# Direct ionization of heavy noble gases by positron impact

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We present results for direct ionization of the heavy noble gases neon, argon, krypton, and xenon by positron impact. The computational method used is a hybrid approach, describing the projectile by a distorted wave but the initial bound state and the ejected-electron–residual-ion interaction by an *R*-matrix (close-coupling) expansion. A relatively small sensitivity of the theoretical predictions on the details of the computational model is noticed. Overall, fair agreement with recent experimental data is obtained.

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## I. INTRODUCTION

Positron collisions with heavy noble gases have been investigated for several decades. In contrast to electron collisions, one of the major experimental difficulties is the generation of a sufficiently intense monoenergic beam. Recent progress in trap technology has resulted in significant advances to overcome this problem, and new benchmark data of unprecedented accuracy are now being generated. An example are the absolute cross-section data measured by Marler, Sullivan, and Surko [1] for direct ionization and positronium formation in positron collisions with heavy noble gases. A summary of the current experimental state-of-the-art for positron-atom collisions can be found in the above paper and the accompanying references.

Computational methods to attack this problem are generally classified as either perturbative, i.e., based upon the Born series, or nonperturbative, i.e., based upon the close-coupling expansion. The former includes work by Campeanu *et al.* [2,3] for direct ionization and by Gilmore *et al.* [4] for positronium formation, while positronium formation was also calculated in the coupled static-exchange approximation by McAlinden and Walters [5]. Overall satisfactory agreement with experiment was obtained for direct ionization processes, while problems remain regarding both the energy dependence and the absolute values of the cross section for positronium formation. For details, we refer again to the recent publication by Marler *et al.* [1].

In this paper, we investigate the ability of a hybrid approach to predict the total cross section for direct ionization by positron impact. Originally developed by Bartschat and Burke [6] for electron-impact ionization of arbitrary atoms and ions, the projectile is described by a distorted wave while the initial bound state and the interaction between the residual ion and the ejected electron are described by an *R*-matrix (close-coupling) expansion. The essential ideas of this method will be summarized in the next section. This is followed by selected results for ionization of argon to illustrate the model dependence of theoretical predictions, before a comparison with the most recent experimental data of Marler *et al.* [1] is made for direct ionization of neon, argon, krypton, and xenon by positron impact.

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## II. COMPUTATIONAL METHOD

As mentioned above, the computational approach used in the present work is based upon the formalism outlined by Bartschat and Burke [6] and the computer program RMATRX-ION of Bartschat [7]. The basic idea is to describe a "fast" projectile positron by a distorted wave and then calculate the initial bound state and the interaction between the residual ion and a "slow" ejected electron by an *R*-matrix (close-coupling) expansion. Although second-order effects in the projectile-target interaction can now be taken into account approximately [8,9], this was not done in the present work, because the approximations that currently still need to be made can make it difficult to distinguish between physical and numerical effects in the interpretation of the results.

We therefore used a first-order distorted-wave representation for the projectile and a two-state close-coupling approximation for electron scattering from the residual ion, coupling only the ionic ground state $(ns^2np^5)^2P^o$ and the first excited state $(nsnp^6)^2S$ with $n=2$ for Ne, $n=3$ for Ar, $n=4$ for Kr, and $n=5$ for Xe, respectively. The ionic target description for $Ne^+$ and $Ar^+$ is the one used first by Burke and Taylor [10] for the corresponding photoionization problem and then later by Bartschat and Burke [11] in the calculation of single-differential and total ionization cross sections of argon by electron impact. For Kr and Xe, we generated similar multiconfiguration (CI) expansions, allowing for single and double promotion of the outer-shell ($n$) electrons into specially designed pseudo-orbitals $\overline{5}s,\overline{5}p,\overline{4}d$ for Kr and $\overline{6}s,\overline{6}p,\overline{5}d$ for Xe. As shown in [10], the use of the latter pseudo-orbitals significantly improved the description of the initial bound state, the theoretical energy splitting between the two ionic states, and the results for the oscillator strength in the ion for Ne and Ar. Similar improvements were achieved in the present work for Kr and Xe, although cancellation effects make it apparently very difficult to calculate the oscillator strength in the residual ion accurately. The results from single-configuration (SC) and multiconfiguration expansions for all four targets are summarized in Table I and compared with datasets compiled by NIST [12]. Since the improvement of the initial state and the final ionic states is a potentially important difference between the present work and calculations reported by other authors, we will compare below selected ionization results obtained with the two target descriptions.

 

TABLE I. Ionization potentials, excitation energies, and oscillator strengths (L for length form, V for velocity form) for the various targets. The experimental data are taken from [12] after averaging over the fine structure of the $^2P^o_{3/2,1/2}$ levels.

| | Ionization potentials (eV) | | | |
|---|---|---|---|---|
| | Ne | Ar | Kr | Xe |
| Single configuration | 21.001 eV | 15.107 eV | 13.529 eV | 9.336 eV |
| Multiconfiguration | 21.782 eV | 15.839 eV | 14.133 eV | 12.314 eV |
| NIST | 21.532 eV | 15.700 eV | 13.778 eV | 11.694 eV |
| | Excitation energies (eV) | | | |
| | Ne | Ar | Kr | Xe |
| Single configuration | 29.507 eV | 18.429 eV | 16.862 eV | 13.085 eV |
| Multiconfiguration | 27.126 eV | 13.556 eV | 12.966 eV | 9.825 eV |
| NIST | 26.878 eV | 13.421 eV | 13.292 eV | 10.831 eV |
| | Oscillator strength | | | |
| | Ne | Ar | Kr | Xe |
| Single configuration (L) | 0.175 | 0.3118 | 0.3813 | 0.4346 |
| Single configuration (V) | 0.116 | 0.1935 | 0.2347 | 0.2517 |
| Multiconfiguration (L) | 0.104 | 0.0297 | 0.0434 | 0.0470 |
| Multiconfiguration (V) | 0.112 | 0.0254 | 0.0425 | 0.0436 |
| NIST | 0.086 | 0.0091 | 0.0014 | 0.0018 |

