

Computer simulations of the Stark effect in the helium- β complex of krypton in inertial confinement fusion conditions

G. Pérez-Callejo^{1,*}, E. Stambulchik^{2,†}, R. Florido³, and M. A. Gigoso¹

¹*Departamento de Física Teórica Atómica y Óptica, Universidad de Valladolid, 47011 Valladolid, Spain*

²*Faculty of Physics, Weizmann Institute of Science, Rehovot 7610001, Israel*

³*iUNAT-Departamento de Física, Universidad de Las Palmas de Gran Canaria, 35017 Las Palmas de Gran Canaria, Spain*



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There is an ongoing interest in using spectroscopy in inertial confinement fusion (ICF) experiments, where dopants such as krypton can provide vital information about the temperature and density of the imploding plasma. While the most advanced tools for calculating Stark profiles are computer simulation models (CSMs), their application to complex lineshapes under the extreme conditions of ICF experiments is computationally challenging. In this manuscript, we present results of several CSM realizations applied to the Stark shape of the krypton He- β line and its satellites at ICF-relevant conditions ($n_e = 10^{24}$ to 10^{25} cm $^{-3}$, $T_e = 3$ keV). We demonstrate that codes with the same underlying physics but different numerical approaches yield identical results and analyze the differences in the line profile caused by various physical effects.

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I. INTRODUCTION

K-shell transitions of He-like species have been widely used to diagnose high energy density (HED) plasmas, including those in inertial confinement fusion (ICF) experiments [1–12]. In particular, He- β (a transition between the states with the principal quantum number $n = 3$ and $n = 1$ in a two-electron ion) is useful for density measurements. In many studies of plasma having a temperature of the order of 1 keV, Ar XVII He- β has been used for this purpose [13–17]. However, argon is strongly ionized in hotter plasmas, and higher- Z tracer species must be used for diagnostics. Indeed, Stark broadening of krypton He- β was used for inferring the electron density of compressed capsules at the National Ignition Facility (NIF) [10,11] and suggested for diagnostics in Laser MegaJoule experiments [18].

The He- β transition is always accompanied by its Li-like satellites with one spectator electron occupying various orbitals. These satellites partially overlap with the He- β line shape, requiring one to model and analyze the entire He- β complex for reliable diagnostics.

The satellite transitions significantly increase the complexity of the lineshape calculations. For example, Li-like satellites $1sn'\ell'3\ell \rightarrow 1s^2n'\ell'$ with $n' = 2, 3$, and 4 ($0 \leq \ell \leq 2$, $0 \leq \ell' < n'$) comprise 69, 68, and 209 atomic levels with 841, 760, and 6206 nonzero electric dipole matrix elements, respectively—not counting for the projection of the total angular momentum. The increased complexity makes applying Stark-broadening models [19] computationally challenging in general and becomes nearly prohibitive for computer simulations [20]. In fact, while computer simulations for the Stark

broadening of the Kr He- β line itself were recently produced [11], we are not aware of published computer simulation results for the Li-like satellite emission—neither for this nor for any other atomic system.

Recently, Gallardo-Díaz *et al.* [21] performed Stark broadening calculations of Kr He- β and its $n = 2, 3$ Li-like satellites using the so-called “standard theory” approximation [22] that assumes static ions and impact electrons. In particular, the effect of the interference terms in the electron impact operator of satellite transitions [23] was analyzed and found to be minor, in agreement with a similar study of the Ar He- β complex [24]. When justified, omitting the interference terms in “standard theory” models allows one to reduce the electron-operator matrix dimensions several times, significantly improving the computational speed.

In the present study, we report on computer simulations applied to the same atomic system (Kr) under conditions relevant to ICF: tracer amounts of Kr in a deuterium plasma, with electron densities in the range from 10^{24} to 10^{25} cm $^{-3}$ and temperature of 3 keV. We model the He- β line and its $n = 2$ and $n = 3$ Li-like satellites using different codes with different physical, mathematical, and numerical approaches. We show the effect of four different levels of particle interaction in the model: independent particles, interaction with the emitter, full N -body interaction, and N -body interaction with recombination broadening. Additionally, we present a hybrid code combining elements of computer simulations and standard theory. We also present the simulation-equivalent interference terms (SEIT), an approach based on the concept of interference terms from impact theory of Stark broadening, in the framework of computer simulations. We observe that the SEIT have a minor effect on the shape of the $n = 2$ satellites. However, it is not negligible in the case of the $n = 3$ satellite transitions, contrary to the recent findings [21]. We discuss the origin of this discrepancy.

*Contact author: gabriel.perez.callejo@uva.es

†Contact author: evgeny.stambulchik@weizmann.ac.il

This manuscript is structured as follows. In Sec. II, we describe the physical framework for the codes used in this analysis. The results obtained for the He- β line of Kr and its $n = 2$ and $n = 3$ satellites are presented and discussed in Sec. III. Section IV is devoted to the analysis of the interference terms. Finally, Sec. V summarizes the primary outcomes of this work and discusses future paths.

II. CODE DESCRIPTION

This paper presents results obtained with three different codes—SIMULA [25], SIMULAM, and SimU [26]. All semiclassical computer simulation models (CSMs), starting from the pioneering work of Stamm and Voslamber [27], share the same approach: the motion of charged plasma particles is modeled by numerically solving a classical N -body problem, while their fields affect the evolution of the atomic system of the emitter, treated quantum mechanically.

