Effects of Ion Motion on Hydrogen Stark Profiles
Joachim Seidel
Institut für Theoretische Physik der Universität Düsseldorf
(Z. Naturforsch. 32 a, 1207-1214 [1977]; received July 21, 1977)

The influence of ion motion on Stark broadened hydrogen lines is studied using the Method of Model Microfields which allows a uniform treatment of electrons and ions. Contrary to former theoretical investigations, strong effects are found in the line centres of L-α, H-α, and H-β which agree well with recent experimental findings, especially those of Wiese, Kelleher, and Helbig.

For the Stark broadening of hydrogen lines the unified theory developed by Voslamber and Smith et al. provides a refined description of line profiles including the transition region from the “static” wing to the “impact” centre. Evaluating the results of the unified theory, Vidal, Cooper, and Smith (VCS) have compiled extensive tables of Stark profiles of low Lyman and Balmer lines which greatly facilitate the comparison to experimental results. A detailed experimental investigation of the Stark broadening of Balmer lines has been carried through by Wiese, Kelleher, and Paquette (WKP) who give a short account as well of former measurements which have been done in the same range of plasma densities and temperatures (typical values are $N_e = 10^{17}$ cm$^{-3}$, $T = 10^4$ K). As a general result, good agreement between theory and experiment is found in the line wings but the measured profiles exhibit much less structure in their central portions than those of VCS. A similar finding has been reported for low electron densities, too, and the conclusion seems to be inevitable that not all the approximations used in the VCS calculations work as good in the line centre as has been estimated.

Possible candidates are especially the neglect of time ordering in the evaluation of the effects of radiator-perturber collisions, and the assumption of a static ion microfield. The first of these is not a constituent part of the unified theory but may be removed at the expenditure of greater calculational efforts. Corresponding results of Roszman indicate that the inclusion of time ordering improves the agreement of experiment and theory, but certainly is not sufficient to remove the discrepancies. This has been made most obvious by a recent experiment of Grützmann and Wende who succeeded to measure the line centre of L-α for the first time. While they report a half width of more than twice the theoretical value, its increase by the consideration of time ordering in the VCS calculations amounts to only 14%. This points out to an influence of ion dynamics much stronger than has been expected, and indeed there is convincing experimental support of this conjecture: Precision measurements of Wiese, Kelleher, and Helbig (WKH) revealed distinctly different line centres for various values of the radiating atom-perturbing ion reduced mass $\mu$. Moreover, these authors found that an extrapolation to $\mu = \infty$, based upon the assumption of a linear dependence on $\mu^{-1/2}$ of their data points, yields half widths etc. in rather good agreement with those of Roszman, i.e., the unified theory with time ordering included.

Contrary to this, theoretical efforts to take ion motion into account do not find any appreciable effect at densities of some $10^{16}$ cm$^{-3}$. Lee’s approach based on second order perturbation theory gives but a partial filling of the central depression of H-β insufficient to bridge the gap to the experimental results, while Hey and Griem even expect a deepening of the minimum (from a treatment, however, that is based on the presumption of small deviations only from the static ion approximation which becomes invalid in the line centre). The unified theory itself cannot be applied to ion broadening except at very low densities (where, on the other hand, fine structure splitting comes into play, and Doppler broadening washes out all details of Stark broadening). Nevertheless, Cooper et al. have applied it in the density range of $10^{14}$ to $10^{15}$ cm$^{-3}$, and for H-β at $N_e = 10^{15}$ cm$^{-3}$ report a much stronger effect than Lee who considered this case, too.
Unsatisfactory as the theoretical situation may appear from this sketch, it becomes really confusing by taking the generalized impact theory of Keple and Griem 15,11 (KG) into considerations together with the interpretation of an experiment by Hey and Griem 12 (HG) based on it. Instead of being identical to the VCS profiles at least in the line centres, the KG profiles show markedly less structure. Especially for H-\alpha they are much more shallow than those of the unified theory and even the experimental ones of WKP. This difference has been retraced to mainly the omission of a complex conjugation in the KG calculations 3, but has been defended by physical reasoning 16 which in turn has led to some dispute on the subject 17,18. The shock tube experiment of HG neither contradicts nor confirms the results of WKH with respect to the dependence of the central minimum of H-\beta on the reduced atom-ion mass. Its interpretation, however, is radically different: Relying on the good agreement of the measured half width of H-\alpha with the theoretical KG value (corresponding to a poor agreement with the VCS half width), and the assumption that ion dynamics are negligible, these authors claim that the observed discrepancies with theoretical profiles of H-\beta (for this line, KG and VCS calculations agree) are due to a thin transition layer which does not affect H-\alpha too much.

