Fully differential cross section for O^{8+}-impact ionization of Li

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We present various differential cross sections for the single ionization of Li by O^{8+} ions. We use a time-dependent, close-coupling approach to model the evolution of a one-active-electron wave function in the field of the incoming projectile for a range of impact parameters. In addition, a Fourier transform approach is used to extract differential cross sections for a specific projectile momentum transfer value. This scheme allows us to incorporate information about the interaction of the two heavy nuclei [the so-called nuclear-nuclear (NN) interaction] and to assess its influence in the differential cross sections. We find noticeable differences in the shape of the differential cross sections when we include (neglect) the NN interaction. Our single-differential cross-section calculation shows excellent agreement with experimental data. In addition, recent measured double-differential cross sections as a function of electron energy and transverse momentum transfer are reasonably well reproduced by our theoretical calculations.

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I. INTRODUCTION

The single ionization of light atoms by fast bare ions provides an interesting probe of the few-body breakup processes. Theoretically speaking, the single and double ionization of atoms by highly charged ions is one of the most challenging many-body quantal problems. It is well known that when we use photons as projectiles, the electrons are promoted to the continuum via a dipolar interaction. On the other hand, when a fast bare ion impinges on an atom, the electron-projectile interaction must include multipolar terms.

The nonperturbative time-dependent, close-coupling (TDCC) method was applied both to ion-atom and ion-molecule single- and double-ionization processes (for a recent review see [1]). On one hand, the TDCC method based on an expansion of a one-electron, three-dimensional wave function was used in single-ionization processes in single-electron systems, namely, H [2] and H_2^+ [3], and in the single-active-electron approximation in He [2], Li [2], and H_2 [4]. On the other hand, the TDCC method, based on an expansion of a two-electron six-dimensional wave function, was applied to single- and double-ionization ionization processes in He [2,5–9] and H_2 [3,4,10]. The TDCC method, based on an expansion of a two-electron six-dimensional wave function scheme, represents a challenge from a computational viewpoint and massive parallel computers are employed to obtain the theoretical quantities needed to compare with the experimental measurements. The latter range from fully differential cross sections (FDCSs) [11] to total cross sections, and for all the cases the TDCC outcomes are found to be in very good agreement with experimental data.

Before the advent of experiments that were able to measure fully differential cross sections, such as cold-target recoil-ion momentum spectroscopy (COLTRIMS) [12] techniques, the nuclear-nuclear (NN) interaction was often neglected in calculations of single ionization of atoms by ion impact. This is because many less differential cross sections, such as single- and double-differential cross sections as well as the total cross section, are not sensitive to the NN interaction. On the other hand, the incorporation of the NN interaction on the FDCS appears to be mandatory in order to reproduce satisfactorily the COLTRIMS experimental data that are differential in projectile scattering angle (or equivalently, in projectile momentum transfer), both in perturbative [13] and nonperturbative approaches [9]. It is worth mentioning, however, that there is not a unique consensus about the most adequate model to be incorporated in the NN-*free* FDCS. An exhaustive study about this issue using helium as a target was shown in [14], where a detailed explanation of several models and numerical calculations of differential cross sections as a function of the projectile momentum transfer are presented.

In this contribution, we use the TDCC method to calculate the differential cross sections for single ionization in O^{8+}+ Li collisions at 1.5 MeV/amu to compare with the inaugural magneto optical trap-reaction microscope (MOTReMi) experiment of Fischer *et al.* [15]. The MOTReMi implementation appears to be an interesting framework from which to study alkali-metal atoms and several lines of action are planned. For instance, single-ionization differential cross sections starting from Li atoms in the $1s^2 2s$ ground state and $1s^2 2p$ excited configuration can be directly obtained. In this direction, recent measurements of double-differential cross sections as a function of electron energy and transverse momentum transfer for Li($2s$) and Li($2p$) atoms were presented [16]. Since the two remaining electrons in the residual Li ion form a closed shell, we apply a TDCC method based on an expansion of a one-electron, three-dimensional wave function in the field of Li^+ to calculate differential cross sections for single ionization at various projectile impact parameters. The TDCC method based on an expansion of a one-electron, three-dimensional wave function was used to calculate the single-ionization cross section of Li by antiproton impact, showing excellent agreement with other nonperturbative calculations (see, e.g., [2] for details). Starting from the differential cross sections as a function of the impact parameter and employing a Fourier

transform approach, we then compute FDCS as a function of the projectile momentum transfer, including (neglecting) the NN interaction. The FDCS represents the most detailed measurement of any few-body breakup problem and it presents a challenge for any theory, as was shown for the case of single ionization of He by bare C atoms [9].

The rest of the article is organized as follows. In Sec. II we briefly summarize the TDCC method based on an expansion of a one-electron, three-dimensional, wave-function method for calculating fully differential cross sections for the single ionization of atoms with one active electron, including the procedure to extract FDCS as a function of the projectile momentum transfer, starting with the ones based on the impact parameter. In Sec. III we apply the TDCC method based on an expansion of a one-electron, three-dimensional, wave-function approach to calculate FDCSs for single ionization in O^{8+} + Li collisions at 1.5 MeV/amu. We present FDCS both as a function of individual impact parameters and the projectile momentum transfer. Furthermore, double-differential cross sections as a function of electron energy and transverse momentum transfer and a single-differential cross section in electron energy are calculated and compared with recent experimental data. In Sec. IV, we finish our contribution with a summary and an outlook for future work. Unless otherwise stated, all quantities are given in atomic units.

