

Article

# Distortion of the Ionization Cross Section of He by the Coherence Properties of a $C^{6+}$ Beam

Francisco Navarrete <sup>1</sup>, Raúl Barrachina <sup>2,3</sup> and Marcelo F. Ciappina <sup>4,\*</sup> 

<sup>1</sup> Department of Physics, Kansas State University, Manhattan, KS 66506, USA; navarrete@phys.ksu.edu

<sup>2</sup> Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica (CNEA) and Universidad Nacional de Cuyo, Av. Bustillo 9500, 8400 Bariloche, Argentina; raul.barrachina@gmail.com

<sup>3</sup> Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Godoy Cruz 2290, C1425FQB Ciudad Autónoma de Buenos Aires, Argentina

<sup>4</sup> Institute of Physics of the ASCR, ELI-Beamlines, Na Slovance 2, 182 21 Prague, Czech Republic

\* Correspondence: marcelo.ciappina@eli-beams.eu

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**Abstract:** We analyze the influence of the coherence of the projectile's beam in scattering phenomena. We focus our study in the ionization of He by  $C^{6+}$  projectiles at 100 MeV/amu. We assess the influence of this effect by performing a Born initial state and continuum distorted wave final state (CDW-B1) calculation together with a rigorous procedure to account for the initial coherence properties of the projectile's beam. These calculations, which had been previously performed for only the scattering and perpendicular collision planes and within the First Born approximation (FBA), were repeated for an ampler set of collision planes. Additionally, a more refined method to describe the applicability of the aforementioned procedure, is used. We achieve a better qualitative agreement with the experimental results.

**Keywords:** coherence; ionization; collisions

## 1. Introduction

The awareness of the relevance of the projectile's beam coherence effects in ion-atom and ion-molecule collisions has motivated an extensive study on this subject in the recent years [1–14]. The traditional way to compute the fully differential cross section (FDCS) [15] of a reaction, describes the incoming beam of projectiles as a purely coherent quantum system, i.e., a plane-wave. Nevertheless, this assumption seems not justified enough when we look at this postulate under the light of the density matrix theory.

As we described in a previous work [11], the time propagation of an incoherent mixture of an ensemble of massive particles, composed by identical wave packets localized at various positions within a much larger region of dimension  $D$ , can eventually develop coherence at a given distance  $L$ , in the same way as the incoherent light coming from the Sun becomes coherent when it arrives to the Earth. When an initially spatially constrained wave packet scatters through a structured target, the outcome of this process should depend strongly on the distance between the target region and the projectile source. This can be understood by noting that if their separation is small, then the wave packet could not "illuminate" the whole target in a coherent way, but only a fraction of it. But as it evolves in time, it will become wider and wider, reaching a point at which it will be able to "illuminate" the target coherently.

Even though the description we gave in the above paragraph may sound as a subtlety of quantum theory, which should be left for an appendix of an undergraduate quantum physics book, this effect is of great relevance on the field of scattering theory [16], and can, in fact, have a decisive role under certain circumstances. In order to bring clarity to this assertion, we will describe a basic ionization process

in ion-atom collisions, which is the single ionization of a neutral target. The primary contribution to the FDCS in this process comes from the interaction between the projectile and the target electron. We must highlight that, in general, there is a surprising agreement of the predictions made even for the most basic first order theoretical models like, for instance, the first Born approximation (FBA), which ignores the interaction between the nuclei in the collision. This agreement should improve as we decrease the Sommerfeld parameter  $Z_P/v$ , being  $Z_P$  the charge and  $v$  the initial velocity of the projectile. Nevertheless, even higher order, or relativistic approaches have failed to explain [17] an experiment which has been coined as the  $C^{6+}$ –puzzle [18] in which we will concentrate in this work, consisting of the ionization of a neutral Helium atom by 100 MeV  $C^{6+}$  ions. A Sommerfeld parameter of  $\approx 0.1$  should make it ideal to be described by almost any calculation method while, as we mentioned, they fail to give even a qualitative description of the FDCS at certain collision planes.

## 2. An Incoherent Mixture of Quantum States

Why do traditional models fail to explain this, in principle, simple ionization collision? Is it possible that the Sommerfeld parameter is not a good reference to test the suitability to use perturbative models for calculating ionization cross sections? Well, fortunately the situation seems not to be so disadvantageous. Even though perturbative methods do give a better description at smaller Sommerfeld parameters, there is an extra effect that should be considered, the coherence properties of the projectile's beam, as described by the so called coherence length [11].

In this section we will show how the latter allows us to quantify the effects of the coherence, and we will provide an operational definition of the incoherent cross section in terms of traditional coherent calculations. This procedure allows us to, while keeping the same calculation methods used up to date, give a more accurate description of the process and therefore to obtain more precise FDCSs.

