Ionization from the outer shell of Ar by proton impact

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(Received 25 June 2003; published 4 November 2003)

Recent results for proton-argon total ionization cross sections [Kirchner *et al.* Phys. Rev. Lett. **79**, 1658 (1997)] show large disagreement between theory and experiment for energies below 80 keV. To address this problem we have employed a recently developed theoretical method with a more pragmatic approach to the charge screening both in the initial and final channels. The target is considered as a one-electron atom and the interactions between this active electron and remaining target electrons are treated by a model potential including both short- and long-range effects. In the final channel the usual product of two continuum distorted wave functions each associated with a distinct electron-nucleus interaction is used. New results in the present calculation show good agreement in total cross sections for the energy range 10–300 keV with the measurement of Rudd *et al.* [Rev. Mod. Phys. **57**, 965 (1985)].

DOI: 10.1103/PhysRevA.68.052702 PACS number(s): 34.50.Fa, 34.70.+e

I. INTRODUCTION

Over the past few decades, both theoretical and experimental physicists have shown their interest in heavy-particle collisions. Of the various processes that might occur due to such collisions, ionization, in particular, became highly significant due to its practical applications in various fields, such as fusion research [1], astrophysics [2], etc. Recently, there have been intense studies of the processes involving collisions of bare ions impinging on multielectron targets with the primary motivation of investigating the wide range of applications of these in fusion research. It is important to assess which reactions become predominant in the plasma environment. In this respect, the study of ionization of multielectron targets has a special interest. For collision of a bare ion with an atom, it may be expected that the residual Coulomb interaction, either in the entrance channel or in the exit channel or in both, may have some effects on the cross-section values. From the theoretical point of view, the main difficulty is the representation of the final electronic state, where the emitted electron travels under the influence of the Coulomb potential due to both the target and the projectile nuclei. Due to the long-range nature of the Coulomb potential this cannot be represented simply by a plane wave. An exact solution of the problem is not possible, though its asymptotic form can be found. Furthermore, ionization cross sections are expected to be sensitive to the quality of the target wave function and therefore accurate wave functions are needed to calculate these cross sections.

On the theoretical side, ionization of multielectron targets has been studied using a variety of distorted-wave models. One such widely used model, developed originally by Crothers and McCann [3], is known as the continuum distorted-wave eikonal initial-state (CDW-EIS) approximation. This approximation differs from the conventional continuum distorted wave (CDW) theory in that it describes the distortion in the initial channel by an eikonal phase factor rather than by a full continuum wave. Of course the phase factor comes from the asymptotic expansion of the CDW. Since its development, CDW-EIS has been used by many groups to investigate ionization from multielectron targets. Fainstein *et al.* [4] generalized the CDW-EIS [3] approximation to multielectron targets using Roothaan-Hartree-Fock (RHF) wave functions [5] for the ionization of helium. This work was followed by a number of works [6,7] by the same group to investigate other many-electron atoms. McCartney and Crothers [8] presented a systematic study of doubly differential and total cross sections for the ionization of lithium, beryllium, and neon. Their results agree fairly well with the available measurements [9–11]. It is to be noted here that the two calculations on neon by McCartney and Crothers [8] and by Fainstein and Rivarola [6] produced noticeably different results for the outer-shell ionization even though both groups used the same CDW-EIS approximation. However, both groups did obtain the same results for the K-shell ionization.