II. THEORY

The time-dependent Schrödinger equation for a bare ion projectile colliding with a one-active-electron atom is given by

$$i\frac{\partial\Psi(\vec{r},t)}{\partial t}=\left(-\frac{1}{2}\nabla^2-\frac{Z_t}{r}+V(r)+\frac{Z_p}{|\vec{r}-\vec{R}(t)|}\right)\Psi(\vec{r},t), \tag{1}$$

where Z_t is the target charge, $V(r)$ is a core potential, and Z_p is the projectile charge. For straight-line motion, the time-dependent projectile position is given by

$$R(t)=\sqrt{b^2+(d_0+vt)^2}\,, \tag{2}$$

where b is an impact parameter, d_0 is a starting position, and v is the projectile speed.

If we expand $\Psi(\vec{r},t)$ in spherical harmonics, the time-dependent close-coupled equations for the $P_{lm}(r,t)$ radial expansion coefficients are given by

$$i\frac{\partial P_{lm}(r,t)}{\partial t}=\left(-\frac{1}{2}\frac{\partial^2}{\partial r^2}+\frac{l(l+1)}{2r^2}-\frac{Z_t}{r}+V_l(r)\right)P_{lm}(r,t)+\sum_{l',m'}W_{lm,l'm'}(r,R(t))P_{l'm'}(r,t)\,. \tag{3}$$

The electron-projectile coupling operator is given by

$$W_{lm,l'm'}(r,R(t))=-Z_p(-1)^m\sqrt{(2l+1)(2l'+1)}\times\sum_{\lambda}\frac{(r,R(t))_<^{\lambda}}{(r,R(t))_>^{\lambda+1}}\sum_q C_q^{\lambda *}(\theta_p,\phi_p)\times\begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l & \lambda & l' \\ -m & q & m\end{pmatrix}\,, \tag{4}$$

where $(r_1,r_2)_<=\min(r_1,r_2)$, $(r_1,r_2)_>=\max(r_1,r_2)$, and λ,q are multipole expansion parameters. For projectile motion in the xz plane, the spherical tensor can be written as

$$C_q^{\lambda}(\theta_p,\phi_p)=\sqrt{\frac{4\pi}{2\lambda+1}}Y_{\lambda q}(\theta_p,0)\,, \tag{5}$$

where $Y_{lm}(\theta,\phi)$ is a spherical harmonic, $\sin\theta_p=b/R(t)$, and $\cos\theta_p=(d_0+vt)/R(t)$.

The initial condition for the solution of the time-dependent, close-coupled equations for single ionization of the ground state of Li ($1s^22s$) is given by

$$P_{lm}(r,t=0)=P_{2s}(r)\delta_{l,0}\delta_{m,0}\,, \tag{6}$$

where $P_{2s}(r)$ is a bound radial orbital obtained by diagonalization of the one-electron Hamiltonian:

$$H(r)=-\frac{1}{2}\frac{\partial^2}{\partial r^2}-\frac{3}{r}+\frac{l(l+1)}{2r^2}+V_l(r), \tag{7}$$

for $l=0$ where $V_0(r)$ is a pseudopotential. Following time propagation of the time-dependent close-coupled equations, electron momentum space wave functions are calculated by

$$\bar{P}_{lm}(k,b)=\int_0^{\infty}dr\,P_{kl}(r)P_{lm}(r,t\to\infty)-P_{2s}(r)\int_0^{\infty}dr'\,P_{2s}(r')P_{00}(r',t\to\infty)\delta_{l,0}\delta_{m,0}, \tag{8}$$

where $P_{kl}(r)$ is a continuum distorted wave. The above-mentioned procedure can be also employed to calculate single ionization of Li from its excited states, e.g., ($1s^22p$), changing the $P_{2s}(r)$ bound radial orbital to the corresponding $P_{2p}(r)$. This allows us to compare our theoretical calculations with recent experimental measurements [16].

The fully differential scattering amplitude for the single ionization of Li is given by

$$S(k,b,\theta_e,\phi_e)=\sum_{l,m}(-i)^l e^{i(\sigma_l+\delta_l)}\bar{P}_{lm}(k,b)Y_{lm}(\theta_e,\phi_e)\,, \tag{9}$$

where σ_l and δ_l are Coulomb and distorted-wave phase shifts. The fully differential cross section for individual values of the impact parameter b (FDCS-b) is given by

$$\frac{d^4\sigma}{dk\,db\,d\theta_e\,d\phi_e}=|S(k,b,\theta_e,\phi_e)|^2\,. \tag{10}$$

An alternative expression can be written in terms of the transverse component of the projectile momentum transfer η employing a two-dimensional Fourier transform [17]. Consequently, a fully differential scattering amplitude for the single ionization of Li is also given by

$$S(k,\eta,\theta_e,\phi_e)=\frac{1}{2\pi}\sum_n i^n\int_0^{2\pi}d\phi_b e^{-in\phi_b}\times\int_0^{\infty}bdb\;S(k,b,\theta_e,\phi_e-\phi_b)e^{i\Delta(b)}J_n(\eta b), \tag{11}$$

where ϕ_b is the azimuthal angle of the impact parameter, $J_n(\eta b)$ is a Bessel function of nth order, and the internuclear

