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MODIFIED SEMIEMPIRICAL METHOD

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A review of the application, during the years 1980 to 2000, of the modified semiempirical method developed by Dimitrijević and Konević in 1980 for calculating the parameters of Stark broadening is given and the possibility of using this method to calculate the Stark width and, in some cases, the shift of a large number of spectral lines of various atoms and a number of ions is shown.

Keywords: *line profile, Stark broadening, plasma.*

Introduction. More than twenty years have elapsed since the formulation of the modified semiempirical (MSE) approach [1] to calculation of the Stark broadening parameters for nonhydrogenic ion spectral lines. During these decades, the method has been found to be useful in solving various problems in physics and astrophysics.

In comparison with the fully semiclassical perturbation approach [2–4] and Griem's (1968) semiempirical approach [5], which need practically the same set of atomic data as the more sophisticated semiclassical one, the modified semiempirical approach requires a considerably smaller number of such data. In fact, if there are no perturbing levels that strongly violate the approximation made, then, e.g., for the line width calculations, we need only the energies of the levels with $\Delta n = 0$ and $l = l_{i,f} \pm 1$, since all perturbing levels with $\Delta n \neq 0$, needed for a full semiclassical investigation or an investigation within Griem's semiempirical approach [5], are lumped together and estimated approximately. Here, n is the principal and l the orbital angular momentum quantum numbers of the optical electron, with i and f denoting the initial and final state of the transition considered.

Owing to the considerably smaller set of needed atomic data in comparison with the complete semiclassical [2–4] or Griem's semiempirical [5] methods, the MSE method is particularly useful for stellar spectroscopy depending on a very extensive list of elements and line transitions with their atomic and line broadening parameters where it is not possible to use a sophisticated theoretical approach in all of the cases of interest.

The MSE method is also very useful whenever line broadening data for a large number of lines are required, and the high precision of every particular result is not so important as, e.g., for opacity calculations or plasma modeling. Moreover, in the case of more complex atoms or multiply charged ions, the lack of accurate atomic data needed for more sophisticated calculations makes the reliability of the semiclassical results decrease. In such cases, the MSE method might be very interesting as well.

The Modified Semiempirical Method. According to the modified semiempirical approach [1, 6–9], for electron impact broadening, the full width at half maximum of the spectral line of wavelength λ is given as

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$$W_{\mathrm{MSE}} = N \frac{8\pi}{3} \frac{\hbar^2}{m^2} \left(\frac{2m}{\pi kT} \right)^{1/2} \frac{\pi}{\sqrt{3}} \frac{\lambda^2}{2\pi c} \left\{ \sum_{l_i \pm 1} \sum_{A_{i'} J_{i'}} \overrightarrow{\mathfrak{R}}^{\,2} [n_i l_i A_i J_i, n_i (l_i \pm 1) A_{i'} J_{i'}] \, \tilde{g} (x_{l_i, l_i \pm 1}) + \right.$$

$$+ \sum_{l_f \pm 1} \sum_{A_{f'} J_{f'}} \overrightarrow{\mathfrak{R}}^{\,2} [n_f l_f A_f J_f, n_f (l_f \pm 1) A_{f'} J_{f'}] \, \tilde{g} (x_{l_f, l_f \pm 1}) + \left(\sum_{i'} \overrightarrow{\mathfrak{R}}_{ii'}^{\,2} \right)_{\Delta n \neq 0} g (x_{n_i, n_i + 1}) +$$

$$\left. + \left(\sum_{f'} \overrightarrow{\mathfrak{R}}_{ff'}^{\,2} \right)_{\Delta n \neq 0} g (x_{n_f, n_f + 1}) \right\}, \tag{1}$$

and the corresponding Stark shift as

$$d_{\mathrm{MSE}} = N \frac{4\pi}{3} \frac{\hbar^2}{m^2} \left(\frac{2m}{\pi kT} \right)^{1/2} \frac{\pi}{\sqrt{3}} \frac{\lambda^2}{2\pi c} \left\{ \sum_{A_{i'} J_{i'}} \sigma_{J_i J_{i'}} \overrightarrow{\mathfrak{R}}^{\,2} [n_i l_i A_i J_i, n_i (l_i + 1) A_{i'} J_{i'}] \, \tilde{g}_{\mathrm{sh}} (x_{l_i, l_i + 1}) + \right.$$

