# **Widths and shifts of spectral lines in He II ions produced by electron impact**

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In this paper, we report relativistic quantum mechanical calculations of widths and shifts of spectral lines in He II ions produced by electron impact. We use the Dirac  $R$ -matrix method to treat  $(N + 1)$ -electron collision systems to obtain scattering matrices. The present calculations ensure that the atomic structure and collisional data on adequate accuracy are used in our electron-impact broadening technique. A detailed comparison of our results with available experimental and theoretical results shows that our results are typically closer to the experimental ones even for the H*α* line.

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## **I. INTRODUCTION**

Atomic data such as spectral line widths and shifts produced by collisions between charged particles and emitters are of special interest for precise plasma spectroscopy of stellar atmospheres as well as for diagnosing astrophysical and laboratory plasmas. Line profile data are a powerful diagnostic tool for the detection of internal plasma parameters like electron density, electron temperature, and ion density. The line broadening parameters not only affect the solar and stellar opacities, but also play a key role in stellar interior modeling, in the determination of the surface gravity and chemical abundance of elements, and in the estimation of radiation transfer in stellar atmospheres. For laboratory plasma diagnostics such as in shock wave tubes, pulsed arc plasma, and dense z-pinch plasma [\[1\]](#page-5-0), the emission spectra of helium and He-like ions are very interesting due to their simple atomic structure. Modern fusion devices, ITER and JET, operate part of the time in helium because of its low activation requirements and lower H-mode threshold [\[2\]](#page-5-0). Recently, spectroscopic electron temperature and electron density measurements in the recombining deviator region and in multifaceted asymmetric radiation from the edge (MARFE) in the National Spherical Torous Experiment (NSTX) using deuterium I and helium II (He II) high-*n* series line emission have been performed [\[3\]](#page-5-0). Broadening of Paschen  $\alpha$  He II at 4686 Å and Paschen  $\beta$  He II at 3203 Å is routinely used to determine electron density  $[4,5]$  $[4,5]$ . In the astrophysical context, for example, investigating the combined He II and H I *Ly*-*α* forest could mainly provide an independent strategy for estimating the temperature and the thermal state of the intergalactic medium [\[6\]](#page-5-0). Many O-type or Wolf-Rayet stars and galaxies or the central region of planetary nebulae having an effective temperature higher than 2 eV emit large features of He II emission lines [\[7\]](#page-5-0), which provide information on the He abundance, plasma characteristics, and radiative properties of these objects. The accurate determination of electron-impact broadening parameters of He II spectral lines is a challenging task from both the experimental and the theoretical aspects.

In laboratory experiments, He II spectral lines are frequently used to determine the electron (ion) density of a variety of plasmas. For this requirement, several studies over the past four decades have attempted to visualize the shifts and widths of spectral lines in He II ions. Pittman *et al.* [\[8\]](#page-5-0) measured the shift of  $H_\alpha$  (1640 Å) and  $P_\alpha$  (4686 Å) spectral lines under a set of plasma conditions. The authors generated the reasonable estimated shift of 0.125 Å for  $P_\alpha$  at an electron density of 10<sup>17</sup> cm<sup>-3</sup>. Fleurier *et al.* measured a line shift of 4686 Å over the electron density range of  $1-6 \times 10^{17}$  cm<sup>-3</sup> at an electron temperature of 4 eV [\[9\]](#page-5-0). The derived value of the line shift at an electron density of  $10^{17}$  cm<sup>-3</sup> is 0.155 Å. In dense z-pinch plasma, the width and shift of the He II Balmer-*α* line was measured by Ahmad [\[1\]](#page-5-0) using a low-density hollow cathode lamp under different plasma conditions. The Stark broadening parameters and Stark line profiles of the first three lines in the He II Paschen series measured in a pulsed discharge lamp were reported by Rodrígues *et al.* [\[5\]](#page-5-0), along with the dip measurements of the  $P_\beta$  (3203 Å) line. On the theoretical side, Griem *et al.* [\[10\]](#page-5-0) used the semiclassical impact-parameter method to study shifts of He II lines in the first three spectral series caused by electron collision. These calculations of shifts in the Paschen and Balmer lines were found to be in agreement with the observed values [\[8\]](#page-5-0), while for the Lyman lines all the present theoretical models were found to be unsatisfactory. In a semiclassical perturbation approach, Dimitrijievic<sup> $et$  *et al.* [\[11\]](#page-5-0) calculated electron-impact line widths</sup> and shifts of He I lines. For low-density plasmas (*<*1018 cm3), Blaha *et al.* [\[12\]](#page-5-0) calculated the line shift of Lyman-*α* of He I by distorted-wave approximation. The shift and width of some spectral lines in He II ions were calculated by Stobbe*et al.* [\[13\]](#page-5-0) using quantum statistical many-particle theory. This approach produced a shift of the  $P_\alpha$  line in excellent agreement with the measured one, whereas the shifts of the  $H_{\alpha}$  line were much less than the experimental results. In principle, various theoretical models indicate significant discrepancies with the experimental results. More accurate and detailed calculations of the width and shift of spectral lines are needed or even new theoretical techniques are required to address the real questions regarding these deviations between theory and experiments. The present relativistic quantum mechanical calculations of the

