

Improved Stark Broadening in Prism Applications

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The bound-bound line profile is an important aspect of any plasma spectroscopic simulation. Spectral broadening generally consists of Doppler, natural, and Stark components. Doppler broadening is due to the motion of the radiator ion, resulting in a Gaussian profile for a thermal plasma, the width of which is rather trivial. Natural width is due to the finite lifetime of the upper level of the spectral line, which can include both radiative and Auger decays, resulting in a Lorentzian profile, and is independent of plasma conditions. Stark broadening is the most complex component, and is often the dominant one at typical HEDP conditions. It is due to the interaction of the radiator ion and the electric fields generated by background electrons and ions. Stark broadened profiles are generally asymmetric, and have non-trivial dependence on plasma density and temperatures. For plasma simulation codes such as *PrismSPECT*, it is computationally prohibitive to generate line shapes using the standard theory of Stark broadening codes such as MERL [1, 2]. Most models approximate the Stark profiles as isolated Lorentzian shapes, the width of which can be determined with various approximations. The final profile of a spectral line is the convolution of three components, leading to a Voigt function.

1 Quasi-contiguous Approximation

The original stark broadening model in *PrismSPECT* is mostly based on the electron impact approximation, and width parameters are taken from the handbook of Griem [3]. For some H-like and He-like transitions of a few elements, analytic fitting formulae based on MERL calculated line profiles are used. The main drawback of the electron impact approximation is that it does not take into account the ion contributions, and breaks down at very high densities. The model is therefore not adequate except for those transitions that have MERL-based analytic fits.

As part of this project, we implemented a new model that is based on the quasi-contiguous (QC) approximation of [4], and the modifications introduced in [5]. The method starts with the electron impact FWHM calculated with the Baranger's formula and supplemented by static ion contributions computed using an analytic fitting formula for the ion micro-field distribution. The parameters entering the quasi-contiguous approximation have been calibrated with detailed Stark broadening calculation using MERL on a variety of K-shell and L-shell transitions covering a wide range of plasma conditions. Comparisons of the *PrismSPECT* Stark broadening FWHM and those from MERL are shown in Figure 1 for