At this point it is worth to remark that the inclusion of coherence effects in collision processes is a subject of growing interest by itself not only in Scattering theory but in quantum mechanics in general, and should not be mistaken by any means for an attempt to patch flaws in available collision theory calculation methods. Our motivation to analyze the so called  $C^{6+}$ –puzzle, stems from the fact that it gives us the opportunity not only to improve our understanding of this intriguing process, but also to get a deeper insight on how to apply the concepts of density matrix theory to a collision problem. The relevance of this experiment, in particular to the latter goal, comes from the fact that the experimental conditions under which it was performed are such that the incoherence of the projectile's beam would not just be "likely", but quite on the contrary. This means that if the projectile's beam is treated in an incoherent fashion, i.e. if the coherence effects are completely neglected, the theoretical predictions would give profound differences with the experimental data.

### 2.1. Mathematical Description

To begin with the mathematical description of the collision process, we will approximate the projectile's beam of initial momentum  $K_i$ , as composed by Gaussian wave packets of minimal width  $\Delta x_0$  transversing a collimator. When it reaches the target, its coherence length  $\Delta r$  is [11,16] (throughout this work, Atomic units are used):

$$\Delta r = \sqrt{(\Delta x_0)^2 + \frac{(\gamma L/K_i)^2}{(\Delta x_0)^2 + D^2}}, \quad (1)$$

where  $L$  is the separation between the collimator and the target,  $D$  is the collimator's characteristic length (e.g., for a circular collimator, its diameter), and  $\gamma$  is a dimensionless parameter [16]. The coherence length achieved by a beam can be thought of as the maximum separation for which two points can interfere. The coherence length of a beam composed exclusively by plane waves is infinite due to the fact that every two points of the wave front interfere, which implies full coherence. On the

other hand, a beam is said to be incoherent when it has a small coherence length compared to the size of the target.

The value of  $\Delta x_0$  is difficult to estimate because it is of microscopical character, meanwhile  $L$  and  $D$  are macroscopical quantities. To this end, Equation (1) can be approximated by

$$\Delta r = \frac{\gamma L}{K_i D} . \tag{2}$$

It is worth to highlight that, unlike collimation, the quantum character of the projectile’s beam implies an inherent degree of coherence that can therefore be not removed.

### 2.2. Calculation of the Incoherent FDCS

The FDCS for single ionization:  $d\sigma/d\mathbf{k} d\mathbf{K} d\mathbf{K}_R$  (being  $\mathbf{k}$ ,  $\mathbf{K}$ , and  $\mathbf{K}_R$ , the projectile’s, the ionized target’s and the electron’s momenta), has been traditionally formulated taking the incoming projectile like a plane-wave, which represents within our framework an entirely coherent wave front. On the other hand, as it has been studied by [19] (for more details see [11,20]), coherence effects can be incorporated in the calculation of the cross section by means of a Kernel  $W$  in momentum space as follows

$$\frac{d\bar{\sigma}}{d\mathbf{k}d\mathbf{Q}d\mathbf{K}_R} = \int d\mathbf{Q}' \frac{d\sigma}{d\mathbf{k}d\mathbf{Q}'d\mathbf{K}_R} W(\mathbf{Q}' - \mathbf{Q}) , \tag{3}$$

where  $\mathbf{K}_i$  is the initial mean momentum, and  $\mathbf{Q} = \mathbf{K}_i - \mathbf{K}$  is the momentum transfer. It is worth to mention that a similar functional form has been derived in other theoretical studies that tried to incorporate experimental uncertainties to the calculation of the FDCS [21–25]. If instead of thinking of the projectile in the initial state as a plane wave, we describe it as an incoherent mixture of states [11]. Under this assumption, finding the functional form of the Kernel can appear elusive. Nevertheless, if we model this mixture of states as a Gaussian distribution of wave packets of Gaussian shape, from density matrix theory it is natural to expect the Kernel to exhibit this functional dependence as well [11]. We will work then by considering the approximation that the initial wave packets have dispersion in the perpendicular direction only, and therefore this Kernel reads

$$W(\mathbf{Q}'_{\perp} - \mathbf{Q}_{\perp}) = \frac{1}{\sqrt{2\pi\sigma_x\sigma_y}} \exp\left(-\frac{(Q'_x - Q_x)^2}{4\sigma_x^2} - \frac{(Q'_y - Q_y)^2}{4\sigma_y^2}\right) , \tag{4}$$

where  $z$  is defined by the projectile’s initial direction, being  $x - z$  the scattering plane, and  $y$  an axis perpendicular to it. Here,  $\sigma_x$  and  $\sigma_y$  are Gaussian dispersion coefficients. We expect, from Heisenberg’s uncertainty principle, that for each component  $i = x, y$  the following relation will hold