With all these contradictory results and conjectures the question of how important ion motion really is represents a true challenge for both experimentalists and theorists. The present paper offers a theoretical solution by employing the Method of Model Microfields (MMM) introduced by Brissaud and Frisch 19 which allows a uniform treatment of electron and ion broadening, and in a preceding paper 20 (henceforth referred to as I) has been shown to be equivalent to the unified theory as far as electron broadening in static ion fields is concerned. For the MMM in contrast to the unified theory the static ion approximation is an unnecessary restriction which may be easily removed. For this reason, the method is perfectly suited for the present purpose.

In I, a critical review of the MMM has been given as well as a description of its application to hydrogen lines without making essential use of the static ion approximation. Referring to this the present paper starts immediately with a discussion of the ion microfield distribution and covariance in Section 1. Section 2 presents theoretical results for L-\alpha, H-\alpha, and H-\beta, which are compared to experimental data in Section 3. A summary may be found in Section 4.

1. Statistical Features of the Model Microfield

For the reasons discussed in I we do not apply the general form of the MMM but use the special Markovian model microfield proposed by Brissaud and Frisch 19 for the high and the low frequency component of the plasma microfield (indexed by e and i). Then all statistical features of the model are determined by just four functions, the probability densities \( p_e, \) \( p_i \) and the jumping frequencies \( \Omega_e, \Omega_i \), from which the line profile is computed according to (1.16) and (1.17) of I. To make the model realistic \( p_e \) and \( p_i \) have to be chosen as the probability densities of the true microfield. For the jumping frequencies there is no equivalent in the real microfield, naturally. There is, however, a one-to-one correspondence between the jumping frequency and the covariance of the respective component of the model field (see Sect. 3 of I), so the jumping frequency is implicitly prescribed by setting the model covariance equal to the true covariance. By this procedure the line profile becomes actually a complicated functional of the true microfield distributions and covariances from which it is calculated.

The use of the field covariance, however, as it is given by plasma kinetic theory 21, say, would entail a large amount of numerical work. For this reason we prefer to work with an approximate form derived from a model plasma of uncorrelated quasi-particles interacting with the radiator through fields of the Debye type. For the high frequency electronic part of the microfield this approach has already been employed in I, where the screening length was set to twice the usual Debye length \( D \) because with this value the microfield distribution computed from the model plasma turned out to be close to the distribution derived by Baranger and Mozer 22,23 (correctly tabulated by Pfennig and Trefftz 24) or Hooper 25,26. This choice corresponds to the assumption that the electrons are shielded statically by their own kind (ion screening of electrons is negligible anyway), but with only \( N_i/4 \) instead of \( N_i \) taken in the formula for the Debye length. For singly charged ions, i.e. \( N_i = N_e = N \), having the same temperature \( T \) as the electrons, an analogous guess for the screening length is \( R_s = (4/5)^{1/2} D \) corresponding to \( N_e + N_i/4 \) instead of \( N_e \) in the formula for \( D \) (electron screen-
In fact this works as well as in the high frequent case, and leads to low frequent microfield distributions in close agreement with those of Baranger and Mozer\textsuperscript{23, 24} or Hooper\textsuperscript{26}.