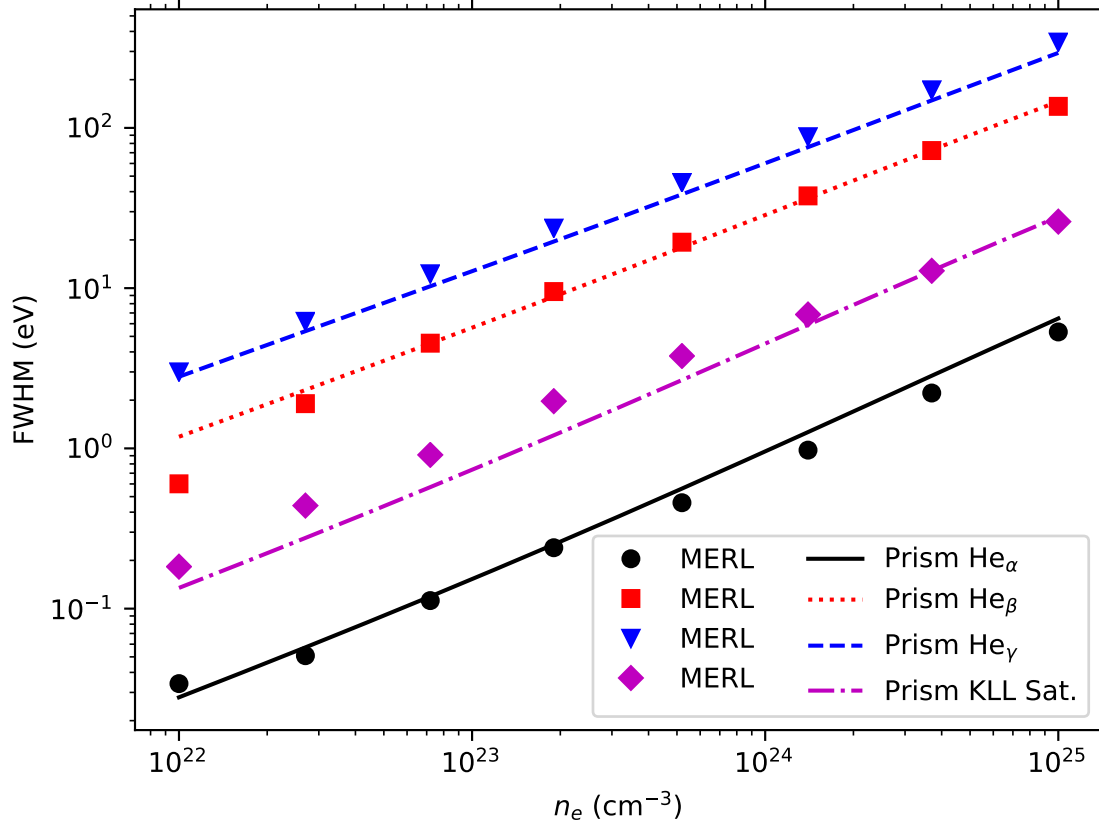


Figure 1: Comparison of Stark broadening FWHM of He-like Ar transitions and the Li-like KLL satellites computed with *PrismSPECT* model and the MERL code.

He-like Ar transitions and the Li-like KLL satellite lines to the He_α , demonstrating good agreements.

2 MERL Profile Database

While the QC model provides reasonably accurate line widths, it is still based on symmetric Lorentzian profile for Stark broadening. It is well known that Stark broadened line profiles generally contain complex structure, and are often asymmetric at high densities. We have developed a numerical line profile database¹ using a modified version of Multi-Electron Radiator Lineshape (MERL) code. MERL is based on the standard theory of Stark broadening, where electron broadening is treated in the impact approximation and effects of ions are

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included with a quasi-static micro-field distribution.

$$I(\omega) = \int d\epsilon Q(\epsilon) J(\omega, \epsilon), \quad (1)$$

where $Q(\epsilon)$ is the static ion micro-field distribution, and $J(\omega, \epsilon)$ is the electron collision broadened line profile in the presence of electric field ϵ . $J(\omega, \epsilon)$ is computed as a trace of an tetradic operator involving the Liouville operator for the time evolution of the system.

$$J(\omega, \epsilon) = \frac{-1}{\pi} \text{Im} \sum_{aba'b'} \rho_a d_{b'a'} [\omega - L_r(\epsilon) - M(\omega)]_{a'b', ab}^{-1} d_{ab}, \quad (2)$$

where ρ_a is the population of level a , d_{ab} is the dipole matrix emelent, $L_r(\epsilon)$ is the Liouville operator, and $M(\omega)$ is the electron broadening operator. A modified version of MERL has been developed as part of this project, with a stream-lined interface to the atomic data generated by the Flexible Atomic Code (FAC), and a parallelization strategy based on the photon energy and micro-field strength points.

The full MERL profile depends on the relative populations of the upper levels of the transition array. This creates a problem for making numerical tables to be used in NLTE kinetic codes like *PrismSPECT*, where populations and line profiles can be coupled. In this work, we decompose the full profile into components, such that the total profile is the population weighted sum of individual components by rewriting Equation 2 as

$$J(\omega, \epsilon) = \sum_a \rho_a J_a(\omega, \epsilon) \quad (3)$$

and the micro-field integrated profile as

$$I(\omega) = \sum_a \rho_a I_a(\omega). \quad (4)$$

Such a decomposition is mathematically equivalent to the original full profile. However, $I_a(\omega)$ may still contain multiple components if there are multiple lower levels in the transition array. Tabulation of such multi-centered profiles require a large photon energy grid. We make a further approximation,

$$I(\omega) = \sum_{ab} \rho_a A_{ab} I_{ab}(\omega), \quad (5)$$

where A_{ab} is the Einstein Coefficient of the transition between fine structure levels, a and b , and $I_{ab}(\omega)$ is the profile of a transition specific component. Although the full MERL profile generally cannot be decomposed in such a way due to interference between different components, we observe that it is a reasonable approximation, at least for the stronger components of the full profile. Figure 2 shows an example of this decomposition for the KLL satellite transitions of He-like Ar. The entire transition array is comprised of a total 22 fine structure transitions.

