

## Article

# The Feshbach Resonances Applied to the Calculation of Stark Broadening of Ionized Spectral Lines: An Example of Interdisciplinary Research

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**Abstract:** In the present paper, we revisit the determination of Feshbach resonances in the elastic and fine-structure cross-sections of the spectral lines of ionized atoms colliding with electrons. The Gailitis approximation will be recalled and used to calculate the Feshbach resonances. A historical point of view will be used, emphasizing the interest of interdisciplinary research, with a back and forth between physics and astrophysics. First, the theory of Feshbach (arising at end of the 1950s and beginning of the 1960s) resonances will be briefly recalled and applied to the calculation of the cross-sections. In the beginning of the 1970s, the insertion of Feshbach resonances in spectroscopic diagnostics calculations permitted researchers to interpret the intensities of solar coronal lines. Then, in the middle of the 1970s, this gave rise to the idea of including the Feshbach resonances in the calculation of electron impact broadening (the so-called “Stark” broadening) of isolated spectral lines of ionized atoms. Finally, in the recent example of the Stark broadening of the Mo VI 5d  $^2D_{5/2} - 5p \ ^2P^{\circ}_{3/2}$  line, the S-matrices will be calculated using the semi-classical perturbation formalism and will be compared to those of the more recent quantum distorted wave formalism.

**Keywords:** stark broadening; impact approximation; isolated spectral lines of ionized atoms; electronic collisions; Feshbach resonances



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## 1. Introduction

Feshbach resonances take part in elastic and fine-structure collisional electron-ionized atom cross-sections. These resonances are due to the fact that for an ion of charge  $Z$ , the colliding electron can be trapped in an excited state of the ion of charge  $Z - 1$ , which will be ejected via autoionization. This process forms Rydberg series, which converge towards the excited state of the ion of charge  $Z$ . This increases the elastic cross-section (and the fine-structure cross-section if the spin is included). First, we will place this study in the context of a historical development of the electron–ion theory of collisions in the 1960s, and in the context of the Gailitis approximation. Then, following the birth and the development of spatial astronomy at the beginning of the 1970s, we will recall that the interpretation of the line intensities of the solar corona often posed insoluble difficulties despite the use of the new developments of collisions and atomic physics developed in the 1960s. Then, we will recall that the inclusion of Feshbach resonances in the fine-structure transitions due to electron collisions permitted researchers to solve the above-cited problem and to interpret the observations. After that, going back in the middle of the 1970s and to the

theory of impact electron collisions applied to the Stark broadening of lines of ionized atoms, these astrophysical results gave rise to the idea of applying this method to the Stark broadening of the “isolated” lines (neighboring levels do not recover) of ionized atoms. So, thanks to the method developed by astrophysicists, Feshbach resonances were included in the expression of the collisional impact line Stark width. This will be detailed in the following sections. This back and forth between physics and astrophysics shows the value of interdisciplinary research. The semi-classical perturbation method developed in the 1960s has been used for the calculation of the collisional S-matrix in a first stage. Then, the quantum distorted wave method for Stark broadening, developed at the beginning of this new century, will be used, and some results of the two methods will be compared at the end of the present paper.

## 2. Historical Background: State of Knowledge at the End of the 1950s: Impact Electron Collisions Applied to Inelastic Cross-Sections and Spectral Line Stark Broadening of Ionized Atoms

### 2.1. Electron Impact (Stark) Broadening of Isolated Spectral Lines of Ionized Atoms

Thanks to the work of Baranger [1], we know that within the impact approximation (colliding interactions with perturbers are separated in time), and for isolated lines (neighboring levels do not overlap), the line profile is Lorentzian. The total width  $2w$  at half-maximum intensity of the  $(\alpha_i J_i - \alpha_f J_f)$  line is given by Baranger’s formula [1,2], where  $N_p$  is the density of the perturbers,  $f(v)$  is the Maxwell distribution of their velocities, and  $b$  is the impact parameter in the case of the semi-classical approximation, where the electron perturber is considered to be a classical particle moving on its classical trajectory. An impact semi-classical code called SCP was created in the 1960s and updated in the 1970s, 1980s, and 1990s. The theory and the method of the calculations have been recalled in [2]. Many widths and shifts for a great number of neutral and ionized atoms have been obtained and published through several research collaborations.