$$- \sum_{A_{i'} J_{i'}} \sigma_{J_i J_{i'}} \overrightarrow{\mathfrak{R}}^{\,2} [n_i l_i A_i J_i, n_i (l_i + 1) A_{i'} J_{i'}] \, \tilde{g}_{\mathrm{sh}} (x_{l_i, l_i - 1}) - \sum_{A_{f'} J_{f'}} \sigma_{J_f J_{f'}} \overrightarrow{\mathfrak{R}}^{\,2} [n_f l_f A_f J_f, n_f (l_f + 1) A_{f'} J_{f'}] \, \tilde{g}_{\mathrm{sh}} (x_{l_f, l_f + 1}) +$$

$$+ \sum_{A_{f'} J_{f'}} \sigma_{J_f J_{f'}} \overrightarrow{\mathfrak{R}}^{\,2} [n_f l_f A_f J_f, n_f (l_f - 1) A_{f'} J_{f'}] \, \tilde{g}_{\mathrm{sh}} (x_{l_f, l_f - 1}) + \left(\sum_{i'} \overrightarrow{\mathfrak{R}}_{ii'}^{\,2} \right)_{\Delta n \neq 0} g_{\mathrm{sh}} (x_{n_i, n_i + 1}) - \tag{2}$$

$$- 2 \sum_{i' (\Delta E_{ii'} < 0)} \sum_{A_{i'} J_{i'}} \overrightarrow{\mathfrak{R}}^{\,2} (n_i l_i A_i J_i, n_{i'} l_{i'} A_{i'} J_{i'} \, g_{\mathrm{sh}} (x_{l_i, l_{i'}}) - \left(\sum_{f'} \overrightarrow{\mathfrak{R}}_{ff'}^{\,2} \right)_{\Delta n \neq 0} g_{\mathrm{sh}} (x_{n_f, n_f + 1}) +$$

$$\left. + 2 \sum_{f' (\Delta E_{ff'} < 0)} \sum_{A_{f'} J_{f'}} \overrightarrow{\mathfrak{R}}^{\,2} (n_f l_f A_f J_f, n_{f'} l_{f'} A_{f'} J_{f'} \, g_{\mathrm{sh}} (x_{l_f, l_{f'}}) + \sum_k \delta_k \right\}.$$

Here, the initial level is denoted by i and the final one by f, and the square of the matrix element is

$$\overrightarrow{\mathfrak{R}}^{\,2} [n_k l_k A_k J_k, n_k (l_k \pm 1) A_{k'} J_{k'}] = \frac{L_>}{2 J_k + 1} Q [l_k A_k, l_k \pm 1) A_{k'}] \, Q (J_k, J_k') \left[R_{n_k l_k}^{* \, n_k^* (l_k \pm 1)} \right]^2, \tag{3}$$

where $k = i, f$; $l_> = \max (l_k, l_k \pm 1)$, and

$$\left(\sum_{k'} \overrightarrow{\mathfrak{R}}_{kk'}^{\,2} \right)_{\Delta n \neq 0} = \left(\frac{3 n_k^*}{2Z} \right)^2 \frac{1}{9} \left(n_k^{*2} + 3 l_k^2 + 3 l_k + 11 \right). \tag{4}$$

In Eqs. (1) and (2),

$$x_{l_k, l_{k'}} = \frac{E}{\Delta E_{l_k, l_{k'}}}, \quad k = i, f,$$

where $E = (3/2)kT$ is the electron kinetic energy and $\Delta E_{l_k,l_{k'}} = \left| E_{l_k} - E_{l_{k'}} \right|$ is the energy difference between the levels l_k and $l_k \pm 1$ ($k = i, f$),

$$x_{n_k,n_k+1} \approx \frac{E}{\Delta E_{n_k,n_k+1}},$$

where, for $\Delta n \neq 0$, the energy difference between energy levels with n_k and $n_k + 1$ is estimated as $\Delta E_{n_k,n_k+1} \approx 2Z^2 E_H/(n_k^*)^3$ and $n_k^* = [\mathrm{EHZ2}/(E_{ion} - E_k)]^{1/2}$ is the effective principal quantum number, Z is the residual ionic charge (for example, Z = 1 for neutral atoms), and E_{ion} is the appropriate spectral series limit.