We have not tried to improve the agreement of the distribution functions any further by altering the value of $R_i$. Ecker and Schumacher\textsuperscript{27}, for example, find $R_i = (2/3)^{1/2} D$ for their probability density, but changing $R_i$ to this value practically does not bear on the line profiles as has been checked numerically for some cases. Some profiles computed by Brissaud and Mazure (private communication, July 1976) with a rather different covariance of the ion microfield and an approximate treatment of electron broadening are very close to ours, too. Hence we have kept to the values

$$R_e = [kT/(\pi e^2 N)]^{1/2}, \quad R_i = [kT/5(\pi e^2 N)]^{1/2}.$$  

(1.1)

For the covariance $\Gamma_e(t)$ of the high frequent microfield this is the same as in I, and all results pertinent to this may be taken from there. Regarding its counterpart $\Gamma_i(t)$, however, there is the coupling of Stark and Doppler broadening mentioned in I. Treating the radiating atom as a point particle with respect to its translational motion, the covariance we need is strictly

$$\Gamma_i(t; u) = \langle E_i(t; u) \cdot E_i(0; O) \rangle$$  

(1.2)

if the atom has velocity $u$ (we neglect collisions) and $E_i(t; r)$ is the field produced by the (quasi-)ions at time $t$ in place $r$ (the plasma is assumed to be homogeneous and stationary). This means that atoms with different velocities and Doppler shifts see different ion fields as well. Though this effect might be incorporated into the MMM, we are not going to consider it here, but rather use the mean of $\Gamma_i(t; u)$ as the ion field covariance:

$$\Gamma_i(t) = \langle \Gamma_i(t; u) \rangle_u.$$  

(1.3)

For our model plasma the evaluation of (1.3) can be done along the lines of Daalenoort's calculation\textsuperscript{28} for uncorrelated particles with Coulomb fields. Utilizing Maxwell distributions for radiator and ion velocities (let the atoms have the same temperature $T$ as the ions and electrons), denoting atom and ion masses by $m_a$ and $m_i$ and their reduced mass by $\mu$, $\Gamma_i$ becomes

$$\Gamma_i(t) = 4 \pi^{1/2} N e^2 R_i^{-1} [s + s^{-1} - \pi^{1/2}(s^2 + s)] 
\cdot \exp(s^2) \text{erfc}(s)$$  

(1.4)

with

$$s := [kT/(2\mu)]^{1/2} R_i^{-1} t$$

$$= \left[ kT \left( \frac{1}{m_a} + \frac{1}{m_i} \right) \right]^{1/2} R_i^{-1} t.$$  

(1.5)

This is just $\Gamma_e(t)$ [Eq. (3.1) of I] with $R_e$ replaced by $R_i$ and $m_e$ by $\mu$, so the calculation of the jumping frequencies from the covariances is essentially the same for both microfield components.

In the frame of the MMM all effects of ion motion on the line profiles arise from $\Gamma_i$. The covariance itself depends on the reduced atom-ion mass solely through $s$, which in turn is proportional to $\mu^{-1/2}$. Because of this peak intensities, half widths etc. depend on $\mu^{-1/2}$ as well. For the full range $(0, \infty)$ of mathematically possible values of the reduced mass this is a trivial assertion as every function of $\mu$ is a function of $\mu^{-1/2}$ as well. But in experiments $\mu$ may change from $1/2$ (H–H$^+$) to 2 (D – heavy ion) at most, corresponding to an interval of 0.7 to 1.4 for $\mu^{-1/2}$, and over that small range of values an approximately linear dependence on $\mu^{-1/2}$ of measurable quantities\textsuperscript{9} derived from (1.4) and (1.5) seems more likely than not, contrary to other conjectures\textsuperscript{12}. By the way it should be noted that (1.5) merely deludes a $T/\mu^{1/2}$-dependence\textsuperscript{9} – due to $R_i \sim T^{3/2}$, $s$ does not at all depend on temperature.

Once the microfield distributions and covariances are known, the calculations can be done in the way described in I.

