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Spectral line shapes of L-shell transitions in Ne-like iron

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Abstract. Photon-energy-resolved large-scale opacity calculations employ Stark broadened spectral line shapes only to account for the contribution of K-shell line transitions. Detailed ion broadening effects are not considered for L- and M-shell transitions. We present Stark broadening calculations for the line profiles of L-shell transitions linking ground state and singly excited states in Ne-like iron ions. These detailed line shapes have been computed in the standard Stark broadening theory approximation taking into account the effect of both static ions and dynamic electrons. The results show the importance of the ion's effect on the line broadening of several L-shell line transitions.

1. Introduction

The calculation of photon-energy-resolved opacities in plasmas depends on atomic physics, equation of state, and spectral line shapes. When the case of application involves L- and M-shell line transitions the calculation becomes challenging because of the very large number of transitions that have to be taken into account. In addition, if the density is sufficiently high so that the broadening of the spectral line shapes by the electric microfields of electrons and ions in the plasma is important, i.e. the Stark broadening effect, then the computation of the spectral line shapes themselves becomes an issue. Spectral line shapes are critical in plasma opacity calculations since their broadening, blending and degree of overlapping can change the opacity by significant amounts. In turn, this can impact the radiation transport and energetics of the plasma.

Currently, spectral line shapes in large scale opacity calculations involving L- and M-shell transitions are modelled as Voigt line profiles that account for natural, Doppler and an impact broadening contribution due to collisions with plasma electrons [1-5]. Detailed ion broadening effects are not considered. However, the splitting and shifting of atomic energy levels due to the Stark effect produced by the ion's microfield distribution can lead to the occurrence of forbidden (field-dependent) line transitions as well as significant changes to the broadening and shape of the line profiles. The key to overcome this limitation in the spectral line shapes of L- and M-shell transitions in large-scale opacity calculations is to develop both suitable theory approximations and fast algorithms that will permit the consideration of detailed ion broadening effects.

Furthermore, the discrepancies found between theory results and observations in iron opacity experiments performed at the Z Facility of Sandia National Laboratories [6] motivate, among other efforts, an examination of the spectral lines shapes of L-shell transitions in Ne-, F- and O-like iron ions. Here, we discuss the case of Stark-broadened spectral line shapes of Ne-like iron for the case of transitions linking the ground state and singly excited states.

2. Line profile calculations

The Stark-broadened spectral line shape calculations were performed with the multi-electron radiator line shape code MERL [7-9]. The physics model implemented in MERL computes the line profile within the scope of the standard Stark broadening theory approximation [10], i.e. assuming the effects of static ions and dynamic electrons. The electric microfield distribution function was computed with the APEX model and code [11], and the required atomic physics data (fine structure energy levels and reduced electric dipole matrix elements) were obtained using Cowan's atomic structure code [12].

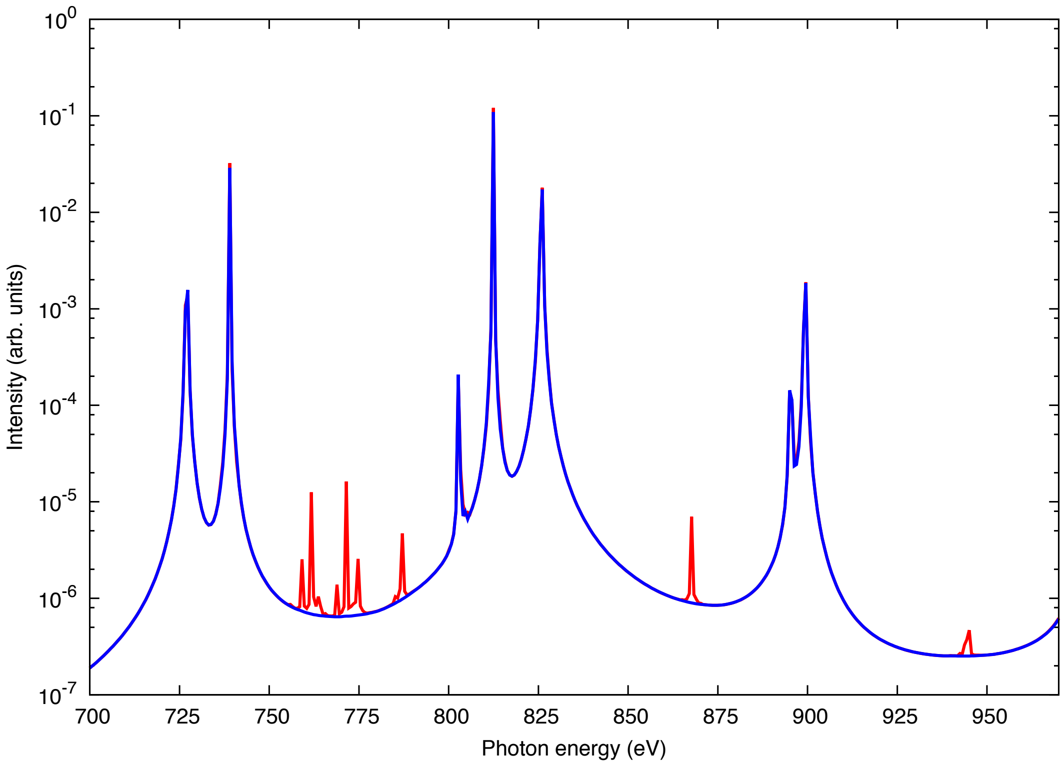

Figure 1. Stark-broadened Ne-like iron L-shell spectrum due to line transitions between the ground state and singly excited n=3 energy levels. Blue: result not including static ion's effect. Red: result including static ion's effect.