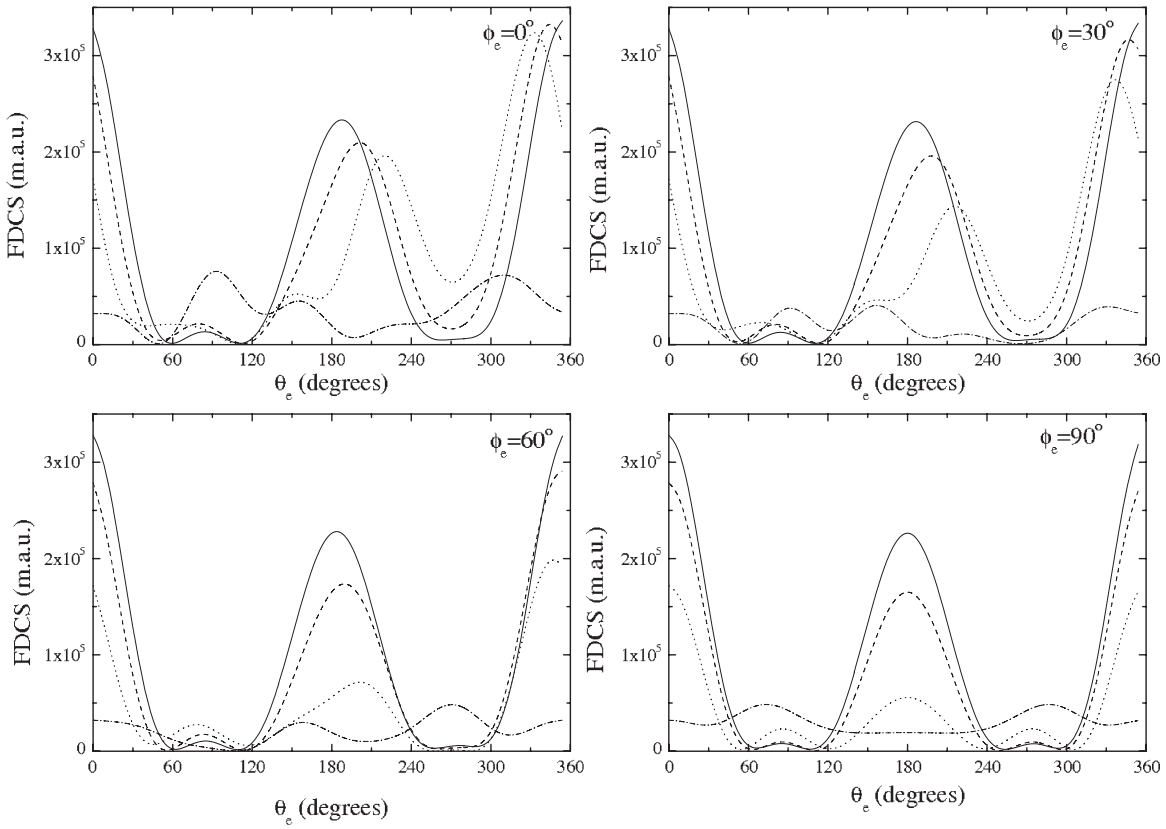

FIG. 1. Fully differential cross sections (FDCS-b) for single ionization in O^{8+}+ Li collisions at a projectile energy of 1.5 MeV/amu, an ejected-electron energy of $\varepsilon = 1.5$ eV, $\theta_e = 0^\circ - 360^\circ$, and for various values of the azimuthal angle ϕ_e. Solid curve, TDCC method based on an expansion of a one-electron, three-dimensional, wave-function calculation at $b = 0.4$ a.u.; dashed curve, TDCC method based on an expansion of a one-electron, three-dimensional, wave-function calculation at $b = 1.0$ a.u.; dotted curve, TDCC method based on an expansion of a one-electron, three-dimensional, wave-function calculation at $b = 2.0$ a.u.; dot-dashed curve, TDCC method based on an expansion of a one-electron, three-dimensional, wave-function calculation at $b = 5.0$ a.u. (m.a.u. = modified atomic units equal to 2.8×10^7 times atomic units such that the total cross section is in units of 1.0×10^{-24} cm^2).

interaction phase factor is given by

$$\Delta(b) = \frac{2Z_{\rm eff}Z_p}{v} \ln vb, \tag{12}$$

where one choice for the charge of the target ion, i.e., the charge of the residual Li^+, is $Z_{\rm eff} = 1$. This approximation appears to be adequate considering the two remaining electrons form a closed shell, but other options are possible (see, e.g., [13]). A more extensive discussion about the characteristics and behavior of similar transition amplitudes in the framework of perturbative approaches has been given in Ref. [14]. In all the calculations presented in this work, we found that inclusion of terms up to $|n| \leqslant 10$ in the Bessel function expansion appears to be sufficient to obtain converged results. The fully differential cross section as a function of the projectile momentum transfer η (FDCS-η) is given by

$$\frac{d^4\sigma}{dk\, d\eta\, d\theta_e\, d\phi_e} = |S(k,\eta,\theta_e,\phi_e)|^2 . \tag{13}$$

If we integrate the last equation over the electron angles θ_e and ϕ_e and use that the electron energy is $\epsilon = \frac{k^2}{2}$ we find

$$\frac{d^2\sigma}{d\eta d\epsilon} = \frac{2\pi}{k} \int_0^\pi \sin\theta_e d\theta_e \int_0^{2\pi} d\phi_e \frac{d^4\sigma}{dk\, db\, d\theta_e\, d\phi_e}, \tag{14}$$

which is a double-differential cross section as a function of electron energy and projectile momentum transfer and was experimentally measured recently for different values of ϵ and η [16].

