

MODIFIED SEMIEMPIRICAL METHOD 1980 - 2000

MILAN S. DIMITRIJEVIĆ

*Astronomical Observatory, Volgina 7, 11160 Belgrade, Yugoslavia**E-mail: mdimitrijevic@aob.bg.ac.yu*

It is more than twenty years from the formulation of the modified semiempirical (MSE) approach (Dimitrijević and Konjević, 1980) for the calculation of Stark broadening parameters for non-hydrogenic ion spectral lines. Within this period the considered method has been applied successfully many times for different problems in astrophysics and physics. Besides the Stark broadening investigation of particular spectral lines in laboratory and astrophysical plasmas, the considered method has been successfully applied e.g. for the research of elemental abundances in normal late-B and HgMn stars (Smith, 1993) and hot white dwarfs (Chayer et al, 1995b), investigations of abundance anomalies in stars (Michaud and Richer, 1992), radiative acceleration calculation in stellar envelopes (Gonzales et al., 1995), consideration of radiative levitation in hot white dwarfs (Chayer et al 1995ab), opacities for classical cepheid models (Iglesias et al., 1990), design of new lasers (Decker and London, 1998), spectroscopic diagnostics of railgun plasma armatures (Bakshi et al., 1993)... The MSE method entered in computer codes, as e. g. OPAL opacity code (Rogers and Iglesias, 1995), handbooks (Vogt, 1996) and monographies (Gray, 1992; Griem, 1997).

In comparison with the full semiclassical perturbation approach and the Griem's (1968) semiempirical approach who need practically the same set of atomic data, the modified semiempirical approach needs a considerably smaller number of such data. In fact, if there are not perturbing levels strongly violating the assumed approximation, for e.g. the line width calculations, we need only the energy levels with $\Delta n = 0$ and $\ell_{if} = \ell_i \pm 1$, since all perturbing levels with $\Delta n \neq 0$, needed for a full semiclassical investigation or an investigation within the Griem's (1968) semiempirical approach, are lumped together and approximately estimated. Here, n is the principal and ℓ the orbital angular momentum quantum numbers of the optical electron and with i and f are denoted the initial and final state of the considered transition.

Due to the considerably smaller set of needed atomic data in comparison with the complete semiclassical or Griem's (1968) semiempirical method, the MSE method is particularly useful for stellar spectroscopy depending on very extensive list of elements and line transitions with their atomic and line broadening parameters where it is not possible to use sophisticated theoretical approaches in all 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 like e.g. for opacity calculations or plasma modeling. Moreover, in

the case of more complex atoms or multiply charged ions the lack of the accurate atomic data needed for more sophisticated calculations, makes that the reliability of the semiclassical results decreases. In such cases the MSE method might be very interesting as well.

In order to complete as much as possible the available Stark broadening data for astrophysical, laboratory, laser produced and technological plasmas investigation and modeling Belgrade group (Milan Dimitrijević, Luka Popović, Vladimir Kršljanin, Nenad Milovanović, Dragana Tankosić) has applied the MSE method (Dimitrijević and Konjević, 1980, 1981; 1987; Dimitrijević and Kršljanin, 1986; Dimitrijević, 1988ab; Popović and Dimitrijević, 1997) for spectral lines Stark broadening parameters, when there is not a sufficiently complete set of reliable perturbing energy levels, for a more sophisticated semiclassical approach.

The Stark broadening data for the most intensive lines for the following atom and ion species are available:

Ar II, Fe II, Pt II, Bi II, Zn II, Cd II, As II, Br II, Sb II, I II, Xe II, La II, Au II, Eu II, Ti II, Kr II, Na II, Y II, Zr II, Sc II, Ra II, Be III, B III, C III, N III, O III, F III, Ne III, Na III, Al III, Si III, P III, S III, Cl III, Ar III, Mn III, Ga III, Ge III, As III, Se III, Zn III, Mg III, La III, V III, Ti III, Bi III, Sr III, Cu III, Co III, Zr III, B IV, Cu IV, Ge IV, C IV, N IV, O IV, Ne IV, Mg IV, Si IV, P IV, S IV, Cl IV, Ar IV, V IV, Ge IV, C V, O V, F V, Ne V, Al V, Si V, N VI, F VI, Ne VI, Si VI, P VI, and Cl VI.

In order to make the use of these data easier we are organizing them now in a database BELDATA.

For the astrophysical purposes, of particular interest might be as well the symplified version of the Modified semiempirical formula (Dimitrijević and Konjević, 1987) for Stark widths of isolated, singly, and multiply charged ion lines applicable in the cases when the nearest atomic energy level ($j' = i$ or f') where a dipolly allowed transition can occur from or to 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. Here, E is the energy of the perturbing electron and $E_{j,j'}$ energies of the initial ($j = i$) or final ($j = f$) levels and the corresponding the nearest perturbing level (j').

