2.7[−1]	2.6[−1]
$3d\rightarrow2p$	1.3[−1]	1.2[−1]	1.1[−2]	9.8[−2]	9.3[−2]	8.9[−2]

ting. Also, the figures show some examples of the results that are obtained when scattering from the lower (final) state is neglected. These are in most cases rather close (although the difference may be of either sign). It is expected that scattering in the initial state would make the dominant contribution in view of the greater spatial extent of the initial state wave function.

In addition, we show the results obtained by Yamamoto[6] for the $3p\rightarrow1s$ and $3s\rightarrow2p$ transitions. His results for the shift are mostly smaller than ours (as might be expected since the maximum angular momentum considered in his calculations was $L_m=6$). However, the lack of convergence in his sum over L appears too small to account entirely for the difference. Moreover, his results show a different temperature dependence. In the case of the $3p\rightarrow1s$ transition, the difference in magnitude of d is a factor of 3; considerably more than can be readily accounted for in terms of his neglect of partial wave contributions with $L>6$.

The calculations of Griem[4] for the electron scattering contribution to the shift are based on a semiclassical approach which neglects contributions to the scattering from monopole components of the scattering potential. The results were smaller than ours by amounts in the range of 20–50 % depending on the transition. After improvement deriving from the work of Boercker and Iglesias[17] which require the inclusion of matrix elements connecting radiator states of the same n, but different l, his results are in reasonable agreement with ours. Because our calculation allows for the coupling of these states, we do not believe that a correction of this type is required to our results. However, Boercker and Iglesias consider corrections to the perturber distribution function which are not included in the impact theory on which the present calculation is based.

The shifts calculated by Nguyen *et al.*[7] are somewhat larger than those obtained here (by 22% for Ly_α and 62% for Ly_β) at a temperature of 4 eV. This is probably

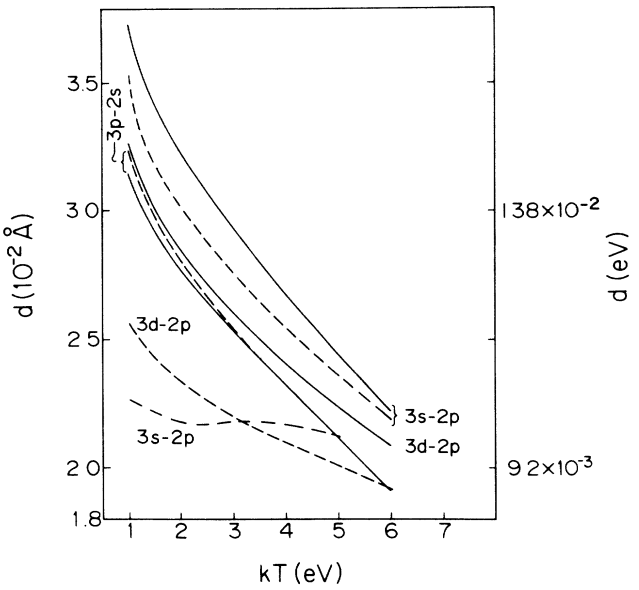

FIG. 2. Shifts of individual components of H_α (left scale, units of 10^{-2} Å) as functions of plasma temperature in eV. All results are for a density of 2×10^{17} cm^{-3}. The right scale shows the shift in eV. The solid curves are the present results including scattering in both the initial and final states. The dashed curves omit the contribution from final-state scattering. The dash-dotted curve is the result of Yamamoto, Ref. 6, shown for comparison.

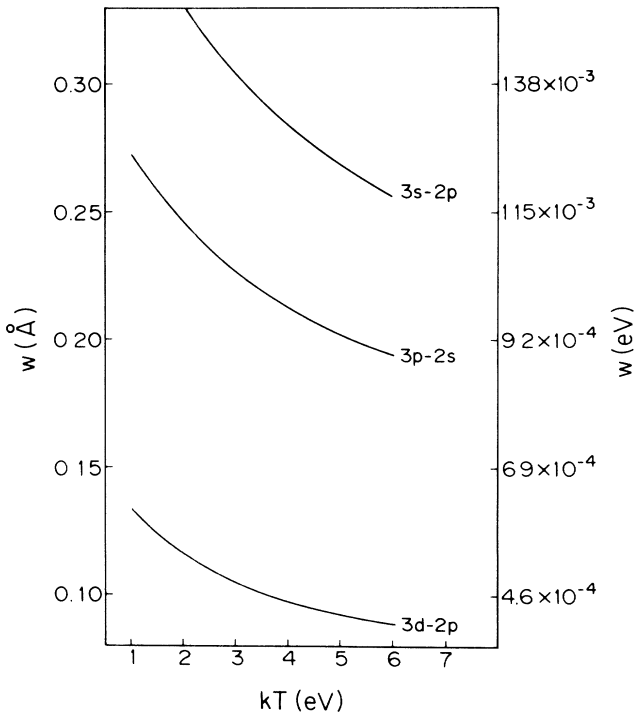

FIG. 3. Electron scattering contribution to the widths of components of H_α (units of Å) as functions of the plasma temperature in eV.

