ASTRONOMY
AND
ASTROPHYSICS

Simple formulae for estimating Stark widths and shifts of neutral atom lines

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Summary. Formulae for estimating Stark widths and shifts of neutral atom lines, based on the simple method of Freudenstein and Cooper and the GBKO semiclassical theory, are presented. For the calculations, most of the available personal computers are sufficient. Obtained formulae have been applied to He I and Mg I lines and results are compared with calculations of Benett and Griem and values obtained according to the method of Freudenstein and Cooper.

Key words: line profiles

1. Introduction

Astrophysicists performing calculations of radiative transfer through stellar plasma or evaluation of physical conditions in stellar atmospheres often require Stark broadening data for a large number of transitions in many atoms. To obtain these data one can use, e.g., so called semiclassical or fully quantum mechanical theoretical approaches (see e.g. Griem, 1974) which both require elaborate calculations even for a single line. To overcome this problem Cowley (1971) offered a very simple approximative formula for evaluation of neutral line widths. Here, atomic structure is taken into account in the crudest possible way only through the effective principal quantum number of the upper level of the transition. As noted by Cowley (1971) this formula gives the wrong temperature dependence. Namely, calculated Stark widths vary as a function of $T^{-1/2}$ while the widths of neutral lines usually increase with temperature (see e.g. Griem, 1974). He therefore advocates using the value at $T = 10^4$ K at all temperatures.

A simple formula for estimating Stark widths of neutral lines derived by Freudenstein and Cooper (1978) gives the correct trend of Stark width dependence upon electron temperature. Furthermore, this formula makes better allowance for atomic structure by taking into account the actual position of the closest interacting level to the upper energy level of the considered transition.

In this paper we report an approximate Stark broadening formula for even more sophisticated estimations of the line widths and extend its applicability to the evaluation of the shifts. These formulae require a complete set of interacting levels and as a consequence larger computation time per spectral line is needed.

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However, with most of the available personal computers this problem is marginal. The drawback for the application of these formulae may be the eventual lack of the complete set of perturbing energy levels for some transitions.

2. Theory

The half-halfwidth (w) and shift (d) of a neutral atom spectral line broadened by electron-impacts (Griem et al., 1962) are given by

$$w + id = \frac{4\pi}{3} N_e \left(\frac{\hbar}{m}\right)^2 \int \frac{dv}{v} f(v) \left\{ \frac{3}{4} \left(\frac{mv}{\hbar}\right)^2 \tilde{\varrho}_{\min}^2 \right.$$

$$+ \sum_{i'} \boldsymbol{R}_{ii'}^2 \left[a_{ii'} \left(z_{ii'}^{\min}\right) - i\,\varepsilon_{ii'}\, b_{ii'}\left(\tilde{z}_{ii'}^{\min}\right) \right]$$

$$\left. + \sum_{f'} \boldsymbol{R}_{ff'}^2 \left[a_{ff'} \left(z_{ff'}^{\min}\right) + i\,\varepsilon_{ff'}\, b_{ff'}\left(\tilde{z}_{ff'}^{\min}\right) \right] \right\}. \tag{1}$$

Here, $\boldsymbol{R}_{jj'}^2$ (in units of the Bohr radius a_0^2) is the square of the coordinate operator matrix element (summed over all components of the operator and over the magnetic substates of total momentum J' and averaged over the magnetic substates of J), N_e the electron density, $f(v)$ the Maxwellian distribution of the electron velocity (v), i, f denote the initial and final states and i', f' are the corresponding perturbing states within the dipole approximation. The quantity $\varepsilon_{jj'}$ determines the signs of individual contributions to the shift, viz.,

$$\varepsilon_{jj'} = (E_j - E_{j'})/|E_j - E_{j'}|$$

where E_j and $E_{j'}$ are the energies of the corresponding states. The minimum impact parameter $\varrho_{\min}$ allowed by the unitarity condition (Griem et al., 1962) is given by