While the idea behind the codes is the same, they operate in different ways. In SIMULA and SIMULAM, the particles are considered independent of each other and, therefore, move following rectilinear trajectories. On the other hand, SimU considers the perturbers to be independent, but it explicitly solves their interaction with the emitter, and, therefore, particles move following hyperbolic trajectories if a Coulomb potential is assumed. For the simulations presented in this work, Debye screening at the appropriate plasma conditions was accounted for, which results in more general curves for the particle trajectories. Evidently, if the emitter were neutral, all codes would reproduce the same trajectories; however, that is not the case for the He- β line of Kr, where the emitter has a charge $Z = +34$. For direct comparison with SIMULA and SIMULAM, we additionally show results obtained with a modified version of SimU, SimU_{SP}, which enforces straight-path trajectories by disabling the radiator-perturber interaction.

For one particular case, we also show the results obtained with the full-molecular-dynamics code DinMol [28]. In DinMol, all electrons and ions in the simulation interact with one another, and the complex, multibody Coulomb field determines their trajectories. Owing to this detailed treatment of all particles, DinMol can detect when an electron becomes bound to an ion [29]. Therefore, it can include the so-called recombination width [30].

An additional difference between the codes is how they calculate the lineshape. SimU and SimU_{SP} use the following expression to obtain the spectrum:

$$I(\omega) \propto \frac{1}{T} \sum_{u,l} p_u \left\{ \left| \int_0^T \langle l | D(t) | u \rangle e^{i\omega t} dt \right|^2 \right\}, \quad (1)$$

where T indicates a time interval, D is the atomic dipole moment, u and l indicate the upper and lower states of the transition, respectively, p_u is the probability of the atom to be in the upper state u (i.e., $\langle u | \rho | u \rangle$, with ρ being the density matrix), and $\{\cdot\}$ indicates the average over the ensemble of emitters (realized as an average over several simulation runs). On the other hand, SIMULA, SIMULAM, and DinMol

calculate the spectrum as

$$I(\omega) \propto \text{Re} \int_0^T \{\text{Tr}[\rho D(t) D(0)]\} e^{-i\omega t} dt. \quad (2)$$

In the limit where $T \cdot N \rightarrow \infty$, with N being the number of emitters included in the ensemble average, these two expressions are mathematically equivalent (as long as the ergodic theorem holds and the density matrix is diagonal). In practice, however, this limit cannot be attained. Furthermore, the ensemble average must be sufficiently thorough, and certain differences might arise from the statistical and numerical treatment of both equations [31,32]. Lastly, while SIMULA solves for the evolution of the dipole moment subjected to the effects of perturbing ions and electrons, SIMULAM includes a mathematical simplification that significantly reduces the computational cost of the calculations. In SIMULAM, the ions evolve as usual in the simulation, and the evolution operator corresponding to the ionic field, $U_I(\tau, t)$, is obtained at each timestep (of size τ) of the simulation. However, the effect of the electronic field is included using the electron broadening operator from standard theory [22], using the formalism described by Gigosos [19]. Effectively, this provides an additional electronic evolution operator $U_e(\tau)$ —which only depends on the size of the timestep—such that the total evolution operator is $U(t + \tau, t) = U_e(\tau) U_I(\tau, t)$. However, given that the operators U_e and U_I do not commute, the electronic operator must be included at each timestep so that the evolution operator is written as

$$\begin{aligned} U(t + \tau, t) &= U_e(\tau) U_I(\tau, t) U(t) \\ &= U_e(\tau) U_I(\tau, t) U_e(\tau) U_I(\tau, t - \tau) U(t - \tau) \dots \end{aligned} \quad (3)$$

This allows for a much shorter computation time since the time scale of the simulation is that of the ion motion.

The differences between the codes are summarized in Table I. The atomic data in all codes used in this work were obtained by cFAC [33], based on the Flexible Atomic Code [34].

Regarding the limitations of this work, the main simplification made here is the widely used dipole approximation, since the full-Coulomb treatment [35,36] could not be applied to keep the calculations computationally feasible. The dipole approximation cannot reproduce the so-called plasma polarization shift [16]. The other effect of the full-Coulomb treatment, a certain reduction of the electron broadening due to the penetrating collisions, is minor for “beta” transitions for which the ion broadening constitutes the major contribution, as will be shown in Sec. IV. In addition, all codes used in this work employ a semiclassical treatment for the particles within the plasma. Specifically, while the radiator’s evolution is obtained by treating it quantum mechanically, the particle trajectories are always strictly classical. This imposes certain limitations on the accuracy with which the physical reality is reproduced in the simulation. Examples of effects not included in this treatment are the effects of the emitted radiation on the thermodynamic equilibrium of the plasma (negligible at these high densities and temperatures) or the exchange interaction effects in electron broadening [37]. However, these

TABLE I. Summary of the characteristics of the different codes presented in this work.

Code	Particle interaction	Correlation function	Ion field	Electron field
SIMULA	None (straight paths)	Eq. (2)	From simulation	From simulation
SIMULAm	None (straight paths)	Eq. (2)	From simulation	Following standard theory
SimU	With Debye-shielded emitter	Eq. (1)	From simulation	From simulation
SimU _{SP}	None (straight paths)	Eq. (1)	From simulation	From simulation
DinMol	Full Coulomb dynamics	Eq. (2)	From simulation	From simulation

are expected to be negligible at the conditions of interest (no magnetic fields, $T > 1$ keV).