Baranger’s formula, giving the full width at half maximum  $2w$ , is expressed as follows:

$$\begin{aligned}
 2w &= N_p \int_0^\infty dv v f(v) \left[ \sum_{\alpha J \neq \alpha_i J_i} \sigma(\alpha_i J_i \longrightarrow \alpha J, v) + \sum_{\alpha' J' \neq \alpha_f J_f} \sigma(\alpha_f J_f \longrightarrow \alpha' J', v) \right. \\
 &\quad \left. + \sigma(\alpha_i J_i \longleftrightarrow \alpha_i J_i, v) + \sigma(\alpha_f J_f \longleftrightarrow \alpha_f J_f, v) - 2 \int_0^\infty db 2\pi b \right. \\
 &\quad \times \sum_{M_i M'_i M_f M'_f m} (-1)^{2J_f + M_f + M'_f} \begin{pmatrix} J_i & 1 & J_f \\ -M_i & m & M_f \end{pmatrix} \begin{pmatrix} J_i & 1 & J_f \\ -M'_i & m & M'_f \end{pmatrix} \\
 &\quad \left. \times \operatorname{Re} \left\{ \langle \alpha_i J_i M_i | T(v, b) | \alpha_i J_i M_i \rangle \langle \alpha_f J_f M_f | T^*(v, b) | \alpha_f J_f M_f \rangle \right\} \right] \tag{1}
 \end{aligned}$$

$N_p$  is the density of the perturbers,  $f(v)$  is the Maxwell distribution of the velocity  $v$  of the incident perturbers, and  $\sigma(\alpha_i J_i - \alpha J, v)$  is the cross-section between the initial  $\alpha_i J_i$  level and the perturbed  $\alpha J$  level (resp. final level  $\alpha_f J_f$  and  $\alpha' J'$ ), and a summation over all the perturbing levels is performed. The last term is the interference term [1–3]. The transition matrix  $T$  is related to the scattering matrix  $S$  by  $T = \mathbb{I} - S$ , and the “3j” coefficients enter the summation.

The interference term is usually negligible when the broadening of one state is vastly larger or smaller than the other; this is usually the case with K-shell transitions.

It is important to note that fine-structure effects (and, a fortiori, hyperfine structure effects) can generally be ignored, and consequently, the fine-structure components (or hyperfine components) have the same width and the same shift, which are equal to those of the multiplet. This is because the electronic spin,  $S$  (and also the nuclear spin,  $I$ ), has no time to rotate during the collision time (in the order of  $b/v$ , i.e., the mean duration of

the collision). This is only true in LS coupling. In the following, the fine structure will be neglected.

The impact broadening theory is an application of the theory of collisions.

## 2.2. Ion–Electron Inelastic Cross-Sections at the End of the 1950s: State of the Art

A review of the theoretical methods can be found in [3]. The Coulomb–Born method was used by Seaton and coworkers. Looking at Figure 4 in [3] ( $1s - 2s$  and  $1s - 2p$  hydrogenic lines), we see that for a neutral atom, the inelastic cross-section is zero at the threshold, whereas it is not the case for an ion. This is due to the Coulomb electron–ion interaction. Consequently, the total cross-section shows a discontinuity at the threshold. This requires an investigation and an explanation.

First, Feshbach [4] developed a “Unified theory of nuclear reactions”. Second, Baz [5] conducted original experiments and found that resonances appear in the elastic cross-sections below the threshold of an excited state of an ionized atom. These were called “Feshbach resonances”.