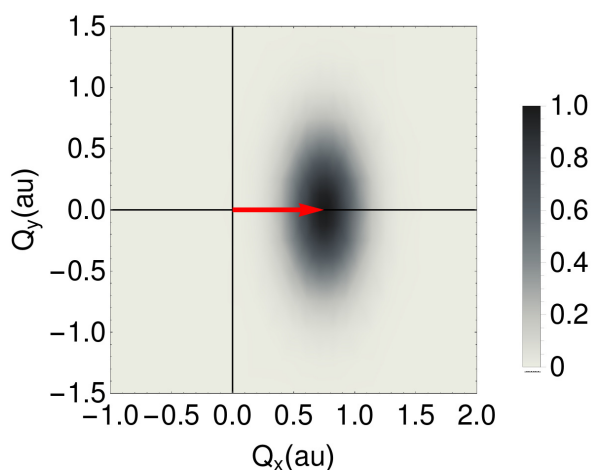
$$\sigma_i \propto \frac{1}{\Delta r_i} , \tag{5}$$

therefore, smaller values of  $\sigma_x$  and  $\sigma_y$  yield a narrower Gaussian distribution, i.e., a more coherent wave packet.

### 3. Results

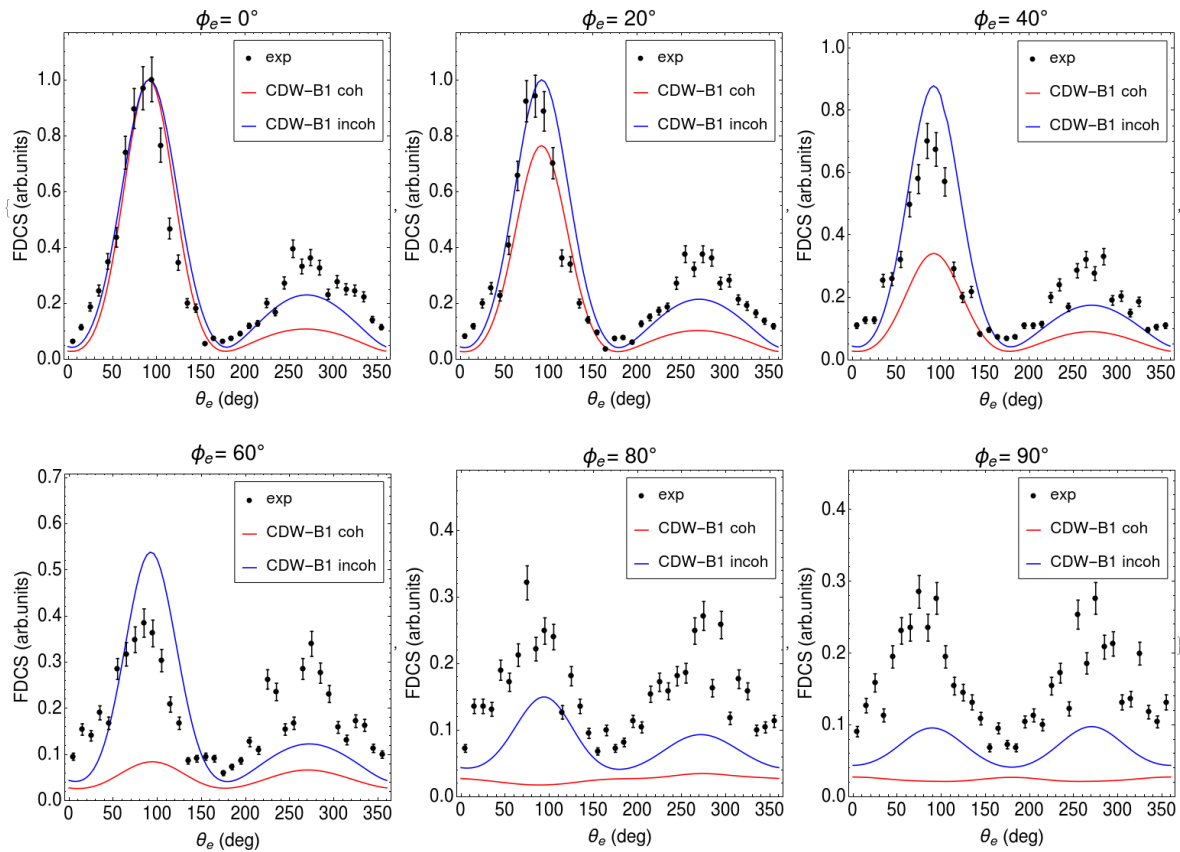
In the current section we compare calculations performed both incoherent and coherently with experimental results [18]. We used a CDW-B1 approximation, refining a previous FBA [20], which has been successfully applied to convolutions similar to the one we perform [22,25,26]. Fully stripped carbon ions at 100 MeV are used as projectiles and neutral He atom as target, which we model as a hydrogen-like atom with an effective charge given by the first ionization energy. The electron’s final energy is fixed at  $E_e = 6.5$  eV, and we evaluated the momentum transfer at  $Q_x = 0.75$  au and  $Q_y = 0.02$  au. We show our results as a function of the polar angle  $\theta_e$  at different angles  $\phi_e$  of the final electron momentum (measured from the  $x$  component of the momentum transfer and the