III. RESULTS

A. He- β line

A comparison of the area-normalized He- β line shapes calculated by different models at $T = 3$ keV and electron densities ranging from 10^{24} to 10^{25} cm $^{-3}$ for tracer amounts of krypton in a deuterium plasma is shown in Fig. 1. The spectral range has been adjusted in each subfigure. Note that since the profiles are area normalized, a narrower lineshape results in a higher peak, highlighting the differences between the codes.

For the lower densities, the two main components of the He- β complex can be clearly resolved, namely, $^3P_1 \rightarrow ^1S_0$ at ~ 15435 eV and $^1P_1 \rightarrow ^1S_0$ at ~ 15435 eV—where we are naming the states using the $(2S+1)L_J$ notation. Additionally, even for $n_e = 10^{24}$ cm $^{-3}$, the $^1D_2 \rightarrow ^1S_0$ forbidden transition starts to appear at $E \sim 15445$ eV, owing to the Stark mixing of the states. This effect becomes clearer at $n_e = 3 \times 10^{24}$ cm $^{-3}$. However, for the highest density case ($n_e = 10^{25}$ cm $^{-3}$), the spectra look significantly different as the contribution from Stark-mixed states becomes more intense than that of the unperturbed states. The main peaks that appear in the spectra correspond to two dipole-forbidden transitions: the aforementioned $^1D_2 \rightarrow ^1S_0$ at ~ 15445 eV and the additional $^3P_2 \rightarrow ^1S_0$ line at $E \sim 15430$ eV, with the original lines contributing only in their wings.

For all plasma densities, all models show qualitatively similar results. Note that SIMULA, SIMULAm, and SimU_{SP} show a remarkable agreement, which is indicative of the fact that,

despite the differences between the codes (both numerical and physical), when the particles are considered independent, all codes reproduce the same shape of the spectral line. On the other hand, it is clear that when interaction with the radiator is included (SimU), the line becomes narrower for all considered densities. This is not unexpected since this interaction causes the radiator to repel perturbing ions, decreasing the ionic microfield (which is a significant broadening agent in these conditions).

In particular, the agreement of SIMULAm, a hybrid code, with CSMs like SIMULA and SimU_{SP}, is remarkable, considering that the electron dynamics are not explicitly resolved in SIMULAm, but instead introduced following the standard theory. As mentioned above, this approach speeds the simulations by a factor of ~ 50 . While a similar approach was used by Stamm and Voslamber [27], the electron effect was introduced as a whole in that case, rather than at every timestep, thus yielding different results owing to the noncommutation of the electron and ion evolution operators.

As mentioned in Sec. II, for the particular case of $n_e = 10^{25}$ cm $^{-3}$, we also performed calculations with the code DinMol which accounts for the full interaction between all particles. Interestingly, the full molecular dynamics simulations follow the same trend for the lineshape that was observed with the simpler CSMs. That is, when all particles are allowed to interact with each other, the line narrows even further since all interactions are smoothed. However, as explained in Refs. [29,30], tracking the full particle interaction enables us to account for the sudden loss of correlation when an emitter captures a free electron, known as recombination broadening. The interplay between these two effects (recombination

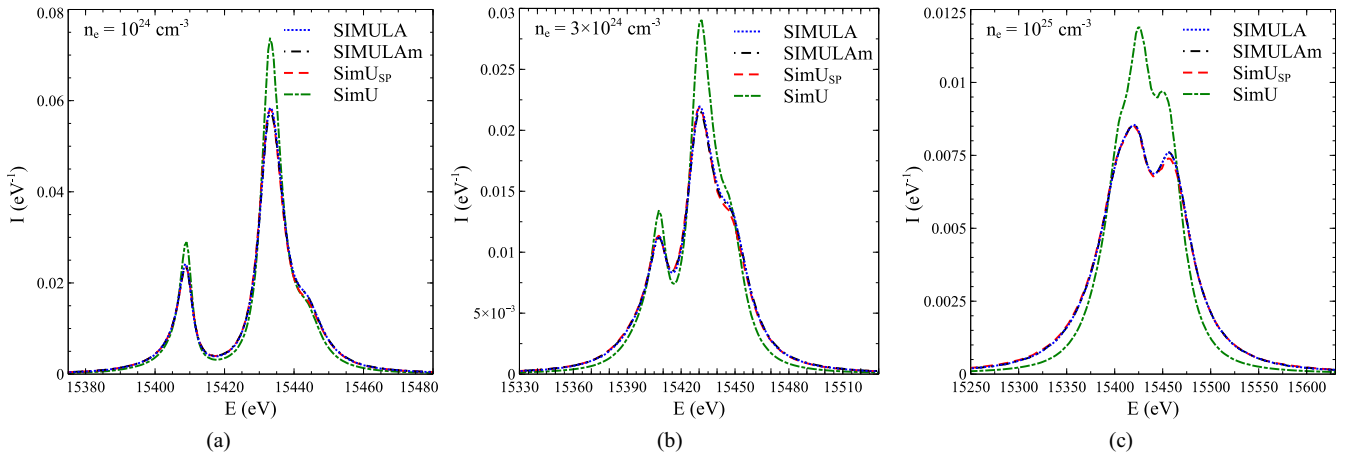


FIG. 1. A comparison of Kr XXXV He- β Stark line shapes, calculated for $n_e = 10^{24}$ cm $^{-3}$ (a), 3×10^{24} cm $^{-3}$ (b), and 10^{25} cm $^{-3}$ (c), using different CSMs. $T = 3$ keV is assumed in all cases. The line shapes are area-normalized to unity.