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<span id="page-1-0"></span>line shift and width may prove to be a much better theoretical model to provide high-accuracy line shift and width data for He II ions than the earlier results.

Spectral lines of ions in a plasma have long been known to be shifted by interactions with charged particles. Theoretical estimates of line shift show large deviations from true values of experiments compared to the line width values. Apart from this reason, a general question relevant to line shift arises, whether or not such line shift is the cause of the deviation from the average charge neutrality of plasma in the vicinity of emitting ions, i.e., plasma polarization [\[14\]](#page-5-0). Despite the existence of various theoretical techniques and experimental approaches to understand the spectral line shift in dense plasmas, like plasma polarization shift, the subject still remains controversial. The major contribution to line shift is believed to be due to electron impact on emitters. According to a theoretical [\[14\]](#page-5-0) study, the line shift and width of He II ions become approximately linearly proportional to the electron concentration in the density range  $10^{17}$  cm<sup>-3</sup>, but at sufficiently higher electron densities, the line shifts and widths do not sustain this linear behavior.

This article reports calculations of the line shift and width of He II ions, and in particular, we focus here on the intent to determine the line shifts in He II ions. We report our results on the line shift and width in He II ions within the framework of impact approximation theory. We have used the relativistic Dirac *R*-matrix method to calculate the electron collision strength of He II ions using DARC codes (DARC hereafter) and the General Purpose Relativistic Atomic Structure Package (GRASP0-10.10) [\[15\]](#page-5-0) included in DARC to calculate target states up to the principal quantum number  $n = 5$ . The rest of the paper is organized as follows. In Sec. II, the basic theoretical and computational methods are described and explained. In Sec. III, we present the results for *Ly*-*α*, *Ly*-*β*, *H<sub>α</sub>*, and *P<sub>α</sub>* lines and compare them with the available experimental and theoretical results. The conclusions are summarized in Sec. [IV.](#page-5-0)

## **II. THEORY AND COMPUTATIONAL METHODS**

Theoretical details on the relativistic quantum mechanical formalism and computational procedure for measuring widths and shifts of spectral lines produced by electron impact can be found elsewhere and do not need to be repeated here. For the sake of completeness of our calculations, we only describe here the final expression relating the widths and shifts of spectral lines. This final quantum mechanical formalism has been obtained by many authors independently, including Baranger [\[16\]](#page-5-0), Seaton [\[20\]](#page-5-0), Barnes and Peach [\[17\]](#page-5-0), and Bely and Griem [\[18\]](#page-5-0), by averaging over the Maxwellian distribution of electron velocities, i.e.,

$$
w + id = \alpha N_e \int_0^\infty T_e^{-3/2} \exp(-\varepsilon/T) \Omega(\varepsilon) d\varepsilon, \qquad (1)
$$

where  $\alpha = 2.8674 \times 10^{-23}$  eV cm<sup>3</sup>,  $T_e$  is the electron temperature (in eV),  $N_e$  is the electron density (in cm<sup>-3</sup>), and  $\varepsilon$  is the energy of colliding electrons [in Rydbergs (Ry)]. The quantities 2*w* and *d* are the full width at half-maximum (FWHM) and the shift of spectral lines, respectively, and both are expressed as electron volts. The dimensionless collision strength  $\Omega(\varepsilon)$  has been derived and defined by many authors [\[19–22\]](#page-5-0):