Kirchner *et al.* [12] studied net ionization and electron loss of Ne and Ar using three different model potentials within the framework of the CDW-EIS approximation. Their Hartree-Fock-Slater (HFS) numerical potential reported earlier by Gulyás *et al.* [13] maintained orthogonality between initial and final states. The other two methods, namely, the local density approximation (LDA) and the optimized potential method (OPM), accounted for exchange correlation effects with the OPM method having the more accurate account of the exchange correlation. Accordingly, their results for net ionization as well as for total electron-loss cross sections in the OPM model show better agreement with the measurements [11,14] above the 100 keV region. Below this energy range the disagreement is worse for the Ar target than for the Ne target. A more pragmatic target screening charge effect both in the initial and final channels might resolve this disagreement, keeping in mind that both targets are closed shell/subshell atoms with $3s^2 3p^6$ and $2s^2 2p^6$ configurations, respectively. This is what motivated us to investigate the ionization of Ar with an improved model potential (described below) which has been used successfully for other neutral targets [15–17]. Further it has been established both by calculations [6,8] and measurement [10,11,18,19] that contributions to the total ionization cross sections come mostly from the $2p$ subshell of Ne, while the $2s$ subshell contribution is at least two orders of magnitude smaller. K-shell contributions practically have a negligible effect on these total ionization cross sections. This is certainly true up to a few hundred keV incident proton energy. A similar trend for the ionization cross sections of Ar can be assumed accordingly. In the present investigation, we therefore consider ionization from the $3p$ sub-shell of neutral argon.

In what follows we present a brief description of our theoretical method applied to the p-Ar ionization problem, evaluation of the transition amplitude, and comparison of our results with available theoretical and experimental data for total ionization cross sections. Atomic units are used throughout unless otherwise stated.

II. THEORY

For simplicity, we consider that the target has only one active electron and that it experiences an effective potential due to the target nucleus and the passive electrons. The interaction of the active electron and the residual target ion of asymptotic charge q_A may be described in different ways; here it has been considered using a model potential of the form

$$V_A=-\frac{1}{r_A}[q_A+e^{(-\lambda r_A)}\{(Z-q_A)+br_A\}], \tag{1}$$

where Z is the nuclear charge of the target and r_A is the distance of the active electron from the nucleus of the target; b and λ are parameters determined variationally with respect to the Slater basis set. This has been done in such a way that the corresponding Hamiltonian of the active electron is diagonalized to reproduce the correct binding energy. The accuracy of the wave function has been verified by the virial theorem to within 0.01%. Clearly, the potential in Eq. (1) contains a long-range part to account for the Coulomb interaction between the active electron and the target core and a short-range part to account for the distortion, the correlation and indeed other effects of the passive electrons. Nevertheless, the present model-potential does not contain explicit exchange correlation as included in the LDA and OPM model of Kirchner *et al.* [12] although some correlation has been taken into account through the dynamic screening.

Following Sahoo *et al.* [15] the Born initial-state (BIS) wave function used here is

$$\Psi_i^+=\left(\sum_j C_j^{nl}\exp(-\beta_j r_A)r_A^l Y_{lm}(\hat{r}_A)\right)\times\exp\left[-i\left\{\frac{\vec{v}.\vec{r}}{2}+\left(\varepsilon+\frac{v^2}{8}\right)t\right\}\right], \tag{2}$$

which is an approximate eigenstate of

$$\left(H_i-i\frac{\partial}{\partial t}\right),$$

where

$$H_i=-\tfrac{1}{2}\nabla_r^2+V_A(r_A) \tag{3}$$

with energy ε and quantum numbers $n,\ l,\ m$; $\mathbf{v}$ is the velocity of the projectile with respect to the target and $\mathbf{r}$ is the position vector of the electron from the midpoint of the two nuclei.

The Hamiltonian for the one active-electron model is represented by

$$H_{el}=-\tfrac{1}{2}\nabla_r^2+V_A(r_A)+V_B(r_B), \tag{4}$$

where r_B is the distance of the electron from the projectile. The impact parameter treatment is considered here and the internuclear motion is treated classically via $\vec{R}=\vec{p}+\vec{v}t$, $\vec{p}$ is the impact parameter and time t has been measured from the instant when the two nuclei are at closest approach.

The transition amplitude as a function of impact parameter p can be expressed as

$$A_{fi}(p)=\int\int\left[\Psi_{\vec{k}}^{-*}\left(H_{el}-i\frac{d}{dt}\right)\Psi_i^+\right]d\vec{r}\,dt, \tag{5}$$

where $\vec{k}$ is the momentum of the ejected electron and $\Psi_{\vec{k}}^-$ is the wave function of the final channel. The initial condition is that at $t=-\infty$, $A_{fi}=0$, and the ionization probability is $|A_{fi}(t=+\infty)|^2$.