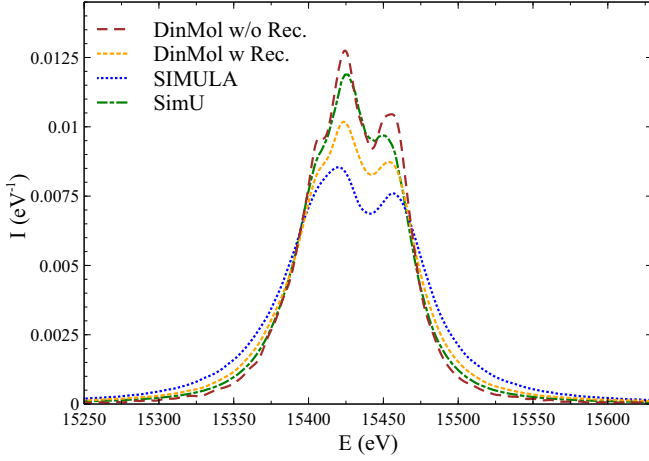


FIG. 2. He- β lineshape at $n_e = 10^{25} \text{ cm}^{-3}$ and $T = 3 \text{ keV}$, comparing the results SIMULA (independent particles), SimU (interaction with the emitter), and DinMol (full molecular dynamics) with and without recombination effects. Effectively, this illustrates the differences in the lineshape resulting from varying levels of complexity in the simulation.

broadening and full particle interaction) results in a lineshape that lies between the predictions of SIMULA and SimU. This is shown in Fig. 2, where we show the line profile obtained for SIMULA, SimU, and DinMol with (w) and without (w/o) recombination broadening.

The results for the He- β line width are summarized in Fig. 3, where we show the full width at half area (FWHA) of the line as a function of density for all codes presented here (FWHA is a metric that is less sensitive to ion dynamics than the full width at half maximum [38]). This shows again that when straight paths are assumed for the perturbers, all codes agree regardless of their computational differences. This figure also includes a line indicating a $n_e^{2/3}$ dependence of

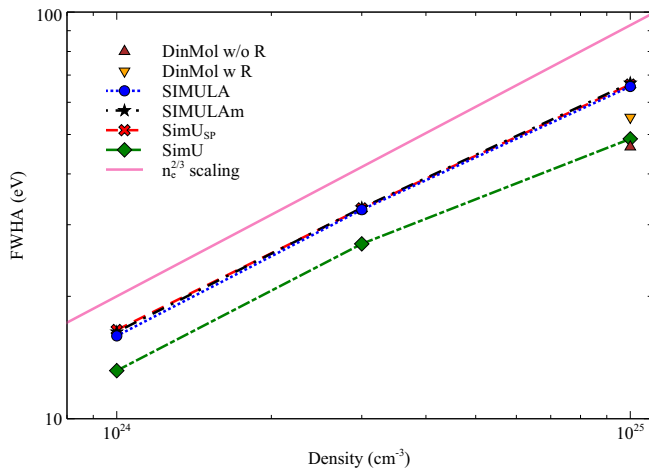


FIG. 3. Comparison of the full width at half area (FWHA) obtained at the different density conditions by the CSMs presented here for the He- β line. A solid-pink line indicating the typical $n_e^{2/3}$ scaling has been added to guide the eye. The plot axes are in logarithmic scale, so the $n_e^{2/3}$ scaling is a straight line.

the line widths on the density typical for the quasistatic Stark effect of hydrogenlike transitions [22]. It can be seen that for all models, the line widths closely follow this trend.

B. $n = 2$ and $n = 3$ Li-like satellites

Calculations of the $n = 2$ and $n = 3$ Li-like satellites are shown in Fig. 4 (top and bottom, respectively), in the same manner as Fig. 1. As for the case of the He- β line, the spectral range has been adjusted for each subfigure. Owing to computational limitations, not all cases are presented for all codes. In particular, SIMULA results are presented only for the highest-density cases (most computationally affordable). Nevertheless, it should be borne in mind that, as discussed in the previous section, the differences between codes are mainly due to the type of perturber trajectories assumed.

We want to emphasize the computational complexity of these calculations. The number of states involved in these transitions is of the order of hundreds. Therefore, for each simulation timestep, the codes must work with matrices of $\sim 300 \times 300$ elements to evaluate the evolution operator, using algorithms that scale as $O(N^3)$, where N is the matrix size. This alone requires significant computer power. Combined with the small size of the timestep necessary to accurately model the time-dependent electric field in plasma at these temperatures and densities, and the need to average over several simulation runs, this results in several thousand hours of computational time for each pair of temperature and density. The calculations presented here are, to our knowledge, the first computer simulations of the lineshape of these transitions, a crucial step for properly studying and modeling full experimental spectra.

C. Complete spectrum of the He- β complex

From the obtained lineshapes of the different components of the He- β complex, it is possible to obtain a synthetic spectrum of the whole emission. To do so, we chose the same conditions used in Ref. [21], that is, a 1:1 mixture of ^3He and deuterium with krypton as a minority at $T = 3 \text{ keV}$ and $n_e = 10^{24} \text{ cm}^{-3}$.

We used the collisional-radiative code ABAKO [39] to solve the atomic kinetics for the temperature and density conditions of interest. Upon doing so, the normalized line profiles were used with ABAKO such that the emissivity and opacity of the corresponding transitions could be properly distributed across photon energies. Additionally, we included the thermal Doppler broadening (of 4.3 eV) in the spectral calculations.