$$
\Omega(\varepsilon) = \sum_{J_i^{\tau} J_j^{\tau} j j' \ell \ell'} \frac{1}{2} (-1)^{J_i + J_{i'} + 2J_j^{\tau} + j + j'} (2J_i^{\tau} + 1) \times (2J_f^{\tau} + 1) \left\{ \frac{J_f^{\tau}}{J_i} \frac{J_i^{\tau}}{J_f} \frac{1}{j} \right\} \left\{ \frac{J_f^{\tau}}{J_{i'}} \frac{J_i^{\tau}}{J_{f'}} \frac{1}{j'} \right\} \times \frac{1}{2} \left[ \delta_{\ell \ell'} \delta_{jj'} \delta_{J_i J_{i'}} \delta_{J_f J_{f'}} - S_I (J_{i'} \ell' j' J_i^{\tau}, J_i \ell j J_i^{\tau}) \times S_f^* (J_{f'} \ell' j' J_f^{\tau}, J_f \ell j J_f^{\tau}) \right],
$$
\n(2)

where the two coefficients of the type  $\{... \}$  are the  $6 - j$ symbols [\[23\]](#page-5-0).  $J_i$  and  $J_f$  are the quantum numbers for a transition between the lower and the upper states of a target ion (i.e., radiator), respectively. The orbital angular momentum quantum number and total angular momentum quantum number of a colliding electron are designated by  $\ell$  and *j*, respectively, and all of the quantum numbers of  $(N + 1)$  $e$ lectron colliding systems (colliding electron  $+$  target ion) are characterized by the superscript  $\tau$ .  $S_I$  and  $S_F$  (the superscript asterisk represents the complex conjugate matrix) are the scattering matrices of the upper and lower state, respectively, and they are calculated under the same free energy *ε* of colliding electrons.

To accomplish our numerical calculations, we initially calculated the atomic structure data (electronic orbital, energy levels, and energy states) of target He II ions using the atomic structure program GRASP0-10.10 included in DARC [\[15\]](#page-5-0). In GRASP0-10.10 calculations, we have adopted the extended average level mode among the four types of optimization modes for self-consistent calculations, which can assign a configuration of a given weight automatically. This provides a compromise set of atomic orbitals describing closely lying states with appropriate accuracy. With these atomic structure data, a set of  $(N + 1)$ -electron colliding systems is constructed and solved by DARC published by P. H. Norrington and I. P. Grant. For a given colliding system, a**K** matrix, i.e., a reactance matrix (a real symmetric matrix), is obtained. To complete our calculations, we have obtained **S** matrices from the **K** matrices by using the following real and imaginary parts of the **S** matrices:

$$
\text{ReS} = \frac{1 - \mathbf{K}^2}{(1 + \mathbf{K}^2)},\tag{3a}
$$

$$
ImS = \frac{2K}{(1 + K^2)}.
$$
 (3b)

These two expressions were used in our numerical calculations. In order to obtain the **S** matrix from the **K** matrix, we have developed a code.

#### **III. NUMERICAL RESULTS AND DISCUSSION**

The atomic structure data on He II target ions are calculated for 12 nonrelativistic configurations (1*s*, 2*s*, 2*p*, 3*s*, 3*p*, 3*d*, 4*s*, 4*p*, 4*d*, 5*s*, 5*p*, 5*d*) which give rise to 19 bound states. The first 14 states are chosen as the target states. Subsequently, the atomic structure data (electronic orbitals, energy levels, energy states) are read by the DARC package as input data to construct the  $(N + 1)$ -electron colliding system, which consists of an upper or lower state of the desired transition

<span id="page-2-0"></span>





×

<span id="page-3-0"></span> $\times 10^{17}$  cm<sup>-3</sup>. Numbers in

TABLE II. Calculated shifts

*d*

d (in Å) for the electron dipole transition line as a function of the electron temperature at an electron density of 2

in the target ion and the colliding electron. In the present study, two constraints are imposed on the colliding electron. First, the quantum number of the orbital angular momentum is  $\ell \leq 15$ . Second, the total number of the continuum basis function of the colliding electron for a given  $\kappa$  ( $\kappa = -\ell - 1$ if  $\kappa$  < 0; otherwise,  $\kappa = \ell$ ) is 14. By employing DARC, the **K** matrices and the corresponding symmetry information on the colliding system are obtained. Since the collision strength  $\Omega(\varepsilon)$ defined in Eq. [\(2\)](#page-1-0) is a function of the incident electron-impact energies  $\varepsilon$ , it is computed in an increasing energy sequence with an energy increment of  $\Delta \varepsilon = 0.008$  Ry by repeating the same procedure. Finally, the trapezoidal integration rule is used to evaluate electron-impact broadening and shift parameters numerically [see Eq.  $(1)$ ].