The profile components $I_{ab}(\omega)$ are calculated on a grid of electron temperature, density, ion temperature, and charge of perturbing ions with MERL. Each component is fitted with

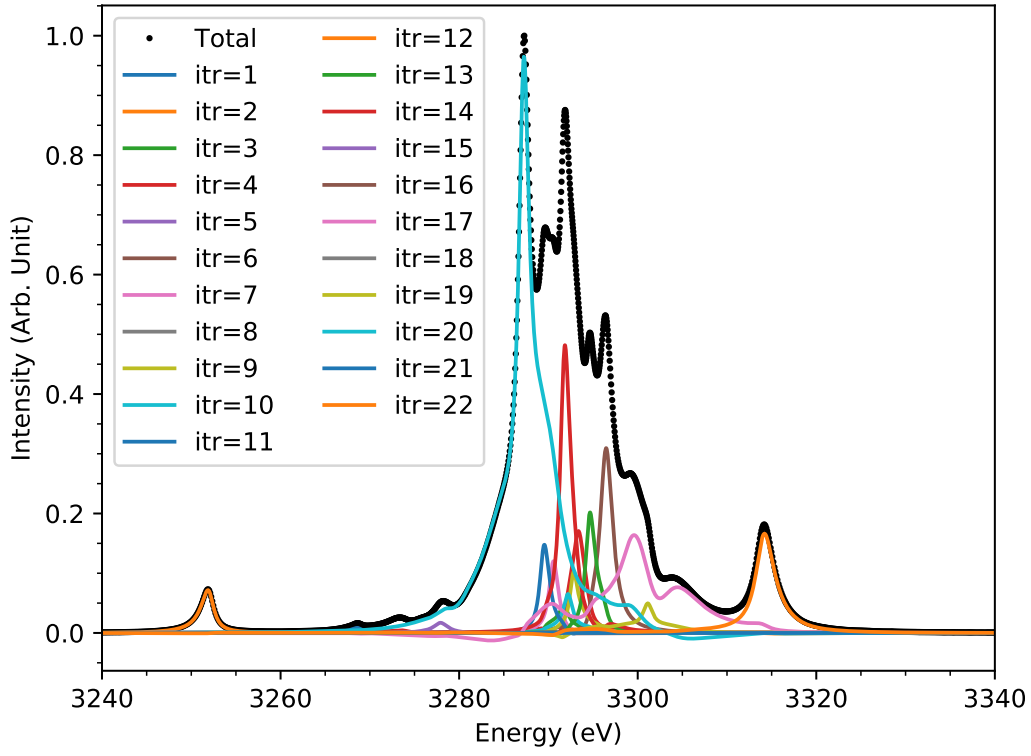


Figure 2: Transition specific decomposition of MERL profile of the KLL satellite lines of He-like Ar at $T_e = 1$ keV and $n_e = 5 \times 10^{23} \text{cm}^{-3}$.

