Hamiltonians by the expression

$$e_0E^0+e_1\bar{E}^1+e_2E^2$$

for d electrons and by

$$e_0E^0+e_1\bar{E}^1+e_2\bar{E}^2+e_3E^3$$

for f electrons. The angular dependence of these operators, which is given by the e_i's, is exactly the same as in the pure Coulomb case.[1,7] The E^i's are the usual sums of Slater integrals used in the Coulomb Hamiltonian,[1,7] and the $\bar{E}^i$'s are defined for d electrons by

$$\bar{E}^1=E^1+(10/7)R_2;$$

and for f electrons by

$$\bar{E}^1=E^1+(14/9)R_2,$$
$$\bar{E}^2=E^2+(14/6435)R_2,$$

where

$$R_2=\mu_0{}^2\int\frac{[R_l(r)]^4}{r^2}dr.$$

The integral R_2 will always be positive; therefore the effect of the spin-spin contact term is always to enhance the value of certain of the E^i's over the purely Coulombic results. Thus, values of E^i obtained from the usual analysis of experimental data must always be corrected downwards in order to find the contribution from the Coulomb interaction alone.

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Effect of Strong Collisions on the H_α Profile*

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Strong collision effects are appreciable for the H_α spectral line. Including these effects in H_α profile calculations, we find agreement between experiment and theory within experimental error.

THE Stark-broadened profiles of several hydrogen lines in a plasma have been calculated by Griem, Kolb, and Shen.[1] They later modified these calculations[2] for the H_β line to include the effects of strong collisions, the Mozer-Baranger ion field-strength distribution functions, and electron-impact broadening of both the upper and the lower levels including the cross terms. With these modifications for H_β the agreement between the measured and the calculated line shapes is $\pm 2\%$,[3] which is within experimental error. The half-width of the H_β line is used where practical to determine electron densities in plasmas because of these refined theoretical calculations of the profiles and the good agreement between theory and experiment. Corresponding modifications were made by us in an attempt to develop a theoretical profile that corresponded more closely to experimental data. The profiles as originally proposed by GKS I had half-widths about 20% smaller than the best experimental data, as shown in Fig. 1. The inclusion of these modifications into the theory alters the calculated line profiles for H_α such that the agreement between the theoretical and experimental half-widths is now within experimental error over the plasma densities tested. The purpose of this paper is to report our results and to demonstrate the relative importance of the various modifications to the GKS I theory.

In the calculations of GKS I for the H_α line, the effects of close or strong collisions (called strong interactions here) were taken to be negligible as compared with distant or weak collisions (called weak interactions here). The electron-impact broadening was considered only for the upper level and the central component of the lower level. Also, the ion field-strength distribution functions of Ecker were used.[4]

To calculate the H_α profiles reported in this paper, the following general equation, due originally to GKS II, was used:

$$S(\alpha)=\frac{1}{\pi}\int df\,W(f)\,\mathrm{Re}\langle\alpha|\mu|\beta\rangle \times\langle\langle\alpha\beta|[i(\alpha+\mathbf{C}f)+\phi_{ab}]^{-1}|\alpha'\beta'\rangle\rangle\langle\beta'|\mu|\alpha'\rangle, \quad (1)$$

where $W(f)$ is the distribution of the ion-field strength f, and μ is the dipole-moment operator. For transitions

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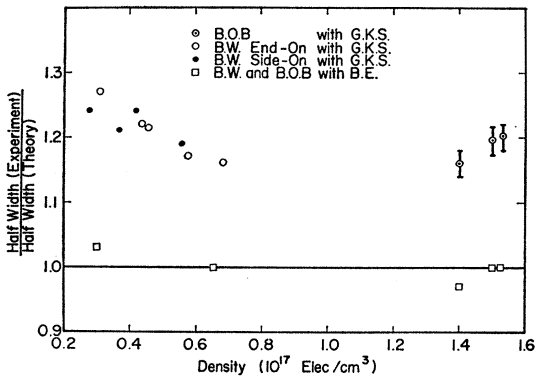