The results of the full He- β spectrum calculated with SimU and SimUsp (i.e., using curved and straight path trajectories, respectively) are shown in Fig. 5 for the conditions above. We also show, for comparison, the resulting spectra using the line profiles from Ref. [21], where the spectral line shapes were modeled with the code MERL [40–42] and the PRISMPECT model [43] was used to solve the atomic kinetics. In order to remove any differences in the spectra arising from the different atomic kinetics, we used ABAKO in all cases with the lineshapes extracted from Fig. 11 of Ref. [21].

It can be seen that the MERL predictions generally lie between those for the simulations with curved and straight

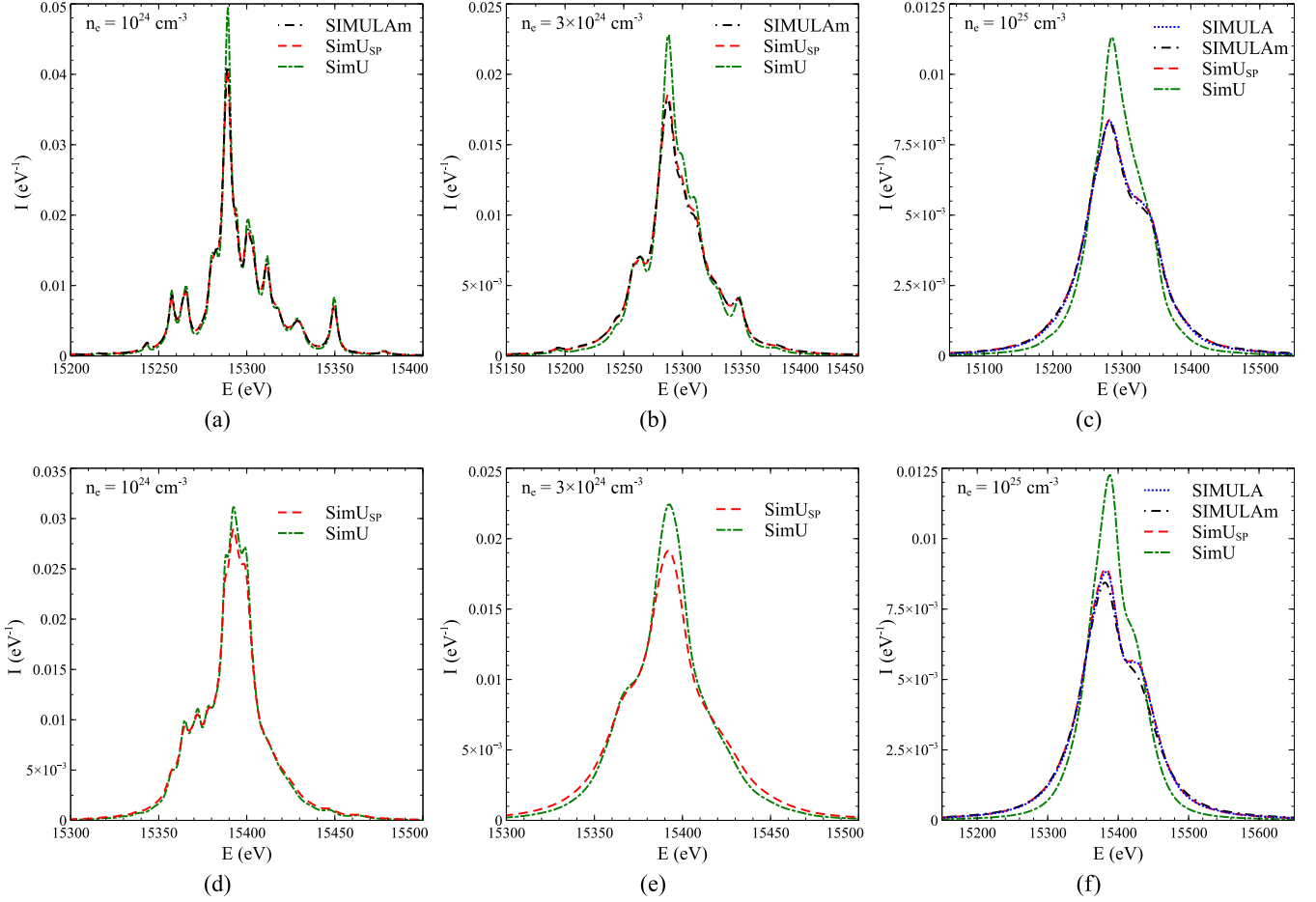


FIG. 4. Same as Fig. 1, but for $n = 2$ (top) and $n = 3$ (bottom) Li-like satellites. Figures 4(a) and 4(d) (left) correspond to $n_e = 10^{24} \text{ cm}^{-3}$, Figs. 4(b) and 4(e) (center) to $n_e = 3 \times 10^{24} \text{ cm}^{-3}$, and Figs. 4(c) and 4(f) (right) to $n_e = 10^{25} \text{ cm}^{-3}$. $T = 3 \text{ keV}$ is assumed in all cases.

paths. However, MERL does not account for the broadening effect of ion dynamics, which is taken into consideration in the simulations. This effect is non-negligible at the conditions of

interest and is likely the cause for the prediction of a shoulder in the high-energy wing of the He- β line (at $\sim 15.45 \text{ keV}$), which is not as prominent in the simulations.