An electron energy single-differential cross section is most easily obtained from

$$\frac{d\sigma}{d\epsilon} = \frac{2\pi}{k} \int_0^\infty bdb \int_0^\pi \sin\theta_e d\theta_e \int_0^{2\pi} d\phi_e \frac{d^4\sigma}{dk\, db\, d\theta_e\, d\phi_e}, \tag{15}$$

and the total cross section σ is computed by a multidimensional integration over the electron scattering angles θ_e and ϕ_e, the electron momentum k, and the projectile impact parameter b, i.e.,

$$\sigma = 2\pi \int_0^\infty bdb \int_0^\infty dk \int_0^\pi \sin\theta_e d\theta_e \int_0^{2\pi} d\phi_e \frac{d^4\sigma}{dk\, db\, d\theta_e\, d\phi_e}. \tag{16}$$

For all fully differential cross sections in both formulations the units are area divided by the units of all the differential quantities. The fully differential cross section of Eq. (10) has the units of area divided by length squared for $2\pi bdb$ times momentum for dk times solid angle for $\sin\theta_e d\theta_e d\phi_e$. The

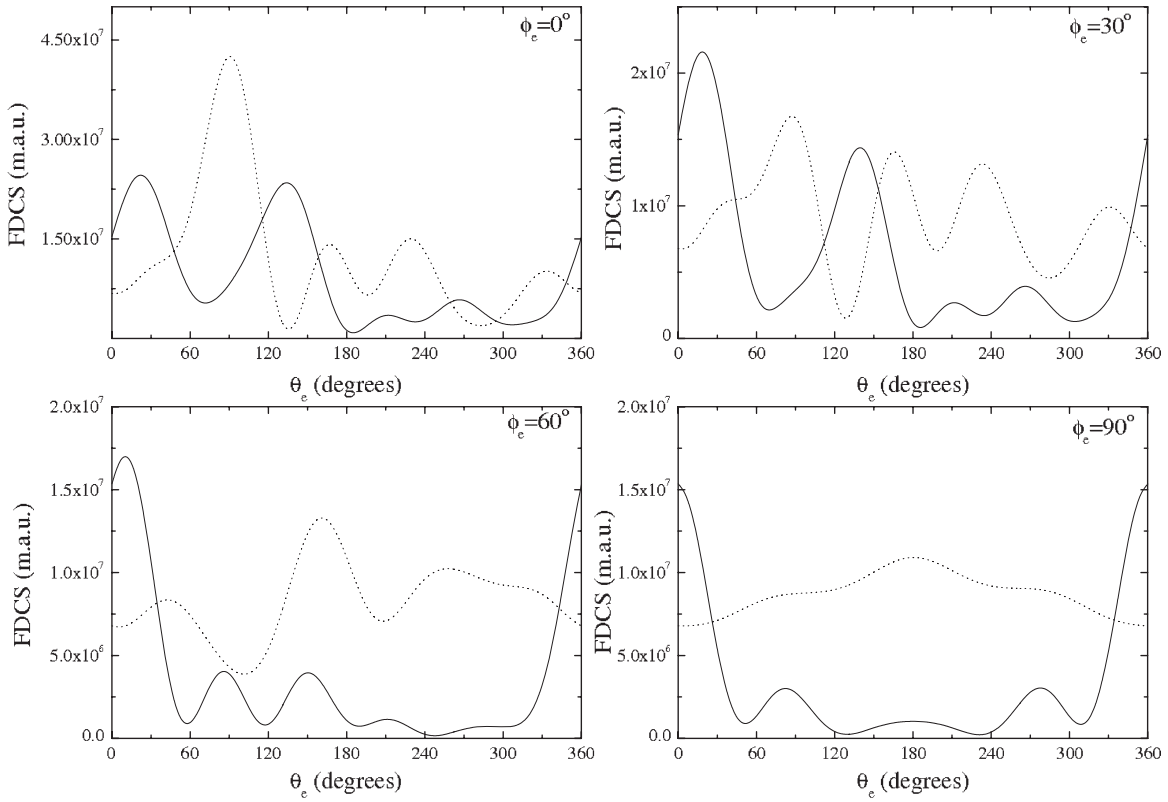

FIG. 2. Fully differential cross sections (FDCS-η) for single ionization of Li($2s$) by 1.5 MeV/amu O^{8+} ions using the TDCC method based on an expansion of a one-electron, three-dimensional, wave-function approach for various values of the ejected electron azimuthal angle ϕ_e, for a momentum transfer of $\eta = 1.0$ a.u., and an ejected electron energy $\epsilon = 1.5$ eV. Full line: calculations including the nuclear-nuclear interaction; dotted line: calculations neglecting the nuclear-nuclear interaction, i.e., with $\Delta(b) = 0$ in Eq. (12). (m.a.u. = modified atomic units equal to 2.8×10^7 times atomic units such that the total cross section is in units of 1.0×10^{-24} cm^2.)

fully differential cross section of Eq. (11) has the units of area divided by $2\pi\eta d\eta$ times momentum for dk times solid angle for $\sin\theta_e d\theta_e d\phi_e$. In order to have the total cross sections in barns (1.0×10^{-24} cm^2) we multiply all FDCS-b and FDCS-η by 2.8×10^7.