2. Theoretical Results

MMM profiles have been computed for L–α, H–α, and H–β which are the lines of most prominent interest for both theory and experiment. For the numerical work the CDC Cyber 76 of the Regionalrechenzentrum Köln was used via the RJE-station installed at the Rechenzentrum der Universität Düsseldorf. The computation time for a profile with ion motion included is nearly the same as for static ions, about one minute for L–α and six minutes for H–β. Most profiles have been computed for a temperature $T = 10^4$ K (identical for atoms, ions, and electrons), but some have been evaluated for lower and higher temperatures as well. The density range covered extends from $N = 10^{15}$ cm$^{-3}$ to $N = 10^{18}$ cm$^{-3}$ (singly charged ions have been assumed so that $N_i = N_e = N$), and the atom-ion pairs considered are H–H$^+$, H–Ar$^+$, and D–Ar$^+$ with reduced masses $\mu$ of 1/2, 1, and 2, respectively ($\mu$ is always given in multiples
of the proton mass). A few checks have shown that results for the H–He+ system are well between those for H–H+ and H–Ar+, from which they can be interpolated.

To give an impression of the effects of ion motion Figs. 1 to 3 show profiles for $N = 10^{17} \text{ cm}^{-3}$ and $T = 10^4 \text{ K}$. The "static ions" profiles depicted are MMM profiles, too, and it should be remembered from I that these already have slightly less structure than the VCS profiles (unified theory without time ordering) and lie close to those of Roszman ⁶ (unified theory with time ordering included). The most drastic effect of ion motion is found for L-α (Fig. 1) whose peak intensity is lowered to nearly half the value it has with static ions, while the characteristic "shoulder" at $\Delta \lambda \approx 0.1 \text{ Å}$ completely vanishes. Owing to this the half width becomes a factor of about 2 greater which is in good agreement with the experimental finding of Grützmacher and Wende ⁷. The line wing, on the other hand, is not afflicted.

Changes of the same direction but smaller in magnitude occur for H-α (Fig. 2) which has a strong unshifted component as has L-α. Contrary to these lines H-β has a distinct central minimum (Figure 3). Here the effects of ion motion are restricted mainly to the region between the two symmetric peaks where the intensity increases markedly with decreasing reduced mass. To maintain normalization the peaks are slightly lowered but only insignificantly shifted, and before reaching the half width the profiles become identical to the one computed with static ions. Qualitatively this is just what one expects, but the extent to which the line cores are affected is far greater than other theoretical approaches ¹⁰⁻¹² predict.

Actually the influence of ion motion becomes still more important at lower densities as may be read from the dependence of the half widths on density, shown in Figs. 4 and 5 for L-α and H-α. At $10^{15} \text{ cm}^{-3}$ the Stark width of L-α is an order of magnitude greater with ion motion included than without; but it is still another order of magnitude below the Doppler width, so there is little chance of experimental verification. For H-α the situation is better: With static ions the Doppler width is about twice the Stark width, but with ion motion included both are nearly equal, an effect that should be measurable. At these low densities it becomes particularly clear that the influence of ion motion is roughly the same for...
Fig. 4. Full half width of $L\alpha$ at $T=10^4$ K as obtained from the MMM with and without ion motion (Stark broadening only). The two horizontal lines indicate the (full) Doppler widths for hydrogen ($H$) and deuterium ($D$).

Fig. 5. Same as Fig. 4, but for $H\beta$.

Fig. 6. Alterations in the dip of $H\beta$ effected by ion motion. All curves are MMM results at $T=10^4$ K neglecting Doppler broadening.

Fig. 7. Temperature dependence of the $H\alpha$ half width for $N=10^{17}$ cm$^{-3}$. Together with the MMM data the results of the Kepple-Griem theory are given (KG). Doppler broadening is accounted for.