Then, Gailitis, in his famous paper [6], extended the multichannel effective radius theory to the case of a Coulomb attractive field. This led to resonances in the cross-section below the threshold of a new excited level. Average cross-sections and widths and shifts of the resonances were obtained. In addition, the main result was that the total cross-section from a given level of a positive ion is a continuous function of the energy once the average of the resonances is performed. The discontinuities due to the inelastic cross-sections are compensated for by the discontinuities in the elastic cross-sections.

The same result was obtained a few years later by Seaton [7] through the quantum defect theory.

## 2.3. The 1960s: First Quantum Close-Coupling Calculations of Ion–Electron Cross-Sections

Bely [8] developed the quantum close-coupling differential equations and a computer code leading to elastic and inelastic Be II electron cross-sections. Looking at Figure 8 in [8], which represents the variation of the collision strength  $\Omega(2s - 2s)$  as a function of the incident energy, many resonances under the threshold of the  $2p$  level are obtained. These resonances are due to excitation from the ground state  $2s$  towards a doubly excited state of neutral Be via dielectronic recombination (because the colliding electron is trapped by the upper level of the ion over the ionization level), followed by autoionization towards Be II  $2s$ .

When averaging over resonances, the total elastic + inelastic cross-section remains continuous through the crossing of the threshold. The distances between the resonances must be large compared to their widths so the series do not overlap, and interferences can be neglected. This is the result of Galitis [6]:

The problem of discontinuity has been solved.

## 3. Interdisciplinarity: Back and Forth Between Physics and Astrophysics

In the 1960s and 1970s, astrophysics researchers focused on calculating the intensities of spectral lines out of local thermodynamic equilibrium (LTE) to compare their results to observations. In the 1970s, thanks to the development of spatial instrumentation, this particularly concerned the solar corona, enabling spectroscopic diagnostics of temperatures and densities. To achieve this, they had to go back to physics, incorporating the latest advancements in the theory of electronic collisions.

### 3.1. Development of Quantitative Solar Physics at the Beginning of the 1970s: Application of Feshbach Resonances with the Gailitis Method for the Spectroscopic Diagnostics of Coronal Line Intensities

#### 3.1.1. Case of the Green Line of Fe XIV 5303 Å

The famous green line of the solar corona is a forbidden line: it is a fine-structure transition of the ground configuration  $3s^2 3p^2 P^{\circ}_{3/2} \rightarrow 3s^2 3p^2 P^{\circ}_{1/2}$ . It is an optically thin emission line formed far from thermodynamic equilibrium.

Using a model of the corona, the so-called statistical equilibrium equations, including collisional and radiative processes, must first be solved to calculate the population of each level. Then, the emitted intensity can be obtained and compared to observations. At the end of the 1960s, the obtained theoretical intensity was incompatible with the observed intensity, which had started to become very accurate. The conclusion drawn was that there was an inexplicable problem with the calculation of the fine-structure electronic cross-section.

This problem remained unresolved for many years.

Without going into details, Petrini [9], using the quantum defect theory [9], generalized the two-channel case to the n-channel case and then introduced the Feshbach resonances through the Gailitis approximation in the fine-structure levels. This permitted researchers to solve the problem (see Figure 2 in [9]).

#### 3.1.2. Case of EUV Lines of OV

At the beginning of the 1970s, thanks to satellite observations, the EUV spectral lines of the solar corona and of the chromosphere–corona transition region could be observed. The interpretation of their intensities permitted researchers to develop new models. In particular, the EUV lines of OV were used to obtain an accurate diagnostic of the electronic density. Using the OSO V satellite, simultaneous observations of the emission lines  $2s^2 \ ^1S \rightarrow 2s2p \ ^1P$ ,  $2s^2 \ ^1S \rightarrow 2s3p \ ^1P$ ,  $2s2p \ ^3P \rightarrow 2p^2 \ ^3P$  were adopted to determine the electronic density  $N_e$  from the observed intensity ratio  $I(2s2p \ ^3P - 2p^2 \ ^3P) / I(2s^2 \ ^1S - 2s2p \ ^1P)$ .