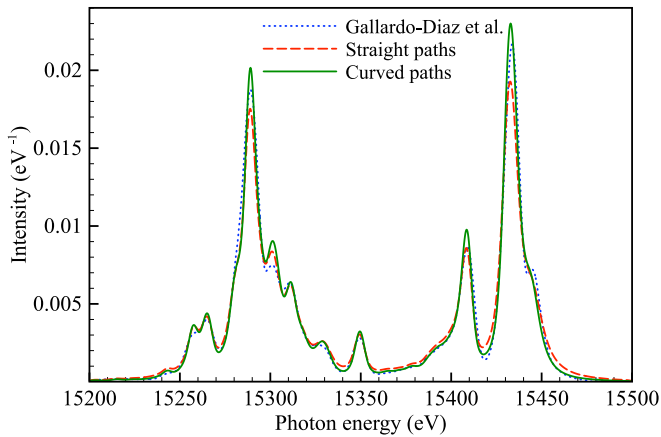


FIG. 5. Comparison of the full spectrum of the Kr He- β complex given in a previous study [21] with our results. A $T = 3 \text{ keV}$, $n_e = 10^{24} \text{ cm}^{-3}$ plasma with a trace minority of Kr in a 1:1 atomic mixture of D and ^3He is assumed. The spectra are area-normalized.

IV. SIMULATION-EQUIVALENT INTERFERENCE TERMS AND THEIR EFFECT ON THE SATELLITE EMISSION

With the results presented in the previous sections regarding the Li-like satellites, we are now in a position to discuss the effect of the so-called interference terms on the lineshape of these complex transitions. The name originates from a discussion [44–47] in the context of the electron impact broadening theory. In this framework, the impact operator Φ , determining the width and shift of spectral lines, contains off-diagonal elements with the $\vec{D}_a \cdot \vec{D}_b$ product, where $\vec{D}_a$ and $\vec{D}_b$ are the dipole moment operators of the upper and lower levels of a transition, respectively, and arise from the interaction of the atom with the plasma microfields. These elements were called interference terms, as they represent a contribution to the spectral line shape caused by the correlation of the wavefunctions of the upper and lower levels evolving at separate rates.

Mathematically, the impact operator Φ can be written as a sum of three terms [42,48], as

$$\begin{aligned}\Phi_{\alpha\beta ij} = & \delta_{ij} \sum_{\gamma} \vec{\mathbf{d}}_{\alpha\gamma} \cdot \vec{\mathbf{d}}_{\gamma\beta} G(\Delta\omega_{\gamma i}) \\ & + \delta_{\alpha\beta} \sum_k \vec{\mathbf{d}}_{ik} \cdot \vec{\mathbf{d}}_{kj} G(-\Delta\omega_{\alpha k}) \\ & - \vec{\mathbf{d}}_{\alpha\beta} \cdot \vec{\mathbf{d}}_{ji} [G(\Delta\omega_{\alpha j}) + G(-\Delta\omega_{\beta i})],\end{aligned}\quad (4)$$

where the Latin and Greek indices represent states from the upper and lower level of the transition, respectively. The function G is related to the evolution operator of the emitter and the elements $\Delta\omega_{\alpha i} = \omega - \omega_{\alpha i}$, with $\omega_{\alpha i}$ corresponding to the transition frequency between the α and i states.

Each of the terms in the sum corresponds to different transitions between the upper and lower levels. The first term involves transitions in which the dipole interaction causes the upper state to evolve by means of an intermediate state ($\alpha \rightarrow \gamma \rightarrow \beta$), but the lower state remains unchanged. Equivalently, the second term involves the evolution of the lower state ($i \rightarrow k \rightarrow j$) but not the upper state. Finally, the last term, involves a transition in which the upper and lower states both evolve separately ($\alpha \rightarrow \beta$ and $i \rightarrow j$). It is this third term that corresponds to the so-called interference terms. Importantly, if $\alpha = \beta$ and $i = j$, the interference terms are zero (since $\vec{\mathbf{d}}$ is an odd operator).

In all computer simulation models of line-shape broadening, the effect of the interference terms is always included. However, to our knowledge, no accepted approach likely exists [49,50] on how to model the omission of this effect in a CSM. In the absence of any prior published study on this subject, we introduce the notion of simulation-equivalent interference terms (SEIT) that retains the physical meaning of the interference terms in the impact approximation and is believed to produce qualitatively and, likely, quantitatively similar results. Namely, from Eq. (2), it can be seen that the shape of the spectral line is given by the Fourier transform of the trace of a matrix. If the density matrix is equal to the unity matrix, this trace can be explicitly written as

$$\begin{aligned}\text{Tr}[D(t)D(0)] &= \sum_{i\alpha\beta} U_{ij}^{\dagger}(t) D_{j\alpha}(0) U_{\alpha\beta}(t) D_{\beta i}(0) \\ &= \sum_{i\alpha\beta} U_{ij}^{\dagger} D_{j\alpha} U_{\alpha\beta} D_{\beta i}\end{aligned}\quad (5)$$

(the explicit time dependence was dropped for brevity). Physically, this involves the transitions $j \rightarrow \alpha$ and $\beta \rightarrow i$, coupled by the evolution operator mixing the states i, j and α, β , respectively.