$$\tilde{\varrho}_{\min}^2 = \frac{2}{3} \left(\frac{\hbar}{mv}\right)^2 \left| \sum_{i'} \boldsymbol{R}_{ii'}^2 \left[A_{ii'} \left(z_{ii'}\right) - i\,\varepsilon_{ii'}\, B_{ii'}\left(z_{ii'}\right) \right] \right.$$

$$\left. + \sum_{f'} \boldsymbol{R}_{ff'}^2 \left[A_{ff'} \left(z_{ff'}\right) + i\,\varepsilon_{ff'}\, B_{ff'}\left(z_{ff'}\right) \right] \right|, \tag{2}$$

where $a_{jj'}$, $b_{jj'}$, $A_{jj'}$ and $B_{jj'}$ are the GBKO (Griem et al., 1962; Griem, 1974) Stark broadening functions of the arguments $z_{jj'}$ and $\tilde{z}_{jj'}$,

$$z_{jj'} = \varrho(E_j - E_{j'})/\hbar v, \quad \tilde{z}_{jj'} = 0{,}75\, z_{jj'},$$

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and ϱ is the impact parameter. In the expression for $z_{jj'}^{\min}$, $\varrho_{\min}$ is used instead of ϱ. Further, we shall approximate the velocity average as $1/\bar{v} \sim (m/3kT)^{1/2}$, following the suggestion of Freudenstein and Cooper (1978), since $\langle 1/v \rangle = (2m/\pi kT)^{1/2}$ tends to weight low velocities, whereas the most important contribution to the width comes from small $z^{\min}$, corresponding to high velocities (Freudenstein and Cooper, 1978), due to the properties of the $a_{jj'}(z)$ function.

In order to simplify Eqs. (1) and (2) we introduce here the approximation

$$\left| \sum_{j'} \boldsymbol{R}_{jj'}^2 \left[A_{jj'} + i\varepsilon_{jj'} B_{jj'} \right] \right| \approx \sum_{j'} \boldsymbol{R}_{jj'}^2 \left| \left[A_{jj'} + i\varepsilon_{jj'} B_{jj'} \right] \right|, \tag{3}$$

i.e. $\tilde{\varrho}_{\min}^2 \approx \sum_{j'} \varrho_{j'}^2$.

For a series of complex numbers z_j we have

$$\left| \sum_j z_j \right| \leqq \sum_j |z_j|,$$

where the sign of equality holds in the case where all z_j have equal arguments. This means that $A_{jj'} \gg B_{jj'}$ which is satisfied for close collisions, high velocities or close perturbing levels which usually give the principal contribution to the line broadening.

The overestimation of $z_{jj'}$ by approximation (3) may be partially compensated by assuming that $z_{jj'} \approx \varrho_{j'} \omega_{jj'}/v$, which lowers the $z_{jj'}$ values.

Define

$$\eta_{jj'} \equiv |E_j - E_{j'}|/3kT.$$

Then

$$w + id \approx \left(\frac{32}{27} \right)^{1/2} N_e \pi \left(\frac{\hbar a_0}{m} \right) \left(\frac{E_{\rm H}}{kT} \right)^{1/2} \left\{ \sum_{i'} \boldsymbol{R}_{ii'}^2 \left[f_w(\eta_{ii'} \, \mathrm{R}_{ii'}) \right.\right.$$
$$\left. - i\varepsilon_{ii'} f_d(\eta_{ii'} \, \mathrm{R}_{ii'}) \right] + \sum_{f'} \boldsymbol{R}_{ff'}^2 \left[f_w(\eta_{ff'} \, \boldsymbol{R}_{ff'}) \right.$$
$$\left.\left. + i\varepsilon_{ff'} f_d(\eta_{ff'} \, \boldsymbol{R}_{ff'}) \right] \right\}, \tag{4}$$