Calculations of widths and shifts for the first two spectral lines ( $Ly-\alpha$  and  $Ly-\beta$ ) in the Lyman series and for the first line in the Balmer and Paschen series ( $H_{\alpha}$  and  $P_{\alpha}$ ) in He II ions, respectively, were carried out under various plasma conditions. [I](#page-2-0)n Tables I and [II,](#page-3-0) we summarize our results obtained with electron temperature  $T_e$  in the range of 1–6 eV at a single electron density,  $N_e = 2 \times 10^{17}$  cm<sup>-3</sup>. Furthermore, the sums over  $J^{\tau}$  in Eq. [\(2\)](#page-1-0) have been checked for convergence by increasing the orbital angular momentum  $\ell$  of the colliding electron up to 31. All of the resulting uncertainty estimates, which were obtained by increasing  $\ell$  from 16 to 31, are also listed in Tables [I](#page-2-0) and II.

For all the lines listed in Tables [I](#page-2-0) and II, one can see that the line shifts are always an order of magnitude lower in comparison to the corresponding line widths. Moreover, all the line shifts are always towards the red wing, corresponding to a small reduction in the energy of the transition, which, under the plasma conditions selected in our work, is an order of magnitude less than the fine-structure splitting.

Fine-structure splitting in relativistic quantum mechanical calculations leads to different fine-structure components. For instance, the *Ly-* $\alpha$  line has two components  $(2p^{\pm} \rightarrow 1s)$ , and the *H<sub>α</sub>* line consists of seven components (3*s*  $\rightarrow$  2*p*<sup>-</sup>, 3*d*<sup>−</sup> → 2*p*<sup>−</sup>, 3*p*<sup>−</sup> → 2*s*, 3*p*<sup>+</sup> → 2*s*, 3*s* → 2*p*<sup>+</sup>, 3*d*<sup>−</sup> →  $2p^+$ ,  $3d^+ \rightarrow 2p^+$ ). From Tables [I](#page-2-0) and II, it is obvious that the electron-impact width and shift are quite different among the fine-structure components in the same  $n \rightarrow n'$  transition. Therefore, the strong (weak) order of components can be naturally defined by their high (low) oscillator strength in the following discussion.

To assess the accuracy of the present results, they must be compared in detail with previous experimental and theoretical studies, in cases where it is possible. The available experimental results have not been adjusted up to now for corrections of relativistic fine-structure splitting. Customarily, the available experimental results are not in our selected range of plasma conditions. For comparison of our results with experimental results, one must recalculate our results by extrapolating the electron density at the same electron temperature because all our calculations assume that the spectral line widths and shifts exhibit linear behavior with electron density [see Eq. [\(1\)\]](#page-1-0). Fleurier *et al.* [\[9\]](#page-5-0) measured the shift of the *Pα* line in He II ions at an electron density of  $10^{17}$  cm<sup>-3</sup> and an electron temperature of 4 eV. The measured value of the line shift,  $0.155 \text{ Å}$ , is similar to the observed value of the line shift, 0.130 Å, reported by Pittman *et al.*  $[24]$ . Our calculated line shift for the strongest component,  $4d^+ \rightarrow 3p^+$ , is 0.235 Å, which is about 50% larger than those reported in Ref. [\[9\]](#page-5-0) (see Table [II\)](#page-3-0). For the second strongest component,  $4p^+ \rightarrow 3s$ , of the  $P_\alpha$  line, our calculated line shift is 0.116 Å, which is about 11% lower than the experimental value,  $0.130 \text{ Å}$  [[24\]](#page-5-0). As a result, we can say that the present results on the shift in the  $P_\alpha$ line are in a good agreement with these two experimental cases.

Some significant inconsistencies between our results and earlier calculations reported by Unnikrishnan *et al.* [\[14\]](#page-5-0) can be seen in Table [II.](#page-3-0) For example, the component  $2p^+ \rightarrow 1s$ is stronger between the doublet components  $2p^{\pm} \rightarrow 1s$  in the  $Ly-\alpha$  line. In Table III, we note that their results for the component  $2p^+ \rightarrow 1s$  are lower than ours, with a maximum difference of 260% at 4 eV. However, our line shifts for the component  $3p^+ \rightarrow 1s$  at all selected temperatures are very similar in magnitude, and a good agreement between these two sets of theoretical results is found, with a maximum difference below 12% at 1 eV. In the case of line shifts of the two components  $(3p^+ \rightarrow 2s, 3d^+ \rightarrow 2p^+)$  in  $H_\alpha$ , our results show the best agreement with their results within a maximum difference of 24%, while the line shifts of the third component,  $3s \rightarrow 2p^+$ , are about two times higher than their results at 6 eV. Concerning the line width data for fine-structure components of the  $Ly-\alpha$  and  $H_\alpha$  lines, our results are not comparable with those reported in Ref. [\[14\]](#page-5-0). For instance, our calculated widths of the components  $3p^+ \rightarrow 2s$  and  $3p^- \rightarrow 2s$  are always lower and higher in magnitude, respectively.