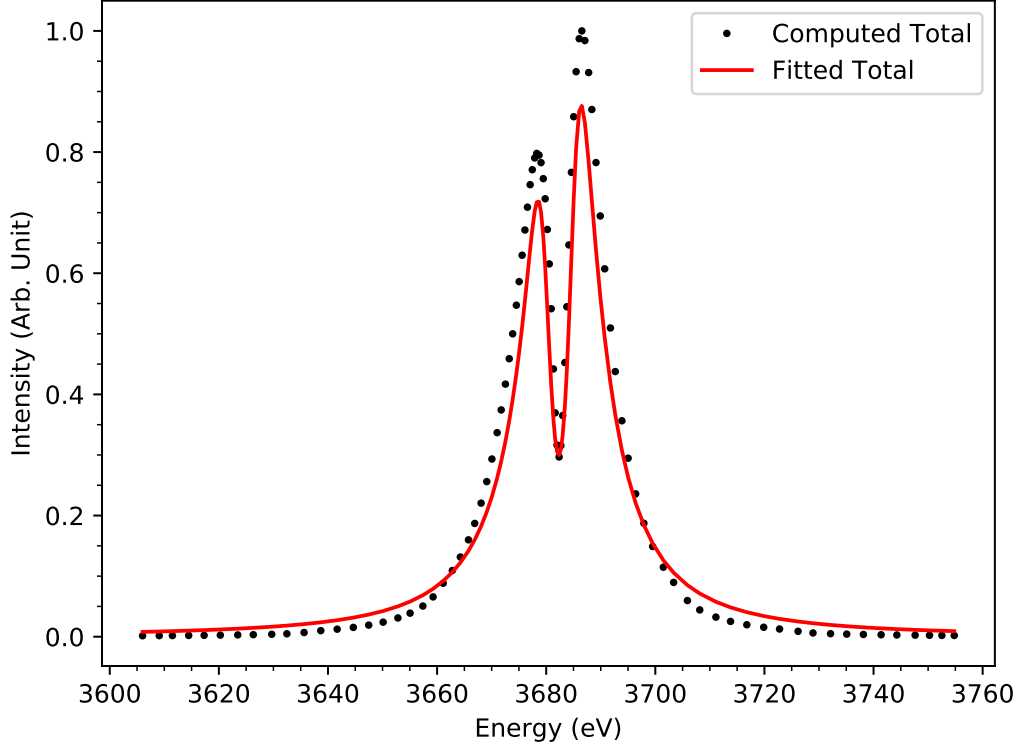


Figure 3: Computed and fitted profiles of He β line of Ar at $T_e = 1$ keV and $n_e = 5 \times 10^{23} \text{cm}^{-3}$.

a parametrized formula

$$I_{ab}(\omega) = C e^{-S} L(\gamma, \omega - \omega_0), \quad (6)$$

$$S = G(A, \sigma, \omega - \omega_0 - \delta) \quad (7)$$

where $L(\gamma, \omega - \omega_0)$ is a Lorentzian profile with HWHM= γ and centered on the transition energy ω_0 . $G(A, \sigma, \omega - \omega_0 - \delta)$ is a Gaussian function with standard deviation σ , amplitude A , and centered on $\omega_0 + \delta$. C ensures proper normalization. We use the Lorentzian profile here because the computed profiles do not include Doppler broadening intentionally. The Stark profiles calculated here will be convolved with Doppler broadening in the final step of producing model emissivities. The purpose of the Gaussian absorption-like feature is to reproduce the complex structure of some profiles calculated with MERL, such as a central dip in He β lines, as shown in Figure 3. Surprisingly, the same parameterization works reasonably well for lines like He γ , which has two shoulders on both sides of a narrower central peak, as shown in Figure 4. To demonstrate the quality of the fit for more complex transitions, we show the sum of the fitted components of KLL satellite lines of He-like Ar, and compare that with the total profile computed with MERL in Figure 5.

A systematic calculation has been carried out for $Z=1-36$ elements. Transitions covered include H-like Lyman α , β , and γ series, Balmer α and β , Paschen α , their He-like counter