where

$$f_w(\eta_{jj'} \, \boldsymbol{R}_{jj'}) = \tfrac{1}{2} [A^2(z_{jj'}^{\min}) + B^2(z_{jj'}^{\min})]^{1/2} + a(z_{jj'}^{\min}) \tag{5}$$

as suggested by Freudenstein and Cooper (1978) and

$$f_d(\eta_{jj'} \, \boldsymbol{R}_{jj'}) = b(\tilde{z}_{jj'}^{\min}), \tag{6}$$

To obtain $f_w(\eta_{jj'} \, \boldsymbol{R}_{jj'})$ and $f_d(\eta_{jj'} \, \boldsymbol{R}_{jj'})$ it is necessary only to solve the following equation

$$(z_{jj'}^{\min})^2 = \tfrac{2}{3} (\eta_{jj'} \, \boldsymbol{R}_{jj'})^2 [A^2(z_{jj'}^{\min}) + B^2(z_{jj'}^{\min})]^{1/2} \tag{7}$$

obtained from Eq. (2) and then to substitute the solution into Eqs. (5) and (6). Using asymptotic forms of GBKO Stark broadening functions, the following analytic expressions may be obtained. For $\eta R \gg 1$,

$$z_{jj'}^{\min} \approx [\pi (\eta_{jj'} \, \boldsymbol{R}_{jj'})^2/6]^{1/3}$$

and

$$f_w(\eta_{jj'} \, \boldsymbol{R}_{jj'}) \approx \tfrac{1}{2} [3\pi^2/32 (\eta \boldsymbol{R}_{jj'})^2]^{1/3} \approx 0,487 (\eta_{jj'} \, \boldsymbol{R}_{jj'})^{-2/3}$$

$$f_d(\eta_{jj'} \, \boldsymbol{R}_{jj'}) \approx 2 \left(\frac{\pi}{6} \right)^{2/3} (\eta_{jj'} \, \boldsymbol{R}_{jj'})^{-2/3}$$

For $\eta R \ll 1$,

$$z_{jj'}^{\min} \approx (\tfrac{2}{3})^{1/2} \eta_{jj'} \, \boldsymbol{R}_{jj'}$$

$$f_w(\eta_{jj'} \, \boldsymbol{R}_{jj'}) \approx \ln (2.27/\eta_{jj'} \, \boldsymbol{R}_{jj'})$$

$$f_d(\eta_{jj'} \, \boldsymbol{R}_{jj'}) \approx \pi/2.$$

In Fig. 1, $f_w(\eta_{jj'} \, \boldsymbol{R}_{jj'})$ and $f_d(\eta_{jj'} \, \boldsymbol{R}_{jj'})$ are presented. Approximate fitted expressions for $f_w(\eta_{jj'} \, \boldsymbol{R}_{jj'})$ (Freudenstein and Cooper, 1978) and $f_d(\eta_{jj'} \, \boldsymbol{R}_{jj'})$ are

$$f_w(x) = e^{-1.33x} \ln \left(1 + \frac{2.27}{x} \right) + \frac{0.487x}{0.153 + x^{5/3}} + \frac{x}{7.93 + x^3}, \tag{8}$$

$$f_d(x) = 1.571 e^{-2.482x} + \frac{1.295x}{0.415 + x^{5/3}} + \frac{0.713x}{8.139 + x^3}, \tag{9}$$

where $x = \eta_{jj'} \, \boldsymbol{R}_{jj'}$.

Using Eqs. (4), (8), and (9), electron-impact width and shift of neutral atom lines may be easily calculated.