Following the philosophy from Eq. (4), the SEIT are defined as the terms in the sum that involve transitions with different upper and lower states, that is

$$\text{SEIT} = \sum_{i\alpha\beta} (1 - \delta_{ij})(1 - \delta_{\alpha\beta}) U_{ij}^{\dagger} D_{j\alpha} U_{\alpha\beta} D_{\beta i}. \quad (6)$$

In practice, it is more convenient to include in the definition of SEIT the terms corresponding to transitions in which either the upper state or the lower state has evolved (not necessarily both of them). While these terms are not, strictly speaking,

of interference, they are negligible [48], and so, in practice, including them in the definition of SEIT makes no difference in the obtained spectra (but simplifies the computation). Therefore, for practical purposes, we define the SEIT as

$$\text{SEIT} = \sum_{i\alpha\beta} (1 - \delta_{ij}\delta_{\alpha\beta}) U_{ij}^{\dagger} D_{j\alpha} U_{\alpha\beta} D_{\beta i}. \quad (7)$$

In doing so, we can remove the effect of SEIT by only considering transitions going from the same upper state to the same lower state, i.e., those elements with $i = j$ and $\alpha = \beta$. This means that Eq. (5) reduces to the “SEIT-free trace” form as

$$\text{Tr}[D(t)D(0)]_{\text{no SEIT}} = \sum_{i\alpha} U_{ii}^{\dagger} D_{i\alpha} U_{\alpha\alpha} D_{\alpha i}, \quad (8)$$

involving only the diagonal elements of the evolution operator U .¹ It is stressed that the evolution operator $U(t)$ is correctly and fully calculated at every timestep of the simulation; only some terms from the trace summation in Eq. (2) [or equivalent ones in Eq. (1)] are omitted.

Using this definition, we studied the effects of the SEIT on the shape of the Li-like satellites. It is found that their effect is almost negligible for the $n = 2$ satellites, but it is not the case for the $n = 3$ satellites. For these, at the lowest density considered ($n_e = 10^{24} \text{ cm}^{-3}$), the effect of the SEIT is observable, although negligible for practical applications, whereas for the highest density ($n_e = 10^{25} \text{ cm}^{-3}$) the SEIT effect significantly modifies the shape of the spectral line. In this case, removing the SEIT caused the satellite emission to lose its structure, such as the shoulder on the high-energy wing of the line. In all cases, removing the SEIT resulted in a broadening of the spectral emission, in agreement with previous findings within the framework of electron impact theory [23]. This can be seen in Fig. 6, where we show the result of removing the SEIT for the highest and lowest densities of consideration using both SimU and SIMULA (curved and linear particle trajectories, respectively).

Importantly, since in the full computer simulations the effects of ions and electrons are considered jointly, this approach is not equivalent to that of removing the interference terms in the electron impact broadening theory within the “standard theory” approach, where ions are always considered in the quasistatic approximation. For a more direct comparison, we ran computer simulations only with electrons. An example of the results obtained in these calculations is shown in Fig. 7 for the $n = 3$ satellites and electron density of 10^{25} cm^{-3} from SimU_{SP}, where the effect of removing the SEIT is clearly observed.

The dashed green line in Fig. 7 shows the full line profile [as shown in Fig. 4(f)] for comparison. Note that for these conditions, the electron broadening is minor compared to that of ions. Furthermore, even that minor contribution is obscured by the energy structure of the numerous atomic levels, indicated by the asymmetric lineshapes in Fig. 7. To further isolate

¹It is important to note that, using this definition, the trace of the dipole correlation function removes intermediate states in the transition from a state in the upper level to one in the lower level. This effectively eliminates the quantum interference caused by the summation of different amplitudes of the evolution operator.

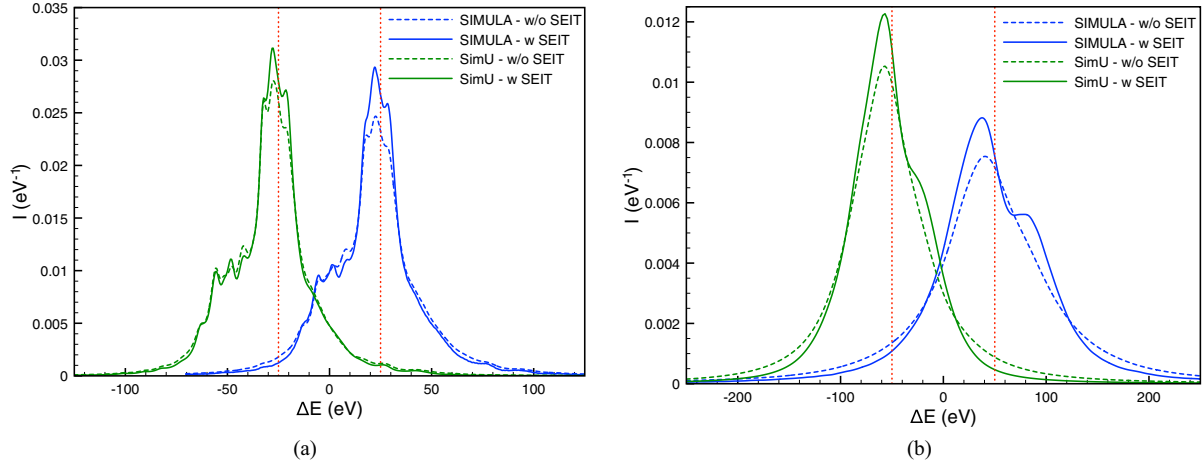


FIG. 6. Area-normalized line profiles of the $n = 3$ Li-like satellite emission for electron densities of 10^{24} cm^{-3} (a) and 10^{25} cm^{-3} (b) with (w, solid lines) and without (w/o, dashed lines) including SEIT. The blue lines correspond to SIMULA, while the red lines correspond to SimU. It can be seen that the SEIT always broaden the line (following the same trend as the classic interference terms); however, this effect is more pronounced for the highest density considered. The lines for SIMULA and SimU have been, respectively, upshifted and downshifted to ease the view, with the center of the lines marked with red dotted lines.

the effect of the electron broadening and the importance of the SEIT on it, the calculations were repeated assuming fully degenerate upper and lower levels of the satellite transitions. The results are shown in Fig. 8. There, it is clearly seen that the SEIT are very important for the electron broadening of the $n = 3$ satellites, affecting the linewidth by a factor of two. Qualitatively similar results are obtained for lower densities.