Figures 1 and 2 display the results of the line shape calculations done for an electron temperature T_e=195 eV and an electron density N_e=1x10^{22} cm^{-3}. The ion temperature was assumed to be equal to that of the electrons, and the plasma composition was 50/50 iron/magnesium. These plasma conditions are relevant to those of the iron opacity experiments performed at the Z Facility [6]. Fig. 1 shows the 700 eV to 970 eV photon energy range which has contributions from n=2-3 line transitions, while Fig. 2 shows the 970 eV to 1350 eV range which is dominated by contributions from n=2-4, n=2-5, n=2-6 and n=2-7 line transitions. The upper energy levels of the transitions were populated with a Boltzmann factor, i.e. an equilibrium distribution of population was assumed. This assumption can be easily removed since MERL can read in as part of the input data that defines a case of application, a non-equilibrium population distribution [8,13]. The ionization potential of Ne-like iron is 1263 eV. In both figures the effect of the static ions is emphasized by showing results not including and including the contribution from the plasma ions to the line shape calculation, i.e. performing the calculation for a zero value of the ion's microfield versus calculating the electron broadened line shape as a function of the ion's microfield value and then integrating it over the microfield distribution function. On the one hand, and for these plasma conditions, the effect of ion broadening in the n=2-3 line transitions is negligible and the Stark broadening is dominated by the collisions with the electrons (see Fig. 1). We note that the peaks between the main spectral features represent forbidden transitions that arise due to the ion's field mixing effect. On the other hand, Fig. 2 shows that the ion's effect is more important for line transitions arising from n=4, 5, 6 and 7. This is illustrated by both the appearance of forbidden components and the effect on the broadening and shape of the line profile of the integration over the ion's microfield distribution function.

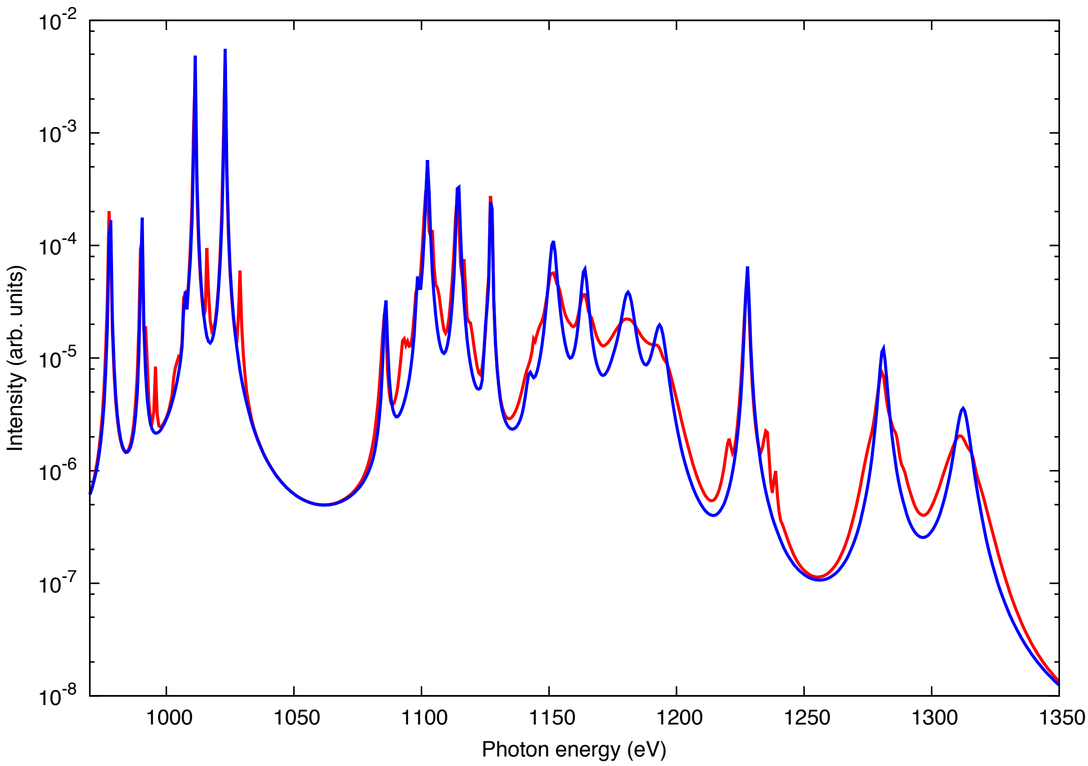

Figure 2. Ne-like iron L-shell spectrum due to line transitions between the ground state and singly excited n=4, 5, 6 and 7 energy levels. Blue: result not including static ion's effect. Red: result including static ion's effect.

3. Conclusions

In order to illustrate the effect of the ion's contribution to the Stark broadening of the L-shell spectrum of Ne-like iron for line transitions between the ground state and singly excited states, a detailed Stark broadening calculation has been performed for plasma conditions relevant to the iron opacity experiments performed at the Z Facility [6]. The ion's contribution impact the spectral line shape through the appearance of forbidden components and by changing the broadening and shape of the line profiles. Including these detailed line profiles in the analysis of the L-shell transitions observed in the iron opacity experiments at Z can further constrain the analysis of the data. To this end, work is in progress to use these line shapes in opacity calculations, consider additional electron density values and transitions involving doubly excited states, and perform line profile calculations for L-shell line transitions in F- and O-like iron ions.

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