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## LETTER TO THE EDITOR

# Electron-impact broadening of Sr<sup>+</sup> lines in ultracold neutral plasmas

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#### Abstract

We report on calculations of electron-impact broadening of  $Sr^+$  spectral lines in ultracold neutral plasmas. Optical absorption imaging of an ultracold Sr plasma has recently been used to infer detailed *in situ* information on the ion dynamics. We modify our recent treatment of collisional broadening in He metastable lines to the collision of electrons from  $Sr^+$  ions. The required scattering matrix elements are obtained from an *ab initio R*-matrix calculation.

(Some figures in this article are in colour only in the electronic version)

Electron collisions with ions can lead to excitation and broadening of ionic spectral lines. The latter effect is of particular importance as a diagnostic tool in high-temperature plasmas. In stellar interiors, electron broadening of lines is a major contributor to radiative acceleration [1]. Knowledge of elastic scattering, excitation, ionization and recombination in collisions between an electron and an atomic or molecular ion is fundamental to our understanding of such diverse processes as the x-ray laser [2] as well as inertial and magnetic confinement. Intense recent interest in creating ultracold Rydberg atoms and corollary plasmas in magneto-optical traps also herald a new area for studying electron collisional broadening [3, 4].

Scattering of electrons from partially screened positive ions presents a non-trivial problem for the theory of atomic collisions. Whereas, for a totally bare nucleus, the differential elastic scattering is described in both classical and quantum mechanical formulations through the well-known Rutherford formula, the scattering from a partially dressed ion embodies the physics of the long-range (Coulomb) and the short-range (polarization) forces. This subject has received scant attention to date [5, 6]. Only recently, direct measurements of the elastic scattering differential cross sections have become possible [7]. Indirectly, the pronounced minima in the differential cross sections [8] were interpreted, using a path-integral formulation, as the result of binary encounters between electrons and the projectile ions [9].

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In a recent experiment with an ultracold neutral Sr plasma, Simien *et al* [10] employed the  $(5s)^2 S_{1/2}$ - $(5p)^2 P_{1/2}$  absorption line in Sr<sup>+</sup> to measure the ion equilibration rate during the initial stage of plasma formation and to obtain detailed information on plasma coupling. In the above experiment, with ion densities around  $5 \times 10^9$  cm<sup>-3</sup>, the principal contributor to line broadening is Doppler broadening during the expansion of the plasma.

In this work, we investigate *electron collisional* broadening of Sr<sup>+</sup> lines. Specifically, we employ the impact approximation [11–13] to obtain the line broadening and shift parameters for various conditions of an Sr<sup>+</sup> ultracold plasma. In this approximation, the shift and broadening of a perturbed atomic line are linearly proportional to the perturber density and depend on the scattering phase shift for binary collisions before and after the absorption or emission of radiation. The impact approximation is a valid approximation near the line centre for the parameters of the above experiment, since  $\omega \tau_c \sim 0.02$ . Here  $\omega$  is the angular frequency corresponding to the Sr<sup>+</sup>(5s–5p) transition wavelength of 421.7 nm while  $\tau_c$  is the average collision time in a plasma of density  $n = 5 \times 10^9$  cm<sup>-3</sup> at an electron temperature of  $T_e \sim 70$  K.

Treating the e<sup>-</sup>–Sr<sup>+</sup> collision in the *LS*-coupling scheme, the broadening (*w*) and shift (*d*) of the  ${}^{2}S_{1/2} - {}^{2}P_{1/2}$  spectral line due to electron collisions can be written [12] as