We employ the TDCC method based on an expansion of a one-electron, three-dimensional, wave-function method to calculate various (multiple) differential single-ionization cross sections in O^{8+} + Li collisions at 1.5 MeV/amu. Our first step is to diagonalize the radial Hamiltonian of Eq. (7), where our choice for the Hartree-local exchange potential is given by

$$V_l(r) = \int \frac{dr'}{r_>} 2P_{1s}^2(r') - \frac{\alpha_l}{2}\left(\frac{24\rho(r)}{\pi}\right)^{\frac{1}{3}}, \qquad (17)$$

where $\rho(r) = \frac{2P_{1s}^2(r)}{4\pi r^2}$ and the $P_{1s}(r)$ bound radial orbital is found from an atomic structure calculation [18] for $Li^+(1s^2)$. Diagonalization of the $l = 0$ Hamiltonian of Eq. (7) with $\alpha_0 = 0.58$ in Eq. (17), on a 768-point radial mesh with $\Delta r = 0.10$ atomic units (a.u.), yields an ionization potential for the $2s$ subshell of Li($1s^2 2s$) of 5.388 0 eV, in excellent agreement with experimental results [19]. In order to prevent collapse of the $P_{lm}(r,t)$ radial wave functions into the closed $1s^2$ inner subshell, we replaced the $l = 0$ Hartree with local exchange potential with a pseudopotential following standard procedures [20]. Diagonalization of the $l = 1$ Hamiltonian of Eq. (7) with $\alpha_1 = 0.20$ yields an ionization potential for the $2p$ subshell of Li($1s^2 2p$) of 3.530 6 eV, again in agreement with experimental results. For $l \geqslant 2$, the Hamiltonian of Eq. (7) is diagonalized with $\alpha_l = 0.0$. Differential ionization cross sections were obtained by propagating the $P_{lm}(r,t)$ radial wave functions using Eq. (3) on the 768-point radial mesh with 16 lm (l = 0–3) coupled channels. Continuum orbitals are obtained by direct integration of the radial Schrödinger equation given by

$$H(r)P_{kl}(r) = \epsilon P_{kl}(r) \qquad (18)$$

for 300 box-normalized functions with a uniform spacing of $\Delta k = 0.05$ a.u. to span an electron energy $\epsilon = \frac{k^2}{2}$ up to 3 keV. The $P_{kl}(r)$ continuum orbitals are used to obtain momentum-space wave functions in Eq. (8).

The multiple-differential cross sections computed from the TDCC method based on an expansion of a one-electron, three-dimensional, wave-function approach are obtained by time propagating Eq. (3) from $d_0 = -50$ a.u. to $d_{\text{final}} = +106$ a.u. at 250 different impact parameters with $\Delta b = 0.2$ a.u. reaching a maximum value $b_{\max} = 50$ a.u.

III. RESULTS

We first start analyzing the fully differential cross section for individual values of the impact parameter b (FDCS-b) of Eq. (10). In Fig. 1 we present FDCS-b for an electron energy