In Eqs. (1) and (2), the sums

$$\sum_{l_k \pm 1} \sum_{A_{k'}J_{k'}} \overrightarrow{\mathfrak{R}}^{\,2} [n_k l_k A_k J_k, n_k (l_k \pm 1) A_{k'} J_{k'}] \, \tilde{g} (x_{l_k,l_k \pm 1}),$$

$$\sum_{A_{k'}J_{k'}} \sigma_{J_k J_{k'}} \overrightarrow{\mathfrak{R}}^{\,2} [n_k l_k A_k J_k, n_k (l_k + 1) A_{k'} J_{k'}] \, \tilde{g}_{sh} (x_{l_k,l_k+1}),$$

$$\sum_{A_{k'}J_{k'}} \sigma_{J_k J_{k'}} \overrightarrow{\mathfrak{R}}^{\,2} [n_k l_k A_k J_k, n_k (l_k - 1) A_{k'} J_{k'}] \, \tilde{g}_{sh} (x_{l_k,l_k-1}), \quad k = i, f,$$

represent contributions of the allowed dipole transitions for $l_k \to l_k + 1$ and $l_k \to l_k - 1$ for $\Delta n = 0$. In the case of the shift, where particular contributions have different signs, all transitions with $\Delta n \neq 0$ are first summed, with the squared matrix elements lumped together. From the sum obtained, the group of transitions with $\Delta E_{kk'} < 0$, $k = i, f$, is subtracted so that in Eq. (2) the sums

$$\sum_{k'(\Delta E_{kk'}<0)} \sum_{A_{k'}J_{k'}} \overrightarrow{\mathfrak{R}}^{\,2} n_k l_k A_k J_k, n_{k'} l_{k'} A_{k'} J_{k'}) \, g_{sh} (x_{l_k,l_{k'}})$$

would be present. In both equations, (1) and (2), the sums $(\Sigma_{k'} \mathfrak{R}^2_{kk'})_{\Delta n \neq 0}$ represent the combined contributions for the energy levels with $\Delta n \neq 0$.

If we know the oscillator strength, e.g., from the literature, the corresponding squared matrix element may be calculated as

$$\overrightarrow{\mathfrak{R}}^{\,2}_{kk'} \approx 3 \frac{E_H}{E_{k'} - E_k} f_{k'k}, \quad E_{k'} > E_k, \quad k = i, f,$$

or

$$\overrightarrow{\mathfrak{R}}^{\,2}_{kk'} \approx 3 \frac{E_H}{E_k - E_{k'}} \frac{2k' + 1}{2k + 1} f_{kk'}, \quad E_{k'} < E_k, \quad k = i, f,$$

where $f_{k'k}$ and $f_{kk'}$ are the oscillator strengths, E_H is the hydrogen ionization energy, and $2k + 1$ is the statistical weight for the level k.

The ultimate configuration mixing may be taken into account (see, e.g., [9]) if one represents $\mathfrak{R}^2_{\alpha\beta}$ as

$$\overrightarrow{\mathfrak{R}}^{\,2}_{\alpha\beta} = K_\alpha \overrightarrow{\mathfrak{R}}^{\,2}_{\alpha\alpha'} + K_\beta \overrightarrow{\mathfrak{R}}^{\,2}_{\beta\beta'},$$

where K_α and K_β are the mixing coefficients for the two configurations and $K_\alpha + K_\beta = 1$.

In Eqs. (1)–(4), N and T are the electron density and temperature, respectively, whereas $Q(lA, l'A')$ and $Q(J, J')$ are the multiplet and line factors. The value of A depends on the coupling approximation (see, e.g., [10]): $A = L$ for LS coupling, $A = K$ for jK coupling, and $A = j$ for jj coupling. $\left[R^{n_k^* l_k \pm 1}_{n_k^* l_k}\right]$ is the radial integral; and $g(x)$ [5], $\tilde{g}(x)$ [1] and $g_{\rm sh}(x)$ [5], $\tilde{g}_{\rm sh}(x)$ [8] denote the corresponding Gaunt factors for the width and the shift, respectively. The factor $\sigma_{kk'} = (E_{k'} - E_k)/|E_{k'} - E_k|$, where E_k and $E_{k'}$ are the energies of the level being considered and of the level perturbing it. The sum $\Sigma_k \delta_k$ is different from zero only if there are perturbing levels with $\Delta n \neq 0$ strongly violating the assumed approximations, so that they should be taken into account separately. The δ_k, $k = i, f$, may be evaluated as

$$\delta_i = \pm \vec{\mathfrak{R}}_{ii'}^{\,2} \left[g_{\rm sh}\left(\frac{E}{\Delta E_{i,i'}}\right) \mp g_{\rm sh}\,(x_{n_i, n_i+1}) \right] \tag{5}$$

for the upper level, and

$$\delta_f = \mp \vec{\mathfrak{R}}_{ff'}^{\,2} \left[g_{\rm sh}\left(\frac{E}{\Delta E_{f,f'}}\right) \mp g_{\rm sh}\,(x_{n_f, n_f+1}) \right] \tag{6}$$

for the lower level. In Eqs. (7) and (8), the lower sign corresponds to $\Delta E_{kk'} < 0$, $k = i, f$.