$$w - \mathrm{i}d = \frac{\hbar^2 \pi n}{m_e^2} \int_0^\infty \frac{f(v)}{v} \,\mathrm{d}v \sum_{L_{\alpha,\beta}Sll'} \frac{(2L_{\alpha} + 1)(2L_{\beta} + 1)(2S + 1)}{(2S^{(i)} + 1)(2S + 1)} (-1)^{l_{\alpha}^{(i)} + l_{\alpha}^{(i')} + l_{\alpha}^{(i')} + l_{\beta}^{(i)} l_{\beta}} \left\{ \begin{array}{c} L_{\beta}L_{\alpha} 1\\ l_{\alpha}^{(i')} l_{\beta}^{(i)} l_{\ell} \end{array} \right\} \\ \times \left\{ \begin{array}{c} L_{\beta}L_{\alpha} 1\\ l_{\alpha}^{(i')} l_{\beta}^{(i')} l_{\ell} \end{array} \right\} \left[ \delta_{ll'} \delta_{l_{\alpha}^{(i)} l_{\alpha}^{(i')} \delta_{l_{\beta}^{(j)} l_{\beta}^{(i')}} - S_{l_{\alpha}^{(i')} l \to l_{\beta}^{(i)} l_{\ell}} (v) S_{l_{\beta}^{(i)} l \to l_{\beta}^{(i)} l_{\ell}}^{*(L_{\beta}, S)} (v) \right].$$
(1)

Here *L* and S = 0, 1 denote the total orbital and spin angular momenta of the electron-ion collision complex, the superscript (*i*) refers to the quantum numbers for the ion, *l* and  $m_e$  are the electron angular momentum and mass,  $s^{(i)}$  and *s* are the ion and electron spins,  $\alpha$  and  $\beta$  refer to the states before and after absorption or emission of radiation and primed quantum numbers are used for states after the collision. Furthermore,  $S_{l_{\alpha}^{(i)} \mid -l_{\alpha}^{(i)} \mid l}^{(L_{\alpha}, S)}(v)$  and  $S_{l_{\beta}^{(i)} \mid -l_{\beta}^{(j)} \mid l}^{*(L_{\beta}, S)}(v)$  are, respectively, the short-range scattering matrices before and after the absorption or emission of radiation. The scattering matrix elements for this work were calculated using the *R*-matrix method. Some details of the model are described below. We also average over the relative electron-ion Maxwell-Boltzmann velocity distribution, f(v) [13]. For the particular collision we consider here,  $l_{\alpha}^{(i)} = 0$ ,  $L_{\alpha} = l$ ,  $l_{\beta}^{(i)} = 1$  and  $L_{\beta} = l - 1, l, l + 1$ . A more compact and instructive form can be written after tailoring the above form for the

A more compact and instructive form can be written after tailoring the above form for the width and shift parameters to the  $e^- + Sr^+$  collision. This yields

$$w - \mathrm{i}d = \pi \left(\frac{\hbar}{m_e}\right)^2 n \sum_l \int_0^\infty \frac{f(v)}{v} \,\mathrm{d}v \left[1 - \frac{1}{4} S_l^{(\alpha,0)}(v) S_l^{(\beta,0)}(v) - \frac{3}{4} S_l^{(\alpha,1)}(v) S_l^{(\beta,1)}(v)\right]$$
(2)

where

$$S_l^{(\alpha,\delta)}(v) \equiv S_{0l \to 0l}^{(l,\delta)}(v) \tag{3}$$

and

$$S_{l}^{(\beta,S)}(v) \equiv \frac{1}{3} \sum_{L=|l-1|}^{l+1} \frac{2L+1}{2l+1} S_{1l\to 1l}^{*(L,S)}(v).$$
(4)

In the above expressions, we have assumed isolated lines, an assumption that imposes l = l'. Since the collisions occur both before and after absorption or emission of radiation, at some relative energy,  $\epsilon = \hbar^2 k^2/2$ , the long-range contribution to the total scattering matrix,  $\exp(i\eta_l)$ , with  $\eta_l$  denoting the Coulomb phase shift, does not enter in the calculation of the total scattering matrix. Note that for the low energies of interest, scattering from the 5s ionic state is purely elastic, while inelastic, superelastic and *l*-changing elastic transitions are all possible in electron scattering from ions in the 5p state.