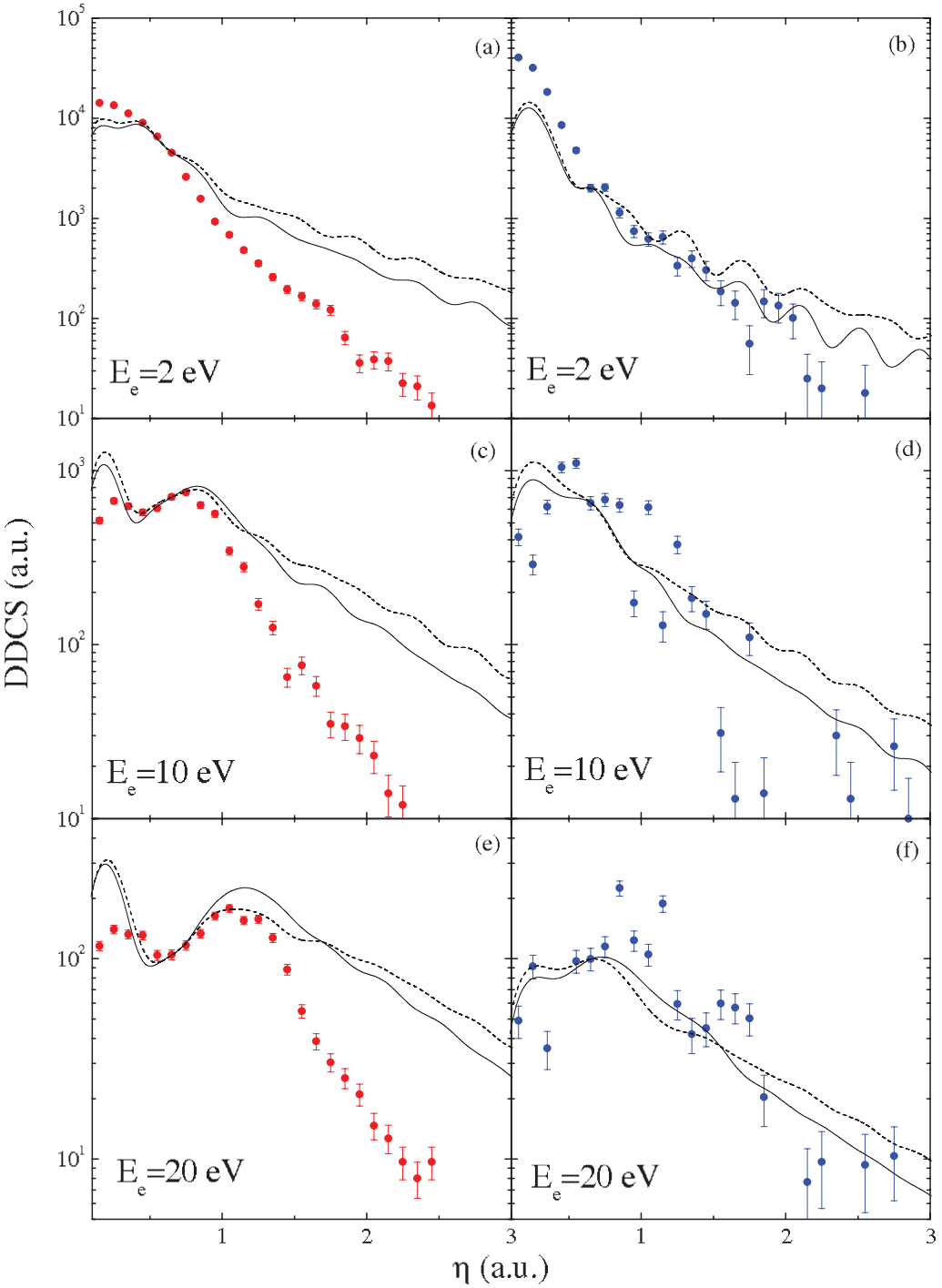

FIG. 3. (Color online) Double-differential cross sections as a function of electron energy and transverse momentum transfer ($d^2\sigma/d\eta d\epsilon$) of single ionization of Li($2s$) and Li($2p$) by 1.5 MeV/amu O^{8+} impact. Panels (a), (c), and (e) are for Li($2s$) and electron energies of 2 eV, 10 eV, and 20 eV, respectively, and panels (b), (d), and (f) are for Li($2p$) and electron energies of 2 eV, 10 eV, and 20 eV, respectively. Solid lines are the TDCC method based on an expansion of one-electron, three-dimensional, wave-function results with a target effective charge in the NN model of $Z_{\text{eff}} = 1$; dashed lines are the TDCC method based on an expansion of one-electron, three-dimensional, wave-function results with a target effective charge in the NN model of $Z_{\text{eff}} = 1.26$; solid circles are the experimental data of Ref. [16].

$\varepsilon = 1.5$ eV, as a function of the electron angle θ_e and for different values of the electron azimuthal angle ϕ_e. $\phi_e = 0^\circ$ corresponds to the so-called scattering plane, while $\phi_e = 90^\circ$ sets the perpendicular plane (for details of the collision geometry see Ref. [21]). Angles different from the two already mentioned define intermediate planes and we have chosen two of them, namely, $\phi_e = 30^\circ$ and $\phi_e = 60^\circ$, in order to study the behavior of the FDCS-b as a function of ϕ_e.

The FDCS-b for $b = 0.4$ a.u. (solid lines) has large peaks for $\theta = 0^\circ$ and $\theta = 180^\circ$ along the direction of the

projectile motion and for all the azimuthal case studies. Comparing this behavior with the case of C^6+He collisions (for details see [8]), we observe that the FDCS-b look quite similar. Since the mean electron radius of of the Li $1s$ orbital is $\langle r\rangle_{1s} = 0.57$ a.u., we see that a projectile with $b = 0.4$ a.u. penetrates deep enough to feel the full charge of the bare ion, as in the case of helium (with now a charge of $Z = 3$), and consequently, comparable features should be observed. In addition, compared with the case of C^6+He collisions, a larger momentum transfer ($\Delta p = 5.08$ a.u.) is also found.

On the other hand, for larger impact parameters, the projectile would feel a more complex atomic structure. Since the mean electron radius of the Li $2s$ orbital is $\langle r\rangle_{2s} = 3.87$ a.u., the FDCS-b for $0.5 \lesssim b \lesssim 4$ corresponds to the case where the projectile will interact with an electron cloud that is quite different than in the case of a He target, which may significantly modify the FCDS-b distribution.