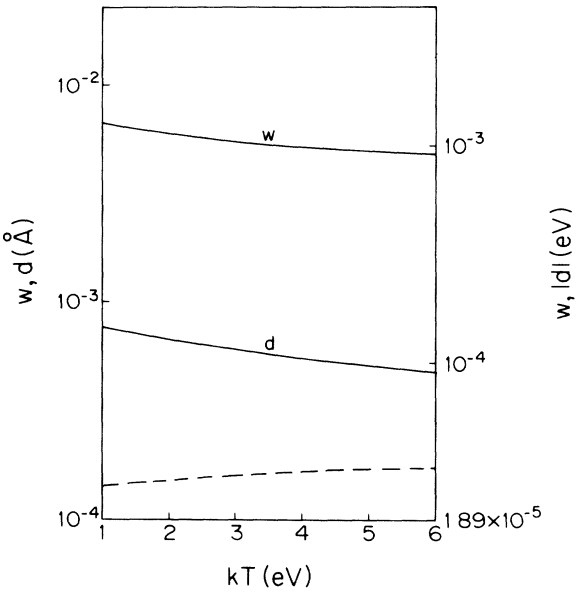

FIG. 4. Shift and electron scattering contribution to the width of the Ly$_\beta$ line (in Å) as functions of the plasma temperature in eV. The dash-dotted curve is the result of Yamamoto, Ref. 6 rescaled to $N_e = 2\times10^{17}$ cm^{-3}.

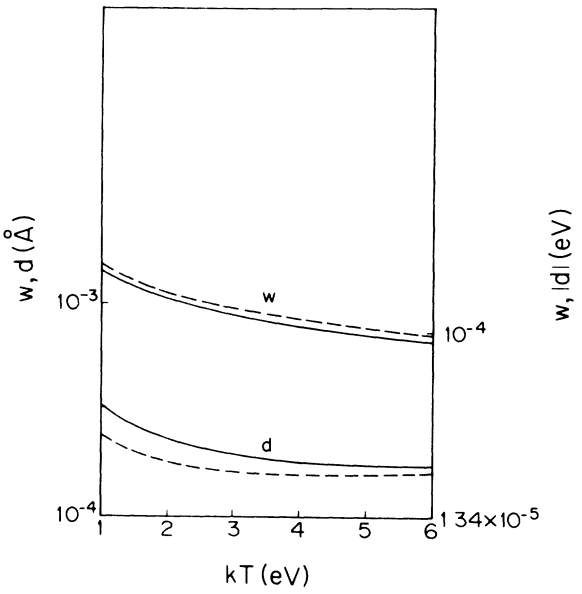

FIG. 5. Shift and electron scattering contribution to the width of Ly$_\alpha$ as functions of temperature. The dashed curves omit the contribution from scattering in the final ($1s$) state. The results of Ref. 5 lie below the bottom of the scale.

due to the unreliability of the elastic scattering calculation in the Coulomb-Born-Oppenheimer approximation at the relatively low energies relevant here. Their approximations would be expected to be more accurate for higher temperatures and for more highly charged radiating atoms. Our finals results for the Ly$_\alpha$ line agree rather well with those of Blaha and Davis,[8] but we have different results for the contributions from different partial waves.

It will be observed from the scale in Fig. 1 that the line shift is smaller; when all contributions to the width are included, the shift is considerably smaller than the width. This is also what is found experimentally. Pittman and Fleurier[18] measured the shift of the H$_\alpha$($n=3\rightarrow n=2$) and P_α($n=4\rightarrow n=3$) lines of He$^+$ in plasmas with densities ranging from 2×10^{16} to 2×10^{17} cm^{-3} for a temperature of 4 eV. A more recent study reported the widths of H$_\alpha$ and H$_\gamma$ lines of He$^+$ in a somewhat hotter and more dense plasma (10 eV, 7×10^{17} cm^{-3}), but did not determine a shift.[19] The data of Ref. 18 (see their Fig. 9) is rather scattered, involves optically thick lines, and apparently shows a nonlinearity in the density. There is, additionally, some uncertainty due to the lack of an absolute wave length reference. Moreover, no consideration is given in Ref. 18 to the possibility (predicted in the present work), that the shift might be different for different components of the line. A reasonable estimate based on this data, and ignoring the points at high density which show the greatest departure from linearity, is a shift of H$_\alpha$, $\Delta\lambda=0.025\pm0.010$ Å at a density of $N_e=10^{17}$ cm^{-3}. This is somewhat larger than our results, although our value for the largest component shift ($3s\rightarrow2p$) would just come to the bottom of the "error bar." The small nonlinear variation of our results with density, due to the dependence of $L_{\max}$ on density, is much too weak—and in the wrong direction—to explain the nonlinearity in the data. An earlier measurement by Van Zandt, Adcock, and Griem[20] at 3 eV and $N_e=2\times10^{17}$ cm^{-3} reported a red shift of H_α in the range of 0.01 and 0.06 Å. Our results are in this range.

The possibility that other effects could make a significant contribution to the shift should not be ignored. Griem,[4] following the work of Demura and Sholin,[21] has considered the contribution to the shift produced by the interaction of an electric quadrupole moment in the radiating atom with the local electric field gradient produced by charges in the plasma. However, he finds this produces a small blue shift; i.e., it acts in opposition to the red shift produced by electron collisions. The shift is rather small, about 12% of the electron contribution in the case of H_α. It is also possible that ion dynamic effects, involving collisions of plasma ions with radiators may contribute to the line shifts as they are known to do to the broadening.[22] More precise experiments, though undoubtedly difficult, are required.

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