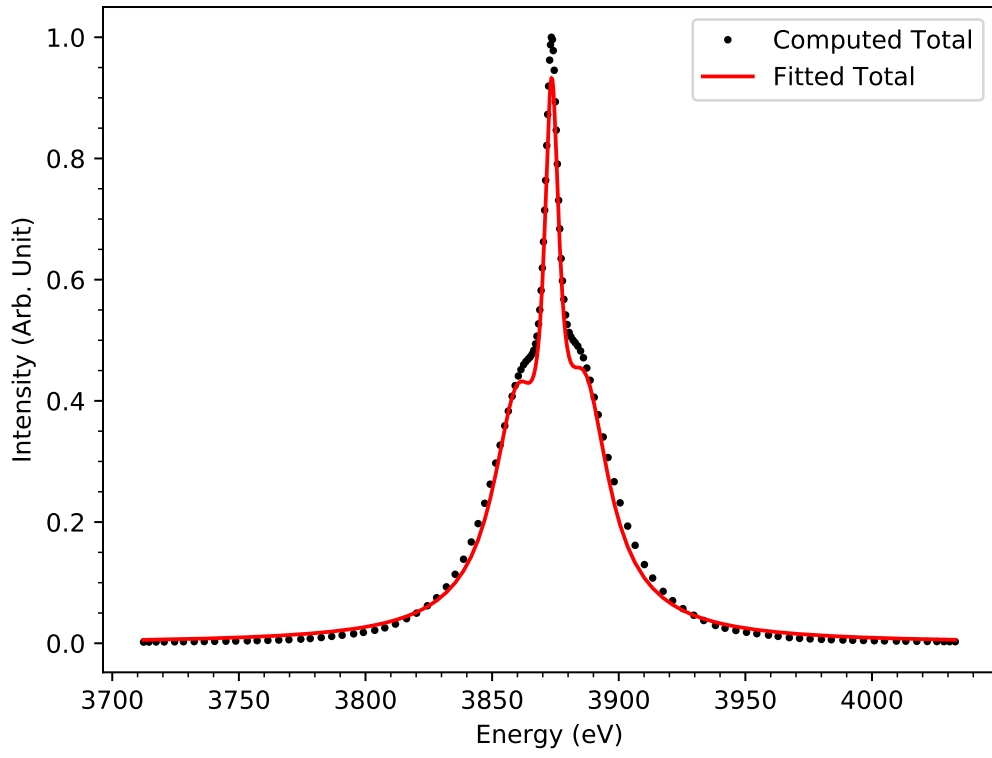


Figure 4: Computed and fitted profiles of He γ line of Ar at $T_e = 1$ keV and $n_e = 5 \times 10^{23} \text{cm}^{-3}$.