This analysis explains the seemingly contradicting results of Gallardo-Diaz *et al.* [21] who concluded that the interference terms played a minor role in the calculation of the $n = 3$ Li-like satellite emission of the Kr He- β line at $n_e = 10^{24} \text{ cm}^{-3}$. Indeed, the effect appears to be small, but only because the electron impact broadening, whether with or without the interference terms, is minor compared to the other line-shape formation factors (ion broadening and atomic

structure). However, under different conditions, such as significantly higher densities or transitions from levels with higher principal quantum numbers, this may no longer be the case, and omitting the interference terms would result in significant errors.

V. CONCLUSIONS AND FUTURE WORK

We have presented computer simulations of the Stark-broadened shape of the krypton He- β line, as well as, for the first time, the associated $n = 2$ and $n = 3$ Li-like satellites at ICF conditions ($T = 3 \text{ keV}$, $n_e = 10^{24}$ to 10^{25} cm^{-3}). These results demonstrate the robustness of current simulation codes and the utility of this technique for HED spectroscopic diagnostics. All codes agree qualitatively and show that the results only depend on the simulation's complexity level. The differences between different codes caused by the treatment of

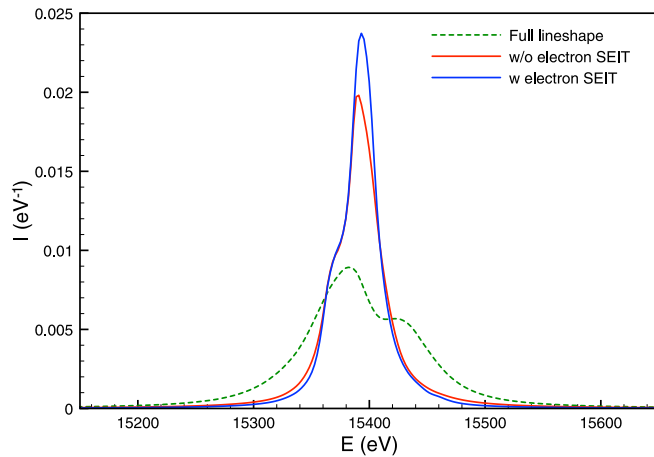


FIG. 7. Area-normalized line profiles from SimU_{SP} of the $n = 3$ Li-like satellite emission for an electron density of 10^{25} cm^{-3} , considering only electron broadening with (w) and without (w/o) SEIT. The full lineshape (including both ions and electrons) shown in Fig. 4(f) has been added to better illustrate this effect.

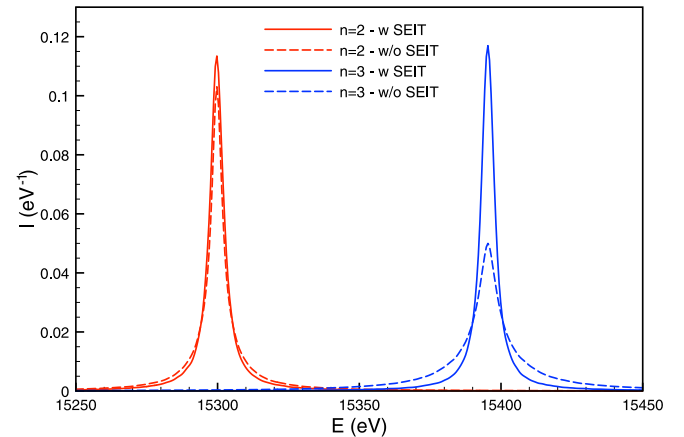


FIG. 8. The effect of removing the SEIT in the electron broadening assuming fully degenerate upper and lower level energies of the $n = 2$ and $n = 3$ Li-like satellite transitions, for an electron density of 10^{25} cm^{-3} .

particle trajectories become more pronounced at higher densities, as the interaction between the emitter and perturbors in the plasma plays a more significant role in the field dynamics.

We have presented SIMULAM, a hybrid code combining computer simulations and standard theory, which shows remarkable agreement with the full simulation codes SIMULA and SimUSP, speeding the simulation up by a factor of ~ 50 . Future work includes testing the approach used by SIMULAM with curved trajectories.

Additionally, we have defined the simulation-equivalent interference terms (SEIT) based on the concept of interference terms from the electron impact broadening theory and analyzed their effect on the shapes of the Li-like satellites. While the effect is practically negligible for the $n = 2$ satellites, the $n = 3$ satellites are noticeably affected. Therefore, omitting these terms in calculations based on the electron impact theory (for the sake of a significant speed up) may result in inaccuracies that tend to increase with higher densities.

Future work on this topic should extend the current results beyond the dipole approximation by accounting for all-order full plasma–radiator interaction and studying the effects of penetrating electron and ion collisions [36,51]. In particular, these effects should result in the plasma polarization shift of the Kr He- β complex that appears to be observed at NIF [11].

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DATA AVAILABILITY

The data that support the findings of this article are openly available [53].

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