all reduced masses considered. The half width curves of Figs. 4 and 5, for example, all have the same slope and run close together parallel over all three decades of density. The corresponding curves for $H\beta$ are not shown here since the spread in half widths (including the “static ions” values) at a given density is always very small, decreasing from about 5% at $N=10^{15}$ cm$^{-3}$ to less than 1% at $N=10^{18}$ cm$^{-3}$. The relative alterations of the line centre of $H\beta$, however, are pronounced at low densities, too. Figure 6 presents the density dependence of the dip, defined to be $(I_{\max} - I_{\min})/I_{\max}$ with $I_{\max}$ and $I_{\min}$ the peak and central intensities. For $N=10^{15}$ cm$^{-3}$ we can compare the MMM result to that of the unified theory, which yields – after convolution with the appropriate Doppler profile – a value of 19% for $H-H^+$ at $T=10^4$ K. From Fig. 6 we find only 17.5% in the corresponding pure Stark profile of the MMM, which are reduced to less than 7% if Doppler broadening is taken into account. The unified theory is, however, of only marginal validity for the ions in this density range so the difference is small wonder. The MMM value agrees very fine with the experimental result of Burgess and Mahon who estimate an upper limit of 5% for the $H-H^+$ dip at this density from their data.

Before we go further into the comparison with experiments let us mention another interesting feature of the MMM profiles including ion motion. Figure 7 gives the temperature dependence (at $N=10^{17}$ cm$^{-3}$) of the $H\alpha$ half width as it is obtained for static ions from the MMM as well as the KG theory, and for
the \( \text{H} - \text{Ar}^+ \) case from the MMM. With static ions this half width decreases towards higher temperatures in spite of the increasing Doppler broadening which is taken care of in the curves (the different magnitudes of the static ion results will be discussed later). Evidently this stems from the fact that the more rapidly fluctuating electronic microfield at high temperature is less effective in Stark broadening than the "slower" field at low temperatures\(^9\). Including ion motion in the MMM calculation, this effect is compensated at least for the temperatures covered here, and the half width is essentially constant. Collecting the relevant data of three different experiments seems to verify this prediction: At \( 10^4 \) K WKP\(^4\) find a half width slightly smaller than that predicted by KG\(^1\), HG\(^12\) report good agreement with the KG value at about \( 2 \cdot 10^4 \) K, and in another recent measurement of Okasaka et al.\(^30\), a half width distinctly greater than that of KG has been observed at \( 3 \cdot 10^4 \) K.

3. Comparison with Experimental Data

For the comparison of the theoretical MMM results to experiments we shall rely upon the measurements of WKP\(^4\) and WKH\(^9\), the latter of which was especially designed to study the influence of ion dynamics on Balmer lines. A more recent experiment by Okasaka et al.\(^30\) shows that an extrapolation to higher densities of the WKH data is possible, and

![Theoretical and experimental half widths of H-α.](image)

Fig. 8. Theoretical and experimental half widths of H-α. Beside the experimental data of Wiese et al. (WKH) and the MMM values, both for the \( \text{H} - \text{Ar}^+ \) case, theoretical curves are given which employ the static ion approximation: Kepple-Griem theory (KG), MMM, and unified theory (VCS). The plasma temperature is \( 10^4 \) K for the theoretical half widths and slightly higher (\( 1.1 - 1.3 \cdot 10^4 \) K) for the experimental ones.
with experimental half widths carries over to the MMM. Sensitive to the reduced mass is the dip of \( \text{H-} \beta \). In Fig. 9 the experimental and theoretical dips are compared for the combinations \( \text{H-} \text{H}^+ \), \( \text{H-} \text{Ar}^+ \), and \( \text{D-} \text{Ar}^+ \). In all three cases both are of the same order, but there remain discrepancies which are greatest at low densities (at \( N \approx 10^{17} \text{cm}^{-3} \) the agreement is very good) and small reduced mass. Particularly for the MMM, a possible reason for this systematic trend might be the use of the unconditioned covariance together with the special Markovian model field which does not describe the mean duration of weak fields correctly. At last let us have a look at the variation of the dip with \( \mu \). Figure 10 presents theoretical and experimental data as functions of \( \mu^{-1/2} \) for densities of \( 10^{16} \text{cm}^{-3} \) and \( 10^{17} \text{cm}^{-3} \). According to what has just been stated agreement is not too good for the lower density but excellent for the higher. Anyhow, in both cases the WKH assumption of a linear dependence on \( \mu^{-1/2} \) does work for the theoretical data.