Before the work of Malinovsky [10], abnormally low electron densities were deduced from the observed ratios. Using [9] and extending [11], the insertion of Feshbach resonances in the fine-structure levels  $2s2p \ ^3P^{\circ}_J - 2s2p \ ^3P^{\circ}_J$  via the Gailitis method permitted researchers to solve the problem (see Figures 5 and 11 in [10]).

### 3.2. Middle of the 1970s: Back from Solar Coronal Lines Intensities to Electron Impact Stark Widths of Lines of Ionized Atoms

The results of [9,10] gave rise to the idea to go back to the electron impact Stark broadening of the lines of ionized atoms and to use the n-channel case to take into account the Feshbach resonances via the Gailitis method. Line 2 of Equation (1) shows that they enter the elastic and fine-structure cross-sections  $\sigma(\alpha_i J_i \leftrightarrow \alpha_i J_i, v)$ ,  $\sigma(\alpha_i J_i \leftrightarrow \alpha_i J'_i, v)$ ,  $\sigma(\alpha_f J_f \leftrightarrow \alpha_f J_f, v)$ ,  $\sigma(\alpha_f J_f \leftrightarrow \alpha_f J'_f, v)$ . Recalling that the atomic spin has no time to precess during the electronic collision, the fine structure can be neglected, and the line width of each fine-structure component is equal to that of the multiplet.

Using LS coupling and neglecting the fine structure, the elastic cross-section of the initial level  $i$  becomes  $\sigma(\gamma_i L_i \leftrightarrow \gamma_i L_i, v)$  and that of the final level  $f$  becomes  $\sigma(\gamma_f L_f \leftrightarrow \gamma_f L_f, v)$ .  $\gamma_i$  and  $\gamma_f$  represent the configurations including the total spin  $S$  (conserved during the collision), and  $L_i, L_f$  represent the orbital angular numbers of the atomic electrons.

Feshbach resonances modify the elastic cross sections  $\sigma(\gamma_i L_i \leftrightarrow \gamma_i L_i, v)$  (resp.  $L_f$ ).

In Ref. [11], a rough two-level approximation was made to obtain the contribution of the Feshbach resonances for the line width. However, although the results of the complete

calculation were introduced into the semi-classical SCP code of Sahal-Bréchet in the second half of the 1970s, they remained unpublished until 2021 [12].

To obtain the contribution of Feshbach resonances, Sahal-Bréchet [12] developed a method analogous to that of [9,10], in which the quantum coupled representation of the ion + electron system is used.

The quantum results are given by Equations (4) and (5) in [12], which is in free access. They are recalled as follows:

$$(\Delta T)^2 = \sum_{\alpha_1 l_1 L_1} \frac{\left| T(k\alpha l L L^T; k_1 \alpha_1 l_1 L_1 L^T) \right|^2 \left| T(k_1 \alpha_1 l_1 L_1 L^T k; \alpha l L L^T) \right|^2}{\sum_{\alpha_2 l_2 L_2} \left| T(k_1 \alpha_1 l_1 L_1 L^T; k_2 \alpha_2 l_2 L_2 L^T) \right|^2} \quad (2)$$

$$\Delta\sigma(k\alpha L \longleftrightarrow k\alpha L) = \frac{\pi}{k^2} \frac{1}{2L+1} \sum_{l L^T} (2L^T + 1) (\Delta T)^2,$$

Index 1 concerns closed shells, and index 2 concerns open shells. The elements of the T-matrix are calculated for energies just above the new threshold and extrapolated under the new threshold. The incident electron kinetic energy is  $\hbar^2 k^2 / (2m)$ .