Simplified Modified Semiempirical Formula. For astrophysical purposes, of particular interest might be the simplified semiempirical formula [7] for the Stark widths of the isolated lines of singly and multiply charged ions. It is appreciable in the cases where the nearest atomic energy level ($j' = i'$ or f') from which a dipolarly allowed transition can occur from or to the initial (i) or final (f) energy level of the considered line, is so far that the condition $x_{jj'} = E/|E_{j'} - E_j| \leq 2$ is satisfied. In such cases, the full width at half maximum is given by the expression [7]

$$W\,[\mathring{\rm A}] = (2.2151 \cdot 10^{-8}) \frac{\lambda^2\,[\rm cm]\, N\,[\rm cm^{-3}]}{T^{1/2}\,[\rm K]} \left(0.9 - \frac{1.1}{Z}\right) \sum_{j=i,f} \left(\frac{3n_j^*}{2Z}\right)^2 (n_j^{*2} - l_j^2 - l - 1)\,. \tag{7}$$

Here, N and T are the electron density and temperature, respectively, $E = 3kT/2$ is the energy of a perturbing electron, $Z - 1$ is the ionic charge, and n^* is the effective principal quantum number. This expression is of interest for abundance calculations and also for stellar atmosphere research, since its validity conditions are often satisfied for stellar plasma conditions.

Similarly, in the case of the shift

$$d\,[\mathring{\rm A}] = (1.1076 \cdot 10^{-8}) \frac{\lambda^2\,[\rm cm]\, N\,[\rm cm^{-3}]}{T^{1/2}\,[\rm K]} \left(0.9 - \frac{1.1}{Z}\right) \frac{9}{4Z^2} \sum_{j=i,f} \frac{n_j^{*2}\varepsilon_j}{2l_j + 1} \times$$

$$\times \left\{ (l_j + 1)\,[n_j^{*2} - (l_j + 1)^2] - l_j\,(n_j^{*2} - l_j^2) \right\}. \tag{8}$$

If all the levels $l_{i,f} \pm 1$ exist, an additional summation may be performed in Eq. (10) to obtain

$$d\,[\mathring{\rm A}] = (1.1076 \cdot 10^{-8}) \frac{\lambda^2\,[\rm cm]\, N\,[\rm cm^{-3}]}{T^{1/2}\,[\rm K]} \left(0.9 - \frac{1.1}{Z}\right) \frac{9}{4Z^2} \sum_{j=i,f} \frac{n_j^{*2}\varepsilon_j}{2l_j + 1} (n_j^{*2} - 3l_j^2 - 3l_j - 1)\,,$$

where $\varepsilon = +1$ if $j = i$ and -1 if $j = f$.

Applications. The modified semiempirical approach has been tested several times on numerous examples [11]. In order to test this method, selected experimental data for 36 multiplets (7 different ion species) of triply charged ions were compared with theoretical linewidths. The averaged values of the ratios of measured to calculated widths are as follows [1]: for doubly charged ions 1.06 ± 0.32 and for triply charged ions 0.91 ± 0.42. The adopted accuracy of the MSE approximation is at about ±50%, but it has been shown in [12] and [13] that the MSE approach, even in the case of emitters with very complex spectra (e.g., Xe II and Kr II), gives very good agreement with experimental measurements (in the interval ±30%). For example, for the 6*s*–6*p* transitions of Xe II the averaged ratio between the experimental and theoretical widths of the lines is 1.15 ± 0.5 [12].