One can remark here that the f_d/f_w ratio is not consistent with the well known adiabatic limit ($d/w = \sqrt{3}$). Namely, the GBKO (Griem et al., 1962) theory is fitted to the classical adiabatic limit using slightly modified unitary condition not used by Freudenstein and Cooper (1978). So we may choose it to be consistent either with Freudenstein and Cooper's (1978) results, Eqs. (8) and (9) derived in the present paper, or to obtain the classical adiabatic limit. Moreover, Dimitrijević and Grujić (1979) have demonstrated recently that the d/w ratio is strongly modified at the adiabatic limit if one takes into account the back reaction of the neutral emitter on a perturbing electron. However, if one wants it to be consistent with the classical adiabatic limit, one must use the unitary condition in the GBKO (Griem et al., 1962) form. Then Eqs. (5) and (7) become

$$f_w(x) = \tfrac{1}{2} (\tfrac{4}{3})^{3/2} [A^2(z_{jj'}^{\min}) + B^2(z_{jj'}^{\min})]^{1/2} + a(z_{jj'}^{\min}), \tag{5a}$$

$$(z_{jj'}^{\min})^2 = \tfrac{2}{3} (\tfrac{4}{3})^{3/2} x^2 [A^2(z_{jj'}^{\min}) + B^2(z_{jj'}^{\min})]^{1/2}. \tag{7a}$$

Using now Eqs. (4), (5a), and (7a) one can easily obtain shift and width in accordance with the classical adiabatic limit.

Another source of Stark broadening in stellar atmospheres are collisions with protons. We can estimate the correction to the Stark width due to the proton-impact contribution using the expression for the "quadrupole" ion-impact width (Griem, 1974) adapted for the case considered:

$$w(\text{Å}) = 0.4074 \, 10^{-26} \, N_e (\text{cm}^{-3}) \, \lambda^2 (\text{Å}) \, (n_i^{*2} - n_f^{*2})^2/Z^2. \tag{10}$$

For typical stellar conditions ($N_e \sim 10^{13} \, \text{cm}^{-3}$) the impact approximation is usually valid also for proton perturbers. The total Stark width is simply obtained by adding electron and proton impact widths.

In Eq. (10) $(Z-1)$ is the ionic charge and n_j^* the effective principal quantum number

$$n_j^{*2} = Z^2 \frac{E_{\rm H}}{E_\infty - E_j},$$

where $E_{\rm H}$ is the hydrogen ionization energy and E_∞ is the appropriate series limit.

When dipole interactions are more important, one can use the approximate formulae of Griem (1962) to calculate the full line width $w_{\rm tot}$ and shift $d_{\rm tot}$

$$w_{\rm tot} \approx 2 [1 + 1.75 \, 10^{-4} N_e^{1/4} A (1 - 0.068 N_e^{1/6} T^{-1/2})] 10^{-16} w N_e, \tag{11}$$