Continuing to refer to [12], to enter the results in the semi-classical SCP computer code, the semi-classical perturbation approximation of Equations (4) and (5) in [12] has to be obtained. Therefore, the incident electron becomes a classical particle moving on a hyperbola with impact parameter  $b = l/k$ . The orbital angular momentum  $l$  of the electron and its projections are conserved. The incident electron kinetic energy is also conserved. The S and T matrices are diagonal in  $l$ , and their elements do not depend on  $m$ .

The decoupling representation must be used for going from the coupled quantum representation towards the semi-classical representation. This requires some angular algebra calculations. The results are given by Equations (7) and (8) in [12], which are recalled as follows:

$$\Delta\sigma(k, \alpha L \longrightarrow k, \alpha L) = \sum_{\alpha_1 L_1} \sigma(k_1, \alpha L \longrightarrow \alpha_1 L_1) \frac{A(\alpha_1 L_1 \longrightarrow \alpha L)}{\sum_{\alpha_2 L_2 < \alpha_1 L_1} A(\alpha_1 L_1 \longrightarrow \alpha_2 L_2)} \quad (3)$$

where  $A(\alpha_1 \longrightarrow \alpha L)$  and  $A(\alpha_1 L_1 \longrightarrow \alpha_2 L_2)$  are the spontaneous emission transition probabilities. The above Equation (3) has been included in the SCP computer code.

Some examples of the SCP effects of Feshbach resonances as a function of temperature can be found in Table 3 in [2] for the Ne VIII ion and in Table 3 in [12] for the C IV ion. Table 3 in [12] shows that the contribution of Feshbach resonances leads to a 50% increase in the line width at  $0.5 \times 10^4$  K and only a 26% increase at  $3 \times 10^4$  K. In addition, for C IV 3s–3p (Figure 1 in [13]), the results are shown for temperatures between  $1.57 \times 10^4$  K and  $1 \times 10^5$  K. This decrease with the increase of the temperature is indeed expected since the contribution of inelastic collisions increases. The conclusion is that the effect of Feshbach resonances is not negligible, but it is not as important as in the case of the intensities of the coronal lines. However, they cannot be omitted and have been included in the SCP computer code.

#### 4. Quantum Distorted Wave Approximation and Superstructure for the Atomic Structure Applied to Electron Impact Broadening in Intermediate Coupling

At the beginning of this new century (2004), a quantum impact broadening theory and a numerical code denoted as QDWS were developed to calculate the widths of ions with the distorted wave approximation for the calculation of the S-matrix and with the SUPERSTRUCTURE code to calculate the atomic structure in intermediate coupling [14].

The method is not based on the calculation of the various cross-sections, as in the semi-classical calculations (Equation (1)), but on the calculation of the elements of the **S**-matrix.

The impact width is given by Equation (12) in [15] in LS coupling and generalized by Equations (4) and (5) in [15] in intermediate coupling.

In a first step, the Feshbach resonances were not included in this QDWS code. Corresponding results of calculations for Be-like lines were published in [15]. On the one hand, the figures linked to these calculations (Figure 1 in [15] for instance) show that the behavior of the quantum distorted wave widths compared to experiments is incorrect at low temperatures because they increase with the temperature and are smaller than the experimental results; on the other hand, the semi-classical ones (which contain the Feshbach resonances), always agree with the experimental results, which decrease with the temperature. At high temperatures, the Feshbach resonances are quite negligible; then, the quantum calculations agree with the experiments, as do the semi-classical ones.

In a second step, the Feshbach resonances were included in the QDWS code with the Gailitis method where the quantum distorted wave S-matrix was extrapolated under the thresholds for the corresponding inelastic processes. The first obtained results were published in [13]. The behavior of the widths, compared to the available experiments and to other theoretical results, such as the semi-classical ones, is correct and always decreases with the temperature. The inclusion of the Feshbach resonances improves the QDWS formalism, and consequently, the QDWS widths are found to be in agreement with experiments and with other theoretical results.