In order to complete as much as possible the needed Stark broadening data, the Belgrade group (Milan S. Dimitrijević, Luka Č. Popović, Vladimir Kršljanin, Dragana Tankosić, and Nenad Milovanović) used the modified semiempirical method to obtain the Stark width and, in some cases, shift data for a large number of spectral lines for various atoms and a number of ions. Up to now the following transitions have been calculated: 6 Fe II [14], 4 Pt II [15], 16 Bi II [9], 12 Zn II, 8 Cd II [16], 18 As II, 10 Br II, 18 Sb II, 8 I II [17], 20 Xe II [12, 18], 138 Ti II [19], 3 La II [20], 16 Mn II [21, 22], 14 V II [23, 24], 6 Eu II [20], 37 Kr II [13], 6 Y II, 6 Sc II [18, 25], 4 Be III, 4 B III [1, 6, 26, 27], 13 S III [28], 8 Au II [29, 30], 8 Zr II [18, 25, 31], 53 Ra II [32], 3 Mn III, 10 Ga III, 8 Ge III [21, 22], 4 As III, 3 Se III [33], 6 Mg III [34], 6 La III [20], 5 Sr III [35], 8 V III [23, 24], 210 Ti III [19], 9 C III, 7 N III, 11 O III, 5 F III, 6 Ne III, 8 Na III, 10 Al III, 5 Si III, 3 P III, 16 Cl III, 6 Ar III [1, 6, 26, 27], 30 Zr III [31], 2 B IV [1, 6, 26, 27], Cu IV [36], 30 V IV [23, 24], 14 Ge IV [21, 22], 7 C IV, 4 N IV, 4 O IV, 2 Ne IV, 4 Mg IV, 7 Si IV, 3 P IV, 2 S IV, 2 Cl IV, 4 Ar IV [1, 6, 26, 27], 3 C V, 50 O V, 12 F V, 9 Ne V, 3 Al V, 6 Si V, 11 N VI, 28 F VI, 8 Ne VI, 7 Na VI, 15 Si VI, 6 P VI, and 1 Cl VI [37]. The shift data have been calculated for the following transitions: 16 Bi II [9], 12 Zn II, 8 Cd II [16], 18 As II, 10 Br II, 18 Sb II, 8 I II [17], 20 Xe II [12], 5 Ar II [38, 39], 6 Eu II [20], 14 V II [23, 24], 8 Au II [29, 30], 14 Kr II [40], and 138 Ti II [19]. Moreover, 286 Nd II Stark widths have been calculated [41] within the simplified modified semiempirical approach.

For comparison with experimental data or testing the theory, calculations within the modified semiempirical approach have been performed also for the Stark width for the following transitions: 14 Al I, 46 Al II, 12 Al III [42], 1 C IV, 1 N V, 1 O VI [43, 44], 1 Ne VIII [44], 3 N III, 3 O IV, 3 F V, 2 Ne VI [45], 12 C IV [46], 4 C II, 5 N II, 3 O II, 4 F II, 3 Ne II [47], 1 N II [48], 8 S II [49], 2 Ne VII [50], 4 N III, 2 F V [51], 2 Ne III, 2 Ar III, 2 Kr III, 2 Xe III [52], 3 Si III [53], 3 Ne III, 2 Ar III, 2 Kr III, and 2 Xe III [54]. Moreover, in [55] the Stark widths and shifts for the 2 Cl II and 6 Ar III lines have been calculated.

In [56–59], reviews of the modified semiempirical approach are given. In addition to the investigation of the Stark broadening of specific spectral lines in laboratory and astrophysical plasmas, the considered method has been successfully applied, e.g., to the study of elemental abundances in early *B*-type stars [60], normal late-*B* and HgMn stars [61], and hot white dwarfs [62], investigations of abundance anomalies in stars [63], elemental abundance analyses with DAO spectrograms for 15-Vulpeculae and 32-Aquarii [64], calculation of radiative acceleration in stellar envelopes [65–69], consideration of radiative levitation in hot white dwarfs [62, 70], quantitative spectroscopy of hot stars [71], non-LTE calculations of silicon-line strengths in *B*-type stars [72], calculation and study of stellar opacities [73–79], investigations of atmospheres and winds of hot stars [80], Ga II lines in the spectrum of Ap stars [81], design and development of new lasers [82–87], spectroscopic diagnostics of railgun plasma armatures [88], investigations of 3*d* photoabsorption in Zn III, Ge V [89], Zn II, Ga III, and Ge IV [90], research of Stark broadening parameter regularities and systematic trends [91–99], calculations of radiative emission coefficients for thermal plasmas [100, 101], considerations

of plasma-wall contact [102, 103], and examination of particle-velocity distribution and expansion of a surface flashover plasma in the presence of magnetic fields [104].

The modified semiempirical method has also entered in computer codes, as, e.g., the OPAL opacity code [75], handbooks [105, 106] and monographs [59, 107, 108].

As can be seen, over the coarse of twenty years a large number of Stark broadening parameter data, calculated within the modified semiempirical approach has been provided to plasma physicists and astrophysicists. In order to make the application and use of these data easier, we are now organizing them in a database, BELDATA.

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