Regarding the comparison of shifts of the  $H_{\alpha}$  line, mea-surements have been reported by Pittman et al. [\[24\]](#page-5-0), about  $2.8 \times 10^{-2}$  Å at  $N_e = 10^{17}$  cm<sup>-3</sup> and  $T_e = 4$  eV. In Table [IV,](#page-5-0) where the shift measured by Pittman *et al.* is compared with our calculations, it is about 1.4 times lower in magnitude for the component  $3d^+ \rightarrow 2p^+$  (the strongest component in  $H_{\alpha}$ ) and about 1.44 times lower for the component 3*d*<sup>−</sup> → 2*p*<sup>−</sup> (the second strongest component in *Hα*). In 1998, Stobbe *et al.* [\[13\]](#page-5-0) calculated the line shifts of the  $H_\alpha$  line

TABLE III. Comparison of our calculated widths 2*w* and shifts *d* in He II lines  $(2p^+ \rightarrow 1s, 3p^+ \rightarrow 1s,$  and  $3p^+ \rightarrow 2s)$  with other theoretical calculations at various electron temperatures  $T_e$  under an electron density of  $N_e = 2 \times 10^{17}$  cm<sup>-3</sup> (all in Å). Numbers in parentheses indicate powers of 10.

	<b>Transition</b>					
	$2p \rightarrow 1s$ $(T_e = 4 \text{ eV})$		$3p \rightarrow 1s$ $(T_e = 1 \text{ eV})$		$3p \rightarrow 2s$ (T <sub>e</sub> = 6 eV)	
	Width	Shift	Width	Shift	Width	Shift
Unnikrishnan et al. [14] This study	$8.0(-4)$ $1.589(-3)$	$1.8(-4)$ $6.502(-4)$	$6.7(-3)$ $6.422(-3)$	$7.7(-4)$ $8.653(-4)$	$1.9(-1)$ $1.096(-1)$	$1.9(-2)$ $1.594(-2)$



<span id="page-5-0"></span>

and their results were much lower than the experimental results reported by Grützmacheret *et al.* [25]. By means of linear interpolation of the experimental data reported in Ref. [25], we evaluated a line shift of  $2.12 \times 10^{-2}$  Å at  $N_e = 2 \times 10^{17}$  cm<sup>-3</sup> and  $T_e = 3.8$  eV. This experimental line shift is similar to our interpolated value,  $2.04 \times 10^{-2}$  Å, for component  $3d^+ \rightarrow 2p^+$  under the same plasma conditions and is about 0.54 times the line shift of component  $3d^-$  →  $2p^-$ . Furthermore, we compare our results for the  $H_{\alpha}$  line with the experimental measurements performed in Ref. [1]. Compared to our results, the widths measured by Ahmad are in a good agreement with our calculated widths, but the shifts are always about two times ours. For example, the measured widths and shifts of the *H<sub>α</sub>* line at  $N_e = 1.85 \times 10^{18}$  cm<sup>-3</sup> and  $T_e =$ 2.34 eV are 1.54 and 0.130 Å, respectively. Our calculated width and shift of the component  $3d^+ \rightarrow 2p^+$  of the  $H_\alpha$  line are nearly 1.65 and  $0.2391$  Å, respectively, evaluated by means of linear interpolation of the line shift data listed in Table [II](#page-3-0) under the same plasma conditions. The difference between the measured and our calculated width is about 7%, while the measured line shift is about 84% lower than ours. Based on these comparisons, we can say that the present results agree well with the available experimental and theoretical results for the  $H_{\alpha}$  line in many cases.

#### **IV. CONCLUSION**

This work reports electron-impact widths and shifts of the *Ly*-*α*, *Ly*-*β*, *H<sub>α</sub>*, and *P<sub>α</sub>* spectral lines in He II ions measured over a range of electron temperatures (1–6 eV) at an electron density of  $2 \times 10^{17}$  cm<sup>-3</sup> using the relativistic quantum mechanical formalism presented above. Generally, our results for line widths and shifts are close to other theoretical results and are in good agreement with experimental measurements. Our calculations show an excellent agreement with other numerical calculations and experimental results for the *Hα* line. Finally, we believe that our results will be useful for new plasma diagnostics and, also, hope that the electronimpact width and shift will be studied both theoretically and experimentally for more new transition lines of He II ions in future.

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