The wave function in the final channel is taken to be the product of two CDWs given by

$$\Psi_{kc}^-=(2\pi)^{(-1.5)}N_1N_2e^{i\vec{k}\cdot\vec{r}}\,{}_1F_1(i\alpha_{B,}1,-i(k_Br_B+\vec{k}_B.\vec{r}_B))\times{}_1F_1(i\alpha_A,1;-i(k_Ar_A+\vec{k}_A.\vec{r}_A))e^{-ik^2t/2}, \tag{6}$$

where $\alpha_B=-z_B/k_B$, $\alpha_A=-q_A/k_A$, $\vec{k}_B=\vec{k}-(\vec{v}/2)$, $\vec{k}_A=\vec{k}+\vec{v}/2$, z_B is the nuclear charge of the projectile, and

$$N_1=e^{-\pi\alpha_B/2}\Gamma(1-i\alpha_B),\quad N_2=e^{-\pi\alpha_A/2}\Gamma(1-i\alpha_A). \tag{7}$$

Compared to Crothers and McCann [3], the electron velocity (and momentum) is refered to the midpoint of the two nuclei, rather than to the target, that is, in Eq. (6), without loss of generality and as a result of Galilean invarience.

The above continuum-state wave function in Eq. (6) satisfies the asymptotic Schrödinger equation

$$\left(-\frac{1}{2}\nabla_r^2-\frac{z_B}{r_B}-\frac{q_A}{r_A}-i\frac{\partial}{\partial t}\right)\Psi_{\vec{k}}^-=0. \tag{8}$$

The doubly differential cross section is obtained by integrating the transition probability over the impact parameter, i.e.,

$$\frac{d^2\sigma}{dE_e d\Omega_e}=k\int|A_{fi}(p)|^2dp, \tag{9}$$

and finally we get the total ionization cross section as

$$\sigma_{total}=2\pi\int\frac{d^2\sigma}{dE_c d\Omega_e}\sin\theta_e d\theta_e dE_e. \tag{10}$$

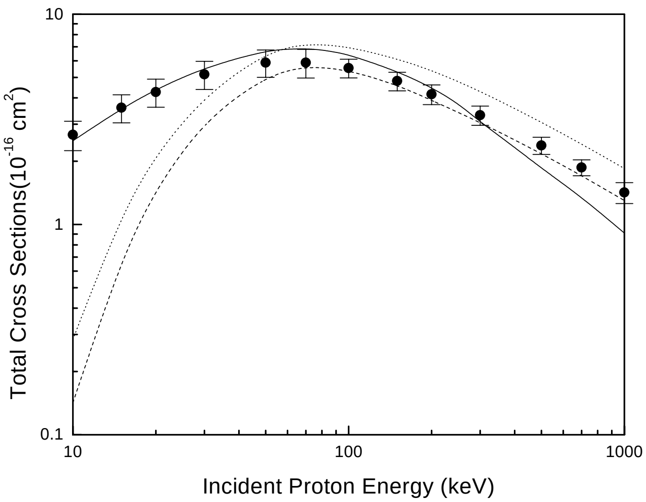

FIG. 1. Total ionization cross section for the proton-impact single ionization of Ar. Present results (——); theoretical results of OPM [10] (- - - - -); HFS (.........); experimental data [9] (••••).

For the total ionization cross sections from the $3p$ shell, we first calculate the average cross section of the electrons in the subshells ($p_{o,\pm1}$) and then multiply by six for the number of p electrons.