FIG. 1. Ratio of the experimental to theoretical half-widths for the H_α line as a function of electron density. The experimental data are those of Birkeland *et al.* (Ref. 9) (B.O.B.) and Bridges and Wiese (B. W.) (Ref. 8). The theoretical half-widths are those of GKS and the present authors (B. E.).

between levels with small principal quantum numbers, the electron-impact broadening is given by

$$\phi_{ab}=\frac{\frac{1}{3}\lambda^2\hbar N^{1/3}}{2.6ecm^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\left[1+\int_{y_{\min}}^{\infty}dy\frac{e^{-y}}{y}\right]\times[\mathbf{R}_a\cdot\mathbf{R}_a-2\mathbf{R}_a\cdot\mathbf{R}_b+\mathbf{R}_b\cdot\mathbf{R}_b],\quad(2)$$

where $\mathbf{R}_a$ and $\mathbf{R}_b$ are the atomic electron coordinate vector operators in atomic units. $y_{\min}$ is a velocity cutoff corresponding to an impact cutoff of 1.1 times the Debye radius and is given by

$$y_{\min}=(4\pi N/3m)(ehn^2/1.1kT)^2,$$

where N is the electron density, n is the principal quantum number of the upper level, and the other symbols have their usual meaning. If parabolic wave functions are employed where the $\alpha(n,n_1,n_2,m)$'s and $\beta(n',n_1',n_2',m)$'s designate the upper and lower levels, respectively, then the operator $\mathbf{C}$ is given by

$$\mathbf{C}=\tfrac{3}{2}(ea_0\lambda_0^2/2\pi\hbar c)[n(n_2-n_1)-n'(n_2'-n_1')]\delta_{aa'}\delta_{\beta\beta'}.\quad(3)$$

The notation $|\alpha\beta\gg$ is due to Baranger[5] and denotes a state of a "double atom," each state of which corresponds to two states of the original atom. This double atom was introduced as a convenience for considering the interaction in the lower level. The states $|\alpha\beta\gg$ form a basis to the so-called line space. For the case of higher principal quantum numbers, the lower-level perturbations are not always additive as they are for H_α as pointed out by Griem.[6]

In Eq. (2) the effect of the strong interaction is given by the term 1 preceding the integral. GKS I assumed that this strong-interaction effect would be small compared with the weak-interaction effect and thus neglected the term 1. They also assumed the lower state was not broadened by impact and thus neglected the terms $-2\mathbf{R}_a\cdot\mathbf{R}_b+\mathbf{R}_b\cdot\mathbf{R}_b$ in Eq. (2) but included a $\mathbf{R}_b\cdot\mathbf{R}_b$ term for the central component. The results of the profile calculations reported here indicate that these are not always negligible effects.

Recently, Birkeland,[7] Bridges, and Wiese[8] have made careful measurements of H_α line shapes. In both cases a stabilized hydrogen arc was used as the plasma source and care was taken to either correct for or to minimize the effect of self-absorption. Simultaneous measurements were made of both the H_α and H_β profiles with the H_β half-widths being used to evaluate the electron density. A comparison of the experimental to the theoretical H_α profiles is given in Fig. 1. Here the ratios of the experimental half-width to theoretical half-width are given for the range of electron densities from 0.3 to 1.6×10^{17} electrons/cm^3. The GKS I theory gives half-widths from 10–30% too small for this density range. Using the theoretical half-widths reported here, the agreement between experiment and theory is improved. The variation is within the experimental error for this same range of densities. At the present time reliable H_α profile data are not available for $0.7<N<1.4\times10^{17}$ electrons/cm^3. Birkeland, Oss, and Braun[9] have reported measurements for this density range but subsequently Birkeland has made further measurements and he does not consider his data near $N=10^{17}$ electrons/cm^3 as reliable as for the higher densities, we have therefore not included the data reported in Ref. 9 for this density range.