Taking all together it is clear that the correct consideration of ion motion effects by the MMM brings theory and experiment to close agreement. This result has some bearing on the valuation of the MMM brings theory and experiment to close agreement. This result has some bearing on the valuation of the Kepple-Griem theory. In Fig. 8 the KG half width of \( \text{H-} \alpha \) is much greater than both the MMM and the VCS half width calculated with static ions, and fits the experimental curve far better. Contrary to this, the \( \text{H-} \beta \) half widths of all theories are nearly identical and coincide well with the measured width. A similar observation in their experiment has led Hey and Griem to the conclusion that there is an inconsistency in the unified theory which the KG theory avoids by a different treatment of elastic and inelastic electron collisions. An important point of the argument is the expectation that ion motion is not important in hydrogen Stark broadening as indeed all previous theoretical investigations suggest. For this reason, HG explain the small dip they observe, too, with the presence of a transition layer near the walls of their shock tube. With the agreement of VCS and "static ions" MMM profiles demonstrated in I the same criticism applies to the MMM though this is not formulated in terms of electron collisions. The present work, however, shows that the incorrect \( \text{H-} \alpha \) half width is due to the neglect of ion motion. As an example let us assume we had measured a half width of 9.4 \( \AA \) from a hydrogen-helium plasma with \( T = 2 \cdot 10^4 \text{K} \); these are approximately the conditions for some of the HG measurements. What electron density do the various theories predict from this? For KG it is \( 10^{17} \text{cm}^{-3} \), while VCS obtain \( 1.9 \cdot 10^{17} \text{cm}^{-3} \), and the MMM with static ions yields \( 1.7 \cdot 10^{17} \text{cm}^{-3} \), these last two values being definitely too high as may be seen also from Fig. 8 (the half widths depend only weakly on temperature, Fig. 7). But with ion motion included, the MMM gets 1.06 to 1.10 \( 10^{17} \text{cm}^{-3} \) according to the hydrogen-helium ratio, and this is consistent with the KG value.

With the MMM profiles (ion motion included) that close to the measured profiles, and the MMM profiles (static ions assumed) nearly the same as the
VCS-Roszman profiles, we conclude that the unified theory is correct in the frame of the static ion approximation while the broader KG profiles of H-α have the correct half width at $N \approx 10^{17} \text{cm}^{-3}$ by chance. If this is true it should show up at densities below $10^{16} \text{cm}^{-3}$ where the KG half width is well beneath that of the MMM. The measurement of Ehrich and Kusch points into this direction, and further systematic investigations of ion motion effects in low density plasmas could help to clarify the theoretical dispute of this point and would be highly valuable. At last it should be mentioned that the MMM results by no means rule out the existence of the transition layer proposed by HG, since the theoretical dips are still more pronounced than the measured ones.

4. Conclusion

The MMM introduced by Brissaud and Frisch provides a uniform unified description of electron as well as ion broadening of hydrogen lines, and allows to drop the static ion approximation of the unified theory. In the present work it has been applied to investigate the effects of ion motion on L-α, H-α, and H-β, which turn out to be much stronger than other theoretical approaches predict.

Most drastic effects result for L-α; these are in good agreement with the first measurement of the centre of this line. For H-α the structure of the line centre is reduced considerably by the influence of ion motion, and discrepancies are removed which exist with experimental profiles if the static ion approximation is employed. The incorrect half widths given by the unified theory are apparently due to this approximation, not an inconsistency in the theory as has been claimed. In the profile of H-β significant changes occur only in the central depression which is partly filled up. Near coincidence with the measured line shapes of Wiese and co-workers is obtained at $N \approx 10^{17} \text{cm}^{-3}$, but some differences remain at lower densities. For very low densities the dip vanishes of Doppler broadening is taken into account. Its dependence on the reduced mass $\mu$ of an ion-atom pair is approximately $\sim \mu^{-1/2}$ over the range of experimentally accessible values as has been conjectured from measured data.

Summing up, ion motion effects are important especially for the central portions of lines with strong unshifted components, and have to be considered if reliable line profiles are to be calculated.