$$d_{\rm tot} \approx [d \pm 2.0 \, 10^{-4} N_e^{1/4} A w (1 - 0.068 N_e^{1/6} T^{-1/2})] 10^{-16} N_e, \tag{12}$$
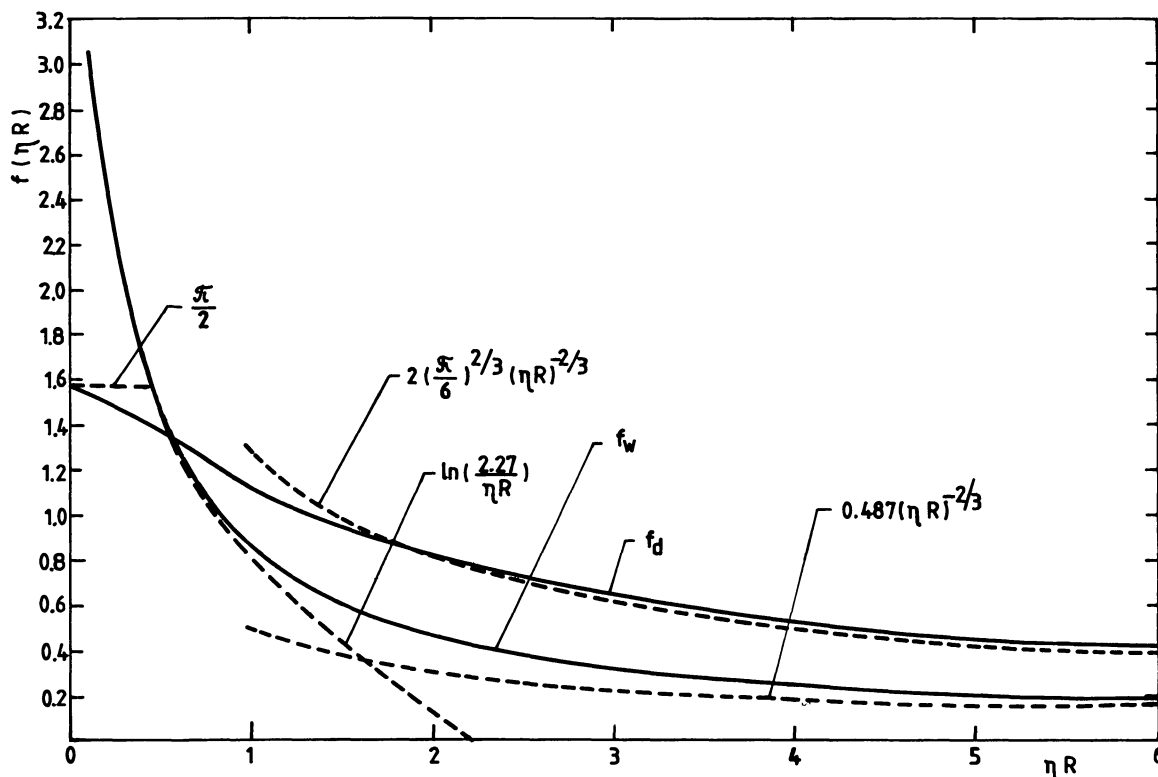
Fig. 1. A plot of the functions $f_w(\eta R)$ and $f_d(\eta R)$ as calculated from Eqs. (5) and (6) or (8) and (9) and their asymptotic limits

where w, d, and A are the electron impact half-halfwidth, shift and ion broadening parameter, respectively, all of them taken at $N_e = 10^{16}\,\mathrm{cm}^{-3}$ and at electron temperature $T(\mathrm{K})$; N_e is the electron density (cm^{-3}) at which w_{tot} and d_{tot} are to be given. There are certain restrictions to the applicability of Eqs. (11) and (12), and they are:

$$B = 8.99\ 10^{-2} N_e^{1/6} T^{-1/2} \lesssim 0.8$$

$$0.05 \lesssim A \lesssim 0.5.$$

Since we have already described the procedure for evaluating w and d, methods for the estimation of the ion broadening parameter A will be discussed here. Freudenstein and Cooper (1978) described the procedure for a crude estimation of A. However, in connection with the present work we would suggest a more sophisticated method described by Griem et al. (1962) and given also by Griem (1974, Eq. (224)). This method requires the evaluation of a number of matrix elements $\sum R_{ii'}^2$ and $\sum R_{ff'}^2$ which are also needed for the calculation of electron impact width and shift, see Eq. (4).

From Eqs. (4), (8), and (9) it is obvious that for reliable calculation of Stark widths and shifts one must use a sufficiently complete set of perturbing energy levels. Therefore, it is of importance to estimate completeness (with regard to dipole matrix elements) of perturbing levels taken for the evaluation of Stark broadening parameter. For this purpose Jones et al. in 1971 (see also Griem, 1974) introduced the parameter $\Delta S/S$ in the following way

$$\frac{\Delta S}{S} = \frac{\sum_{i'} \boldsymbol{R}_{ii'}^2 + \sum_{f'} \boldsymbol{R}_{ff'}^2 - R_{ii}^2 - R_{ff}^2}{R_{ii}^2 + R_{ff}^2},$$

where

$$R_{jj'}^2 = \frac{n_j^{*2}}{2Z^2}\,[5 n_j^{*2} + 1 - 3 l_j(l_j + 1)].$$

If this parameter is close to zero, the set of energy levels used is sufficiently complete. Another indication of the importance of inclusion of a particular perturbing level is the ratio $f_{i'i}/|E_i - E_{i'}|$, where $f_{ii'}$ is the absorption oscillator strength.