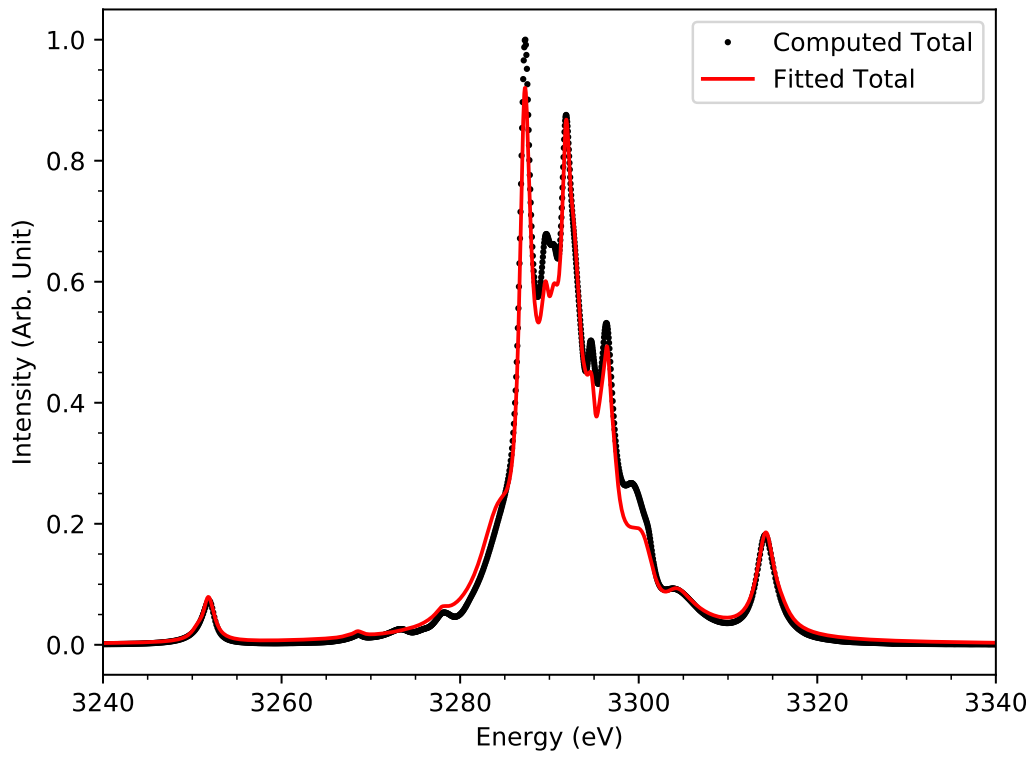


Figure 5: Computed and fitted profile of KLL satellite transitions of He-like Ar at $T_e = 1$ keV and $n_e = 5 \times 10^{23} \text{cm}^{-3}$.

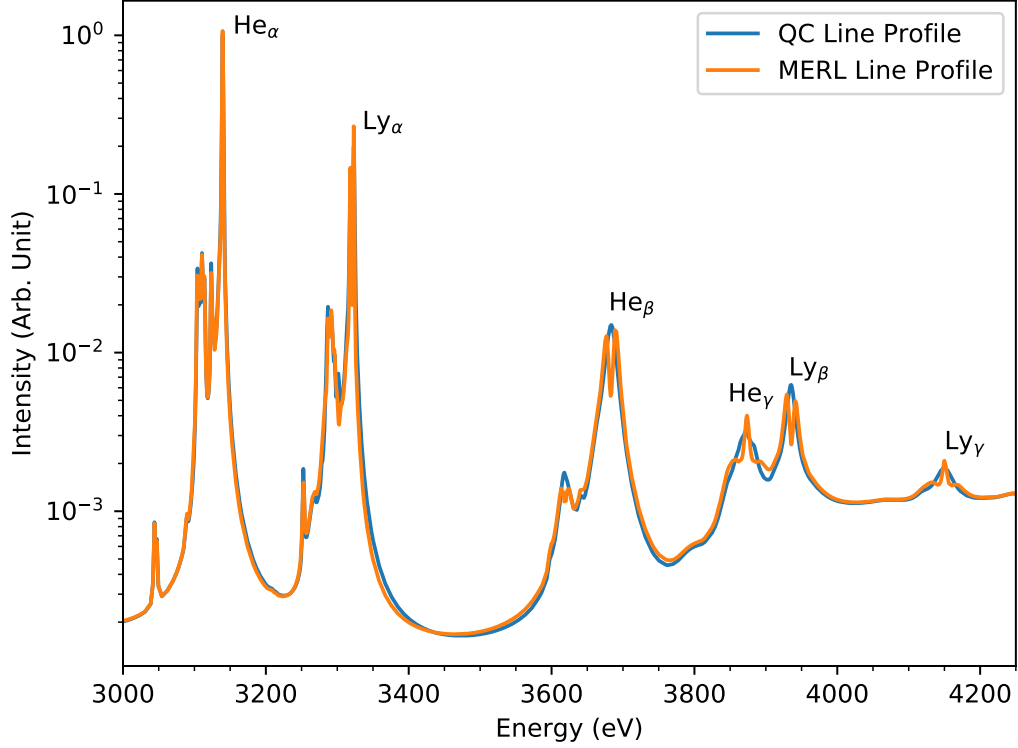


Figure 6: Ar K-shell emission at $T_e = 1$ keV and $n_e = 5 \times 10^{23} \text{cm}^{-3}$. Line profiles computed from the QC model and from the new MERL database are compared.

parts, and KLL, KLM satellite transitions in He-like, Li-like, and Be-like ions. The fitted parameters are tabulated in a database, which are integrated into the Prism spectroscopic software tools, such as *PrismSPECT* and *Spect3D*. Figure 6 demonstrates the effects of this new line profile model on the emissivities of Ar K-shell transitions, as compared to the QC model. One can clearly see that the profiles using the database show more complex structures typical of Stark broadening, instead of symmetric Voigt functions as in the QC model.

References

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