III. RESULTS AND DISCUSSIONS

We have already noted in the Introduction that most of the contributions to the total ionization cross sections come from the outer subshell ionization particularly in the low-energy region. For the Ne target both calculations [6,8] and measurements [10,11,18,19] clearly support this contention. According to Fainstein and Rivarola [6] the total cross sections up to 200 keV almost merged with the contribution from the $2p$ sub-shell (Fig. 1 in their work). The contributions from the $2s$ subshell are more than an order of magnitude smaller towards the lower end of the energy scale and 1s contributions are smaller by at least two more orders of magnitude. Similar behavior was also noted by McCartney and Crothers [8]. These results are in clear agreement with the available measurements [10,11,18,19]. Ar being a target of similar configuration in the M shell ($3s^2 3p^6$) as that of Ne in the L shell ($2s^2 2p^6$), we expect that the $3p$ subshell contributions would be dominant for Ar. In the present calculation, therefore, we considered ionization of Ar only from the $3p$ subshell.

In Fig. 1 we present our total $3p$ subshell ionization cross sections for the energy range 10 keV to 1 MeV. For comparison we also include, in the same figure, the total cross-section data of Rudd *et al.* [11] and HFS and OPM results of Kirchner *et al.* [12]. Notice that both HFS and OPM models (in contrast with the present results) produce cross sections in considerable disagreement with the measured values from 10 keV to 50 keV. Above this energy, OPM results show very good agreement with the measurement. The results of Kirchner *et al.* [12] with the LDA potential (not shown in this figure) are much higher than the other two models except at the highest energy. The LDA results also overestimate the measurement around the cross-section peak. In addition, the peak position in the LDA results seems to have shifted slightly towards lower energy compared to the measurement and other theoretical models. The point we wish to make here is that both LDA and OPM [12] include a static atomic-exchange potential with a more accurate exchange correlation in the OPM model. While the OPM results show very good agreement with measurement [11] at energies above 100 keV and underestimate it below that energy, the LDA results disagree throughout the energy range. On the other hand, the HFS cross sections which include a numerical Hartree-Fock-Slater potential always lie between the LDA and OPM results. Therefore none of the three model potentials (with or without exchange correlation) are doing particularly well over the energy range below 100 keV. In our understanding, the strength of the interactions (effectively more pragmatic screening charge) in the initial and final channels has to be taken into consideration. The present results (solid line) in Fig. 1 show very good agreement with the measurement [11] from 10 keV to 300 keV. Very recently, using a time-dependent independent particle model calculation Kirchner *et al.* [20] reported total cross sections for the net ionization in p-Ar collisions. They also found that the contributions to the total cross sections from the L-shell are at least two orders of magnitude smaller showing the dominance of the M-shell contributions. Again within the M shell, the $3p$ subshell contributions are expected to dominate in agreement with the corresponding Ne case [6,7]. Around the cross section peak our results are marginally higher than the corresponding measured values. Nevertheless, the present peak position agrees perfectly with the measurement. A closer look at the Fig. 2 of Kirchner *et al.* [20] shows that the peak position of their "response+AI" and "no response" results are shifted towards the lower energies compared to the measurement [11]. Their results around the peak are much higher than the present results and the measured values. The final-state wave function in the CDW-EIS [3] and in the present calculations are similar; however, the initial states in the two calculation differ. In the CDW-EIS an atomic bound state is multiplied by an Eikonal phase factor, whereas in the present case the plane wave stands alone. It is well known that the EIS is best suited for the intermediate and the high energy region. The model potential [Eq. (1)] in the calculation of our target wave function is phenomenological and contains correct long- and short-range Coulombic behavior. This means that the wave function in Eq. (2) optimized on the Hamiltonian in Eq. (3) contains radial and energy correlation. We may conclude that the model potential with the corresponding wave function used in the present calculation is the primary reason for the better agreement of our results with the measurement [11] in the low-energy region. For higher energies the CDW-EIS results of Kirchner *et al.* [12] are comparatively better than ours.

ACKNOWLEDGEMENTS

One of the authors (K.R.) acknowledges the IRCEP at the Queen's University Belfast for support to visit Belfast. N.C.D. acknowledges financial support through the DST (Government of India) Grant No. SP/S2/L-12/99.

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