Within the one-electron approximation (Griem, 1974), i.e. using only one energy level for each nl electron, with the other quantum numbers chosen as to select the dominant contributions, the dipole matrix element $R_{jj'}^2$ for the sum of all lines originating or ending in a term SL, is

$$R_{jj'}^2 = \frac{l_>}{2l' + 1}\,R_{l'l}^2.$$

Here, $l_>$ is the greater of l, l' and $R_{l,l'}^2$ is the radial factor (Shore and Menzel, 1965).

For complex atoms it is better (Dimitrijević, 1982) to take into account every particular component of the supermultiplet. In such a case one can use the expression

$$\boldsymbol{R}_{jj'}^2 = \frac{l_> R_{\mathrm{mult}}^2 R_{l,l'}^2}{(2L + 1)},$$

were R_{mult}^2 is the multiplet factor (Shore and Menzel, 1965).

If the energy difference between the perturbing and perturbed level is comparable to the Debye (plasma) frequency, we must take into account Debye shielding corrections (see e.g. Griem, 1974). In such a case it is better to check also whether the line is isolated or not (see e.g. Dimitrijević and Sahal-Bréchot, 1984).

Table 1. Electron impact half-halfwidths w and shifts d in Angstrom units for He I and Mg I lines as a function of temperature (T): W_{DK} – present results; W_{BG} – semiclassical of Benett and Griem (1974); W_{FC} – present calculations according to Freudenstein and Cooper (1978). Electron density is $10^{16}\,cm^{-3}$

T	W_{DK}	W_{BG}	W_{FC}	d_{DK}	d_{BG}
He I 4438 Å $2p\ ^1P^0$–$5s\ ^1S$					
5000	1.46	1.41	1.34	1.73	1.51
10000	1.77	1.57	1.64	1.49	1.43
20000	1.85	1.65	1.72	1.12	1.24
30000	1.79	–	1.66	0.924	–
40000	1.72	1.62	1.60	0.803	0.996
He I 6678 Å $2p\ ^1P^0 - 3d\ ^1D$					
5000	0.468	0.423	0.948	0.236	0.275
10000	0.428	0.386	0.825	0.181	0.233
20000	0.389	0.349	0.696	0.135	0.196
30000	0.364	–	0.623	0.111	–
40000	0.344	0.318	0.573	0.096	0.161
Mg I 3835 Å $3p\ ^3P^0$–$3d\ ^3D$					
5000	0.098	0.107	0.239	-0.0266	-0.0445
10000	0.087	0.0962	0.207	-0.0170	-0.0270
20000	0.076	0.0852	0.173	-0.0111	-0.0139
30000	0.070	–	0.155	-0.0089	–
40000	0.066	0.0752	0.142	-0.0078	-0.00512

3. Results and discussion

In Table 1 present results for half-halfwidths w_{DK} and shifts d_{DK} are compared with our width calculations according to the method of Freudenstein and Cooper (1978) w_{FC} and semiclassical results w_{BG} of Benett and Griem (1972), given also by Griem (1974).

In the case of the He I 4438 Å line, the one-level approximation used by Freudenstein and Cooper (1978) is well satisfied since the $5p$ energy level contribution is dominant and all results are mutually close. In the two other examples, for the He I $2p\ ^1P^0 - 3d\ ^1D$ and Mg I $3p\ ^3P^0 - 3d\ ^3D$ lines, we have no dominant perturbing level and our results are considerably closer to the semiclassical ones than to values calculated from the simple approximate formula (Freudenstein and Cooper, 1978).

We believe that the simple formulae presented here will be useful when astrophysicists or physicists require a number of reliable atom line widths and shifts influenced by the Stark effect.

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