initial direction of the projectile, respectively). The scattering plane corresponds to  $\phi_e = 0$  and the perpendicular plane to  $\phi_e = 90$ . The plotted FDCS at all polar angles are normalized by the maximum of the distribution which occurs at  $\phi_e = 0$ , either for the experimental and both theoretical results, the three of which are normalized independently. The parameters  $\sigma_x$  and  $\sigma_y$  were determined by fitting Equation (3) to experimental cross sections [18], giving the values  $\sigma_x = 0.3$  au and  $\sigma_y = 0.6$  au, at all azimuthal angles. In Figure 1 we plot the Kernel (see Equation (4)) used in our calculation. The values of  $\sigma_x$  and  $\sigma_y$  correspond to a coherence length which is smaller than the Bohr radius of He, which means that the effect of the incoherence is playing a big role in shaping the outcome of the collision. Because of the fundamental role of the projectile's momentum in determining the coherence length (see Equation (2)), for less massive particles and lower velocities, the effect of the coherence can become less noticeable, as we analyzed for protons at 1 MeV on He [20]. In Figure 2 we can see how the incoherent calculation, not only enhances the agreement with experimental data on the scattering plane, but also gives a better qualitative agreement in the perpendicular plane. Furthermore, at the intermediate planes, the results keep showing an enhancement in the description of the experimental data when compared to that of the coherent ones.



**Figure 1.** Density plot of the Gaussian Kernel used in our calculations in the  $x - y$  plane (i.e.,  $\theta_e = 90$ ), for  $\sigma_x = 0.3$  au and  $\sigma_y = 0.6$  au. The red arrow corresponds to the momentum transfer projection in that plane,  $Q_x = 0.75$  and  $Q_y = 0.00$ .

We note, however, that in their work of 2003 by Schulz et al [18], the influence of the coherence of the projectile was not taken into account for the analysis, because the link between collision theory and density matrix theory had not been yet established. In a subsequent work [3], they indeed estimated this coherence length to be in the order of  $\Delta r = 0.001$  au. Such extremely small value for this parameter, which is smaller than that estimated by us, implies that the collision is exceptionally incoherent and thus a simplified procedure for introducing coherence effects, like that used in our approach, would yield an overwhelming distortion of the FDCS, as discussed in [10]. Hence, a more thorough analysis of the coherence properties of the projectile's beam would be key to calculate appropriately the FDCS, in order to give an absolute correlation between the coherence length and its effect on the FDCS. Beyond the above cited limitations in the approach we implemented, we think, however, our work represents a step forward in that direction.



**Figure 2.** FDCS in arbitrary units, normalized by the maximum of the distribution, located at  $\phi_e = 0$ , for the single ionization of He by 100 MeV/amu  $C^{6+}$  ions at different azimuthal angles  $\phi_e$ , for various values of the ejected electron polar angle  $\theta_e$ . The momentum transfer is set at  $\mathbf{Q} = (Q_x, Q_y, Q_z) = (0.75, 0.00, 0.02)$  au and the ejected electron energy at  $E_e = 6.5$  eV. With a red line we show the FDCS calculated in the usual coherent form with a CDW-B1 approach. The blue line corresponds to the incoherent calculation within the CDW-B1, convoluted by Equation (3), with  $\sigma_x = 0.3$  au and  $\sigma_y = 0.6$  au. Black dots represent the experimental results from [18].

#### 4. Conclusions

Even though we should keep relying on and refining traditional perturbative calculation methods in scattering theory, a more complete description of the physics of the process is required under certain circumstances which we described in this work, to get a clear understanding of the underlying physics and give precise results. For testing the goodness of a calculation method, not only the Sommerfeld parameter should be borne in mind, but also the coherence length. Therefore, when testing a given method at high velocities, coherence effects should be introduced properly. On the other hand, perturbative methods which introduce coherence effects in an ab-initio manner should be highly desirable, and are yet to be developed.

The above mentioned considerations were proved by repeating a previous first order (FBA) calculation with a more sophisticated approach (CDW-B1) under similar coherence parameters. Additionally, we extend the parameters range of the theory-experiment comparison. In particular, our work confirms that the disagreements between theory and experiment found for the  $C^{6+}$ –puzzle [18] for 100 Mev/amu  $C^{6+}$  on He are, in a large amount, due to projectile coherence effects.

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**Conflicts of Interest:** The authors declare no conflict of interest.

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