The FDCS-η are the quantities experimentally measured in COLTRIMS and MOTReMi experiments. Such measurements are differential in all the parameters, namely, η, k (or energy ϵ via $\epsilon = \frac{k^2}{2}$), θ_e, and ϕ_e. In Fig. 2 we show the FDCS-η as a function of the electron angle θ_e and for different values of the electron azimuthal angle ϕ_e. The electron energy was chosen as $\epsilon = 1.5$ eV, and the value of the projectile momentum transfer is $\eta = 1.0$ a.u. The two latter values could be considered typical and experimentally accessible [22].[1] In Fig. 2 the FDCS-η are calculated including (full lines) and neglecting (dotted lines) the interaction between the two heavy nuclei, i.e., the NN interaction. The latter was included using the phase factor of Eq. (12) in Eq. (11). We should note, however, the choice of the NN model is not unique [9,13,14].

In some sense, the FDCS-η represents a *weighted* collection of the FDCS-b for different values of the impact parameter b. Incidentally, FDCS-b for precise values of b resembles in shape the FDCS-η in particular collision planes (this behavior was also observed using He targets [8]). In the perpendicular plane ($\phi_e = 90^\circ$), for instance, the FDCS-b for $b = 2.0$ a.u. (dotted line in Fig. 1) appears to be similar in shape to the corresponding FDCS-η counterpart of Fig. 2. On the other hand, for the other planes it appears the complex shape observed in FDCS-η (both including and neglecting the NN interaction) is not closely reproduced by FDCS-b for particular values of b.

From a close inspection both in shape and magnitude of Fig. 2 we can conclude the FDCS-η depends strongly on the NN interaction. For instance, when this interaction is included, the FDCS-η for $\phi_e = 0^\circ$ (scattering plane) presents a double-peak-shaped structure in the range $0^\circ < \theta_e < 180^\circ$; meanwhile, when the NN interaction is neglected only one peak appears to dominate in the same θ_e range. In the perpendicular plane, i.e., $\phi_e = 90^\circ$, the FDCS-η including the NN interaction shows a symmetric structure with a large peak at $\theta_e = 0^\circ$ and other small peaks at $\theta_e \approx 90^\circ$ ($\theta_e \approx 270^\circ$) and $\theta_e = 180^\circ$. On the other hand, the FDCS-η neglecting the NN interaction peaks at $\theta_e = 180^\circ$ and the difference between the value of this peak and the one at $\theta_e = 0^\circ$ is less pronounced.

One major difference, both in the FDCS-b and the FDCS-η, between the case of single ionization of He and Li by ion impact should be pointed out. By comparing the single ionization of He and Li for similar projectile parameters [13,24] we can conclude the FDCS are very sensitive to the initial state. For single ionization of He by relatively high-speed projectiles, the FDCS-η shows the usual binary and recoil peaks at the direction of $\approx\boldsymbol{\eta}$ and $\approx-\boldsymbol{\eta}$, respectively. Certainly the actual position will depend on the projectile velocity and charge, but in a large range of projectile parameters the FDCS exhibits these two peaks at $\theta_e \approx 90^\circ$ (binary peak) and $\theta_e \approx 270^\circ$ (recoil peak) [9,21,24].

In Fig. 3 we present double-differential cross sections (DDCSs) as a function of electron energy and momentum transfer for single ionization of Li($2s$) and Li($2p$) by 1.5 MeV/amu O^{8+} impact ($d^2\sigma/d\eta d\epsilon$). The latter was obtained by integration of the FDCS-η over the electron angles θ_e and ϕ_e [see Eq. (14)]. Our theoretical results are compared with the experimental measurements of Ref. [16]. We have normalized the experimental data to our theoretical cross sections for $\eta = 0.65$ a.u. (see. [16] for more details). From the figure we can observe the very good agreement between theory and experiment for all the Li($2p$) cases [panels (b), (d), and (f)] and fair agreement for the Li($2s$) cases [panels (a), (c), and (e)]. In the latter, major deviations can be seen for values of $\eta \gtrsim 1$ a.u. We can consider our model accounts for the NN interaction in a similar way to the continuum distorted wave-eikonal initial state approximation accounting for the nuclear-nuclear interaction quantum mechanically in terms of the eikonal approximation (CDW-EISNN) of Ref. [16] (dashed lines of Fig. 2), i.e., a quantum-mechanical model based on the eikonal approximation. Consequently, comparable predictions would be expected. This is true for all the Li($2p$) cases (see below) and the Li($2s$) case with $E_e = 2$ eV, but discrepancies appear for the other two energies studied, i.e., $E_e = 10$ eV and

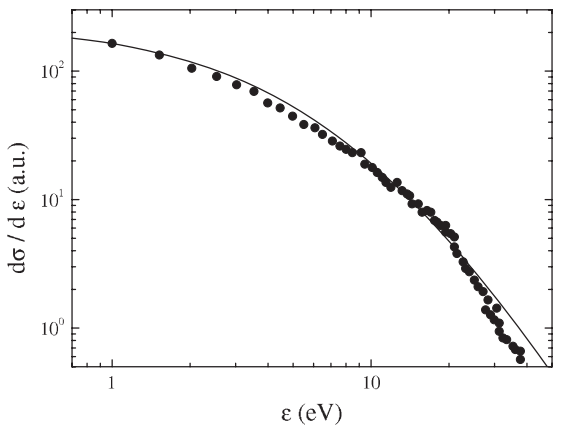

FIG. 4. Single-differential cross section in energy ($d\sigma/d\epsilon$) for single ionization of Li($2s$) by 1.5 MeV/amu O^{8+} ions. The solid line is the TDCC method based on an expansion of one-electron, three-dimensional, wave-function results and the solid circles are the experimental data of Ref. [15].