The shift and broadening of the spectral lines can be re-written in a form resembling formulae for cross sections [13] as

$$w - \mathrm{i}d = n \sqrt{\frac{8kT}{\pi m_e}} \langle \sigma_{\beta\alpha} \rangle \tag{5}$$

where the energy averaged cross section is

$$\langle \sigma_{\beta\alpha} \rangle = \int_0^\infty \sigma_{\beta\alpha} \gamma \,\mathrm{e}^{-\gamma} \,\mathrm{d}\gamma \tag{6}$$

with  $\gamma = \epsilon/kT$ . The broadening and shift cross section

$$\sigma_{\beta\alpha} = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left[ 1 - \frac{1}{4} S_l^{(\alpha,0)}(v) S_l^{(\beta,0)}(v) - \frac{3}{4} S_l^{(\alpha,1)}(v) S_l^{(\beta,1)}(v) \right]$$
(7)

has real and imaginary parts due to the bilinear products of *S*-matrix elements in the above expression. The real part is always positive, while the imaginary part can be positive or negative.

It is also worth mentioning that while the total elastic cross section for  $e^-$ -ion collisions diverges owing to the long-range Coulomb interaction, the broadening and shift parts of the cross section are still finite, because the influence of the Coulomb long-range interaction in the initial and final channels cancels out exactly [12], leaving only the short-range part of the *S*-matrix. In this sense, measurements of the broadening and shift parameters in electron—ion collisions indirectly probe the short-range interactions.

The short-range S-matrix elements used in this work were calculated for a total of seven orbital angular momenta, L = 0 - 6, and both total spin channels (S = 0, 1). These results were obtained by performing a three-state *R*-matrix calculation for  $e - Sr^+$  scattering, in which the 5s, 5p and 4d states of Sr<sup>+</sup> were included in the close-coupling plus correlation expansion. For the very low energies of interest in this work, such a small close-coupling expansion is expected to be sufficient, provided the Sr<sup>+</sup> target is described very accurately. The scattering calculation was performed using the Belfast *R*-matrix code RMATRX-I [14] for the inner region with a box radius  $a = 18.7a_0$  ( $a_0 = 0.529 \times 10^{-10}$  m denotes the Bohr radius) and 25 continuum orbitals to represent each projectile angular momentum. Finally, the scattering matrices for each energy were generated with the FARM code of Burke and Noble [15].

The necessary accurate target description mentioned above was achieved by starting with the Hartree–Fock core orbitals for the ground state of  $Sr^+$ , as given by Clementi and Roetti [16]. These core-orbitals (1s–4s, 2p–4p and 3d) were then used to generate the Hartree core potential before adding semi-empirical local exchange and polarization potentials to simulate the response of the core to the valence electron and, ultimately, the projectile electron. We used the program of Bartschat [17] to optimize the various parameters needed for these potentials and obtained very good (better than 0.1% accuracy) ionization energies for the target states of interest. We can also judge the accuracy of the subsequent collision calculation by comparing the scattering phase shifts obtained in the elastic 5s channel with quantum defects calculated



**Figure 1.** The real and imaginary parts of the broadening and shift cross section  $\sigma_{\beta\alpha}$ .

from the spectrum of neutral Sr [18]. After including the dielectronic core polarization term to account for two electrons outside of the  $Sr^{2+}$  core, excellent agreement was obtained for the various *LS*-symmetries, thereby giving us confidence in the collision results. Note that the scattering from the 5s state can essentially be predicted by extrapolating the quantum defects from the bound spectrum of neutral Sr into the low-energy continuum.

Figure 1 displays the broadening and the shift, i.e., the real and imaginary parts of the  $\sigma_{\beta\alpha}$  cross section as a function of collision energy. The structures seen in the vicinity of 0.45 eV are due to resonances, which strongly affect electron collisions with Sr<sup>+</sup> in the 5p state in several partial waves, even at energies just above threshold.

Finally, figure 2 displays our results for the electron-impact broadening and shift of the  $Sr^+$  (5p  $\rightarrow$  5s) spectral line as a function of electron temperature. The broadening at a currently typical plasma density of  $10^{10}$  cm<sup>-3</sup> is still about two orders of magnitude smaller than the Doppler broadening at a temperature of 70 K. However, already with a modest increase in plasma density and lower temperatures, conditions that are likely to be achieved in the very near future, electron collisions are expected to become an important mechanism for line broadening and the plasma dynamics in general.



Figure 2. The broadening and shift of the Sr<sup>+</sup> (5p  $\rightarrow$  5s) line through electron collisions as a function of electron temperature for a plasma density of  $10^{10}$  cm<sup>-3</sup>.

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