The modified semiempirical approach has been tested several times on numerous examples (Dimitrijević, 1990). The assumed accuracy of the MSE approximation is about $\pm 50\%$, but it has been shown in Popović and Dimitrijević (1996, 1998) that the MSE approach, even in the case of the emitters with very complex spectra (e.g. Xe II and Kr II), gives very good agreement with experimental measurements (in the interval $\pm 30\%$). For example for Xe II, $6s-6p$ transitions, the averaged ratio between experimental and theoretical widths is 1.15 ± 0.5 (Popović and Dimitrijević 1996).

In order to test the modified semiempirical approach, 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 (Dimitrijević and Konjević, 1980): for doubly charged ions 1.06 ± 0.32 and for triply-charged ions 0.91 ± 0.42 .

References

- Bakshi, V., Barrett, B.D., Boone, T.D.Jr., Nunnally, W.C.: 1993, *IEEE Transactions on Magnetics*, **29**, 1097.
- Chayer, P., Fontaine, G., Wesemael, F.: 1995a, *Astrophys. J. Suppl. Series*, **99**, 189.
- Chayer, P., Vennes, S., Pradhan, A.K., Thejll, P., Beauchamp, A., Fontaine, G., Wesemael, F.: 1995b, *Astrophys. J.*, **454**, 429.
- Decker, C. D., London, R. A.: 1998, *Phys. Rev. A*, **57**, 1395.
- Dimitrijević, M. S.: 1988a, *Bull. Obs. Astron. Belgrade*, **139**, 31.
- Dimitrijević, M. S.: 1988b, *Astron. Astrophys. Suppl. Series*, **76**, 53.
- Dimitrijević, M. S.: 1990 in *Accuracy of Element Abundances from Stellar Atmospheres* ed. R. Wehrse, Lecture Notes in Physics 356, Springer, Berlin-Heidelberg p. 31.
- Dimitrijević, M.S., Konjević, N.: 1980, *JQSRT*, **24**, 451.
- Dimitrijević, M. S., Konjević, N.: 1981 in *Spectral Line Shapes* Ed. B.Wende, W. de Gruyter, Berlin, New York p. 211.
- Dimitrijević, M.S., Konjević, N.: 1987, *Astron. Astrophys.*, **172**, 345.
- Dimitrijević, M.S., Kršljanin, V.: 1986, *Astron. Astrophys.*, **165**, 269.
- Gonzales, J.F., LeBlanc, F., Artru, M.-C., Michaud, G.: 1995, *Astron. Astrophys.*, **297**, 223.
- Gray, D.F.: 1992, *The Observation and Analysis of Stellar Photospheres*, Cambridge University Press, Cambridge.
- Griem, H. R.: 1968, *Phys. Rev.*, **165**, 258.
- Griem, H. R.: 1997, *Principles of Plasma Spectroscopy*, Cambridge Monographs of Plasma Physics 2, Cambridge University Press.
- Iglesias, C.A., Rogers, F.J.: 1992, *Revista Mexicana de Astronomia y Astrofisica*, **23**, 161.
- Iglesias C.A., Rogers F.J., Wilson B.G.: 1990, *Astrophys. J.*, **360**, 221.
- Michaud, G., Richer, J.: 1997, in *Spectral Line Shapes*, **9**, eds. M. Zoppi, L. Ulivi, *AIP Conf. Proc.*, **386**, 397.
- Popović, L.Č., and Dimitrijević, M. S.: 1996, *Astron. Astrophys. Suppl. Series*, **116**, 359.
- Popović, L.Č., and Dimitrijević, M. S.: 1997, in *The Physics of Ionized Gas*, eds. B. Vujičić, S. Djurović and J. Purić, Institute of Physics, Novi Sad, p. 477.
- Popović, L.Č., and Dimitrijević, M. S.: 1998, *Astron. Astrophys. Suppl. Series*, **127**, 295.
- Rogers, F.J., Iglesias, C.A.: 1995, in *Astrophysical Applications of Powerful Databases*, eds. S.J. Adelman, W.L. Wiese, ASP Conf. Series **78**, 31.
- Smith, K.C.: 1993, *Astron. Astrophys.*, **276**, 393.
- Vogt, H. H. editor: 1996, *Stellar atmospheres: Atomic and molecular data*, Astronomy and Astrophysics, Extension and Supplement to Vol. 2, Subvolume B, Stars and Star Clusters, Landolt-Boernstein, Group VI: *Astron. Astrophys. Volume 3*, Springer, 57.