[1]Note that very recently fully differential cross sections (in the azimuthal plane) for single ionization of Li by impact of 1.5 MeV/amu O^{8+} ions were presented [23].

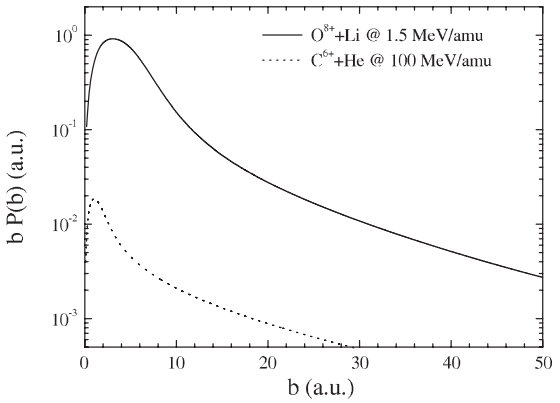

FIG. 5. TDCC method based on an expansion of one-electron, three-dimensional, wave-function calculations of the weighted ionization probability (log-scale) for single ionization of Li($2s$) by 1.5 MeV/amu O^{8+} ions and single ionization of He by 100 MeV/amu C^{6+} ions as a function of the impact parameter.

$E_e = 20$ eV, with $\eta \gtrsim 1.5$ a.u. The reason for this discrepancy could be traced back to the way each individual FDCS-b is weighted by the Fourier transform formalism and indicates that the contribution of the small impact parameters, the so-called "close collisions" (corresponding to the larger values of η), is overestimated. The excellent agreement between a perturbative theory joint with a classical model for the NN interaction (continuum distorted wave-eikonal initial state approximation accounting for the nuclear-nuclear interaction classically (CDW-EISCLNN), i.e., solid lines of Fig. 2 of Ref. [16]) demonstrates, however, that our model for the NN interaction could be also responsible for the differences.

On the other hand, for the Li($2p$) DDCS, our theoretical model is able to reproduce reasonably well the experimental data. As a consequence, the Fourier transform approach seems to adequately weight the individual FDCS-b for this case. We note Z_{eff} in Eq. (12) is a parameter one could vary in order to obtain a possibly better description of the NN interaction, including, for instance, the screening of the passive remaining electrons of the Li residual ion. One simple choice for Z_{eff} can be obtained from $Z_{\text{eff}} = \sqrt{-2n^2\varepsilon_i}$, where n is the principal quantum number and $\varepsilon_i < 0$ the energy of the ground or excited initial state [13]. For the cases studied in this article, however, there are no major improvements compared with the choice of an *unscreened* charge, i.e., $Z_{\text{eff}} = 1$.

In Fig. 4 we present single-differential cross sections for the single ionization of Li($2s$) by 1.5 MeV/amu O^{8+} projectiles in the electron energy ($d\sigma/d\epsilon$). The latter was obtained from multiple integrations (see Sec. II) of the time-propagated electron momentum space wave functions. Our theoretical results are compared with experimental data obtained in MOTReMi experiments [15]. The measured experimental data were normalized to the theoretical differential cross sections at the smallest electron energy. From the figure we observe the excellent agreement of the TDCC method based on an expansion of one-electron, three-dimensional, wave-function results with the experimental data for almost all the range of ejected electron energies. Consequently, our scheme appears to be adequate to model differential cross sections in such an energy range. Performing the integration in energy the total cross section was found to be 1.12×10^{-15} cm^2 using Eq. (16).

Finally, in Fig. 5 we show the weighted ionization probability in logarithmic scale for the single ionization of Li($2s$) by 1.5 MeV/amu O^{8+} projectiles in comparison with the case of single ionization of He by by 100 MeV/amu C^{6+} projectiles [9]. From the figure we could argue that now the probability distribution peaks around $b = 4$ a.u. ($b = 1$ a.u. for the case of helium) and it is much broader. In addition, a large range of impact parameters ($b = 50$ a.u. was our maximum value used in our calculations) is required in order to obtain converged cross sections.

IV. SUMMARY AND CONCLUSIONS

We have shown in this paper how the TDCC approach may be used to calculate fully differential cross sections for single ionization of Li by fast projectile impact. We have employed a three-dimensional treatment of one active electron interacting with the projectile. This approach could be considered adequate considering the remaining two electrons of the Li ion form a closed shell. The three-dimensional approach can also be straightforwardly modified to calculate fully differential cross sections both as a function of the impact parameter and the projectile momentum transfer. The latter are the quantities obtained in COLTRIMS or MOTReMi experiments and consequently, our predictions could be confirmed by future measurements. The interaction between the two heavy nuclei, the so-called NN interaction, can be directly incorporated in our numerical scheme and we have observed substantial differences, both in shape and magnitude, between the calculated quantities when we include (neglect) this interaction. This behavior confirms FDCS as the most sensitive quantity in the few-body breakup processes. Furthermore, our single-differential cross section calculations are in excellent agreement with experimental data over the whole range of electron energy. Finally, we have also incorporated in our scheme calculations for the single ionization of Li in its excited states in order to compare our results with double-differential cross sections as a function of the electron energy and transverse momentum transfer. Reasonable agreement, especially for the Li($2p$) cases, is observed.

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