### 5. Comparison of Results Between the Quantum-Distorted Wave-Superstructure and the Semi-Classical Perturbation Calculations on the Example of Mo VI 5d <sup>2</sup>D<sub>5/2</sub> – 5p <sup>2</sup>P<sup>o</sup><sub>3/2</sub>

We present here a comparison between the QDWS and the SCP results. The atomic data (i.e., the levels and oscillator strengths between the levels) have been calculated with SUPERSTRUCTURE, where seven configurations have been considered: 4p<sup>6</sup>[4d, 5s, 5p, 4f, 5d, 6s, 6p]. Then, the QDWS widths and the SCP widths have been calculated for an electron density equal to 10<sup>17</sup> cm<sup>-3</sup> and six temperatures: 5.0 × 10<sup>4</sup>, 7.5 × 10<sup>4</sup>, 10<sup>5</sup>, 2.0 × 10<sup>5</sup>, 5 × 10<sup>5</sup>, 7.5 × 10<sup>5</sup> K. In Table 1, we display the total widths at half maximum W (FWHM) in Å and the contribution of the Feshbach resonances.

**Table 1.** Stark widths of the Mo VI 5d <sup>2</sup>D<sub>5/2</sub> – 5p <sup>2</sup>P<sup>o</sup><sub>3/2</sub> line according to the QDWS method (W<sub>Q</sub>) and according to the SCP method (W<sub>SCP</sub>). Feshbach<sub>Q</sub>/W<sub>Q</sub> is the relative contribution of Feshbach resonances to the QDWS. (Feshbach<sub>SCP</sub>/W<sub>SCP</sub>): (Resp. to the SCP) width. The last column gives the relative contribution of the elastic collisions to the SCP width.

T(K)	W <sub>Q</sub> (Å)	W <sub>SCP</sub> (Å)	W <sub>Q</sub> /W <sub>SCP</sub>	Feshbach <sub>Q</sub> /W <sub>Q</sub>	Feshbach <sub>SCP</sub> /W <sub>SCP</sub>	Elast/W <sub>SCP</sub>
50,000	0.0151	0.0136	1.107	0.857	0.0933	0.518
75,000	0.0124	0.0114	1.089	0.713	0.0816	0.505
100,000	0.0108	0.0101	1.074	0.703	0.0708	0.497
200,000	0.0079	0.00774	1.020	0.356	0.0437	0.474
500,000	0.0051	0.00566	0.905	0.158	0.0183	0.444
750,000	0.0041	0.00501	0.824	0.107	0.0118	0.435

Several conclusions can be drawn from the results presented in Table 1:

- The relative contribution of the elastic (close) collisions decreases when the temperature increases.
- In general, the two results—QDWS and SCP—are not very different for the chosen temperature range; in fact, the relative error between them varies from 2 to 18%.



- QWDS and SCP results become much closer to each other when the elastic collisions become less important. This is because the elastic collision contributions are taken into account differently in the QWDS and the SCP methods.
- As expected, the contribution of Feshbach resonances decreases when the temperature increases for the two calculations (QWDS and SCP).
- Even the Feshbach resonances have the same behavior with temperature for the two formalisms; their contributions (columns 5 and 6) are much more important for the quantum calculations than for the semi-classical ones. This remains unexplained and requires further investigations.
- The last column (column 7) shows that the relative contribution of the elastic collisions to the SCP full width is important, which is expected because the chosen temperatures are not very high.
- At low temperatures, the QWDS widths are higher than the SCP ones. However, when the temperature increases, the elastic collisions and Feshbach contributions decrease, and the SCP results become higher. This conclusion confirms that the difference between the two formalisms comes principally from the evaluation of these contributions to the full width. This requires further investigations which are beyond the scope of the present paper. However, the existing comparisons with laboratory measurements (3s–3p spectral lines of Li-like ions [13]) show that the SCP and QWDS results both agree with the experimental ones within 10–20%.

Finally, it is recommended to include Feshbach resonances in calculations of line Stark broadening of ionized atoms, even for high temperatures where their contribution is not important.

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