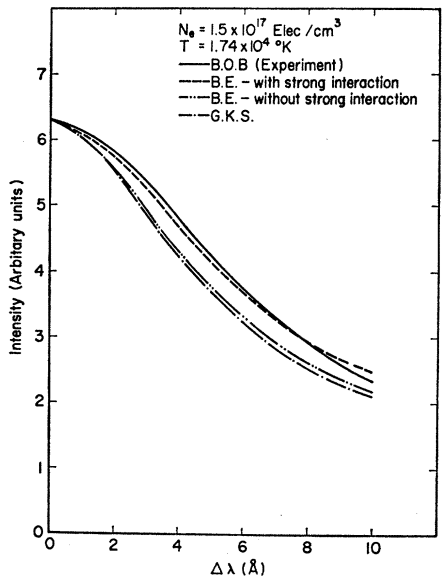

FIG. 2. Theoretical and experimental H_α line profiles for an electron density $N=1.5\times10^{17}$ cm^{-3} and electron temperature $T=1.74\times10^4$°K. The theoretical profiles have been normalized to the peak intensity of the experimental data.

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In Fig. 2 is shown the experimental H_α-line profile of Birkeland *et al.*[6] for an electron density of 1.5×10^{17} electrons/cm^3 and electron temperature of 1.74×10^4°K. Also shown for comparison are several theoretical line profiles calculated from Eq. (1) using different approximations. From this figure one can see the relative importance of the various effects on the theoretical profile. The GKS curve neglects the strong interaction, considers only broadening of the upper level and the central component of the lower level, and uses the Ecker distribution function. Substituting the Mozer-Baranger distribution function for the Ecker function (everything else unchanged) has only a small effect on the line shape as shown by the curve marked "BE-without strong interaction." It is expected that the distribution function proposed by Hooper[10] would also have a small effect at the center and near wings of the line. The effect of considering only broadening of the central component in the lower level is about the same as considering broadening of all the components in the lower level. This profile would coincide with the curve marked "BE-without strong interaction" and is not shown. When the strong-interaction effects, the Mozer-Baranger distribution functions, and broadening for both the upper and lower levels with cross terms are included there is close agreement between the experimental and theoretical profiles. The theoretical profile is then given by the curve marked "BE-with strong interaction." Neglecting strong interaction and broadening of the lower level, but with the Mozer-Baranger distribution function, the profile (not shown in Fig. 2) would have a half-width about 30% smaller than the experimental half-width. From Fig. 2 one can see that the major effects on the profile are the strong interaction and the broadening of the central components in the lower level. It is to be expected that the strong-interaction effects will be appreciable for those lines having an unshifted central component (L_α,L_γ,H_α,H_γ, etc.) and have a smaller effect on those lines with a shifted central component (L_β,L_δ,H_β,H_δ, etc.).

H_α-line profiles have been calculated[11] using this modified theory for electron densities and temperatures within the range from 10^{16} to 10^{20} electrons/cm^3 and 10^4 to 10^5 °K, respectively, wherever the ion-distribution functions of Mozer and Baranger and the GKS II theory are valid. These higher densities and temperatures correspond to typical values in the laser-produced plasmas reported by Edwards and Litvak.[12] Using the ion-field distributions of Hooper[10] should yield more accurate results than the Mozer-Baranger functions, especially for the high-density high-temperature plasmas. Lyman-α profiles were also calculated[11] using this same modified theory. Experimental profiles of L_α corrected for self-absorption were not available for making a comparison similar to that made for H_α. This modified theory is also being used to calculate H_γ profiles in an attempt to find closer agreement between theory and experiment.[3]

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Vacuum Ultraviolet Emission Produced by Proton and H-Atom Impact on H_2†

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The spectrum in the wavelength range 1200 to 1700 Å excited by proton and hydrogen-atom collisions with hydrogen molecules has been investigated under thin-target conditions. The prominent features of the spectrum are bands originating from the B and C states of H_2 and the Lyman α line of atomic hydrogen. Relative cross sections are presented for the emission of Lyman α and the Lyman band emission from the B state of H_2 due to proton and hydrogen-atom impact in the energy range 20–130 keV. Absolute values of these cross sections are estimated by comparison with known cross sections for Lyman α. A calculation of the cross section for proton excitation of the sum of the B and C states of H_2 in the first Born approximation is presented and compared with the experimental results for the B state.

INTRODUCTION

THE homonuclear diatomic molecule is one of the simplest molecular structures. A collision between the proton and H_2 is the least complex ion-molecule interaction and the collision between the hydrogen atom and H_2 is the simplest atom-molecule

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