In this hybrid method, exchange between the ejected electron and the residual target ion is treated computationally exact, since the close-coupling expansion for this part of the problem is based on fully antisymmetrized wave functions. Also, some channel-coupling effects are included, and it is possible to calculate ionization cross sections for the final ionic states (here $^2P^o$ and $^2S$) within the same model individually. On the other hand, the projectile (here the positron) is described by a distorted wave. The distortion potential was always chosen as the static ground-state potential of the respective neutral atom. Note, however, that our model does not account for any postcollision effects between the scattered projectile and the ejected electron. In particular, if the scattered positron is slower than the ejected electron, the choice of the neutral-atom potential for the positron while calculating electron scattering from the residual ion may not seem appropriate. For electron-impact ionization, this problem is typically overcome [13] by only integrating the single-

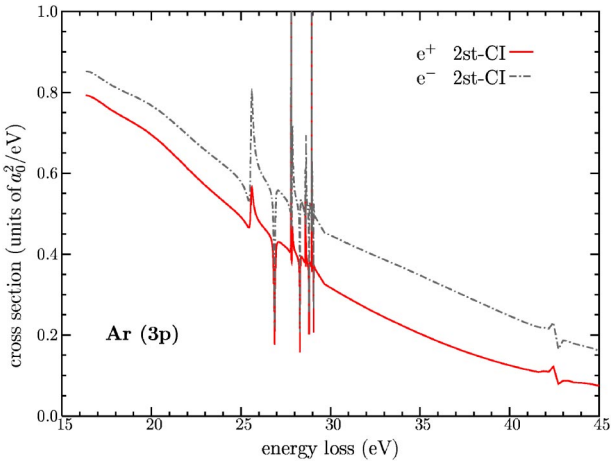


FIG. 1. Single-differential (with respect to energy loss) cross section for direct ionization of Ar(3*p*) by positron and electron impact, as obtained in the hybrid distorted-wave plus two-state close-coupling method for an incident projectile energy of 68 eV. The label "CI" stands for a multiconfiguration interaction description of the initial bound state and the final ionic target states.

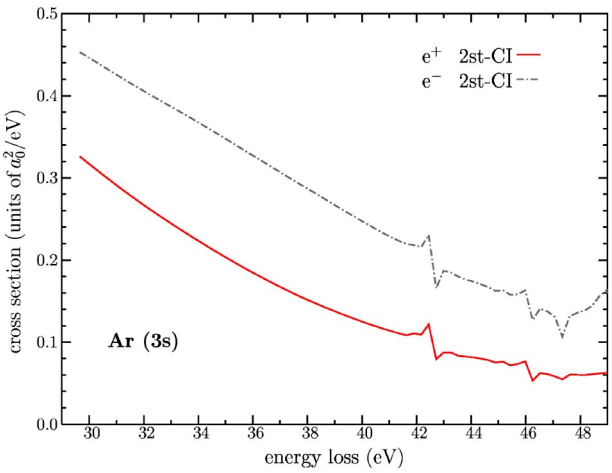


FIG. 2. Single-differential (with respect to energy loss) cross section for direct ionization Ar(3s) by positron and electron impact, as obtained in the hybrid DW-2st-CI method for an incident projectile energy of 68 eV.

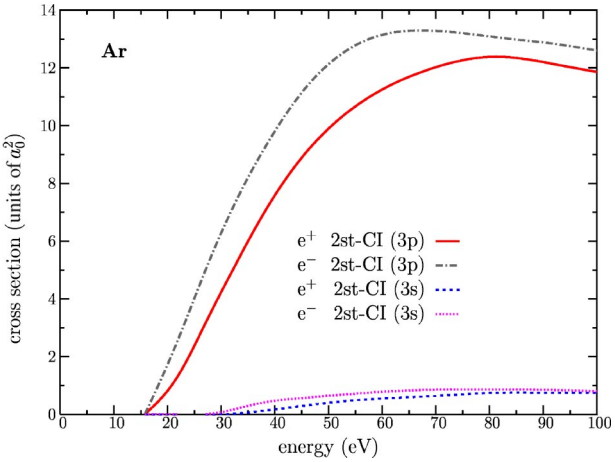


FIG. 3. Direct ionization cross sections for Ar(3*p*) and Ar(3*s*) by positron and electron impact, as obtained in the hybrid DW-2st-CI method.

differential (with respect to the energy loss) cross section (SDCS) up to half the excess energy that is to be shared between the two outgoing electrons. In the case of positron scattering, we estimated the contributions from the higher-energy losses by extrapolation. While this approach adds some uncertainty to the results, we note that the SDCS generally decreases with increasing energy loss (see Figs. 1 and 2 below) for incident energies sufficiently high above threshold, and hence the error in the estimate is not expected to be intolerably large.

Finally, partial waves up to orbital angular momenta of $\ell=90$ for the fast projectile guaranteed the convergence of its partial wave expansion. Furthermore, the Coulomb interaction between the fast projectile and the target was accounted for through the multipole components $\lambda=0-5$. This range of multipole components proved to be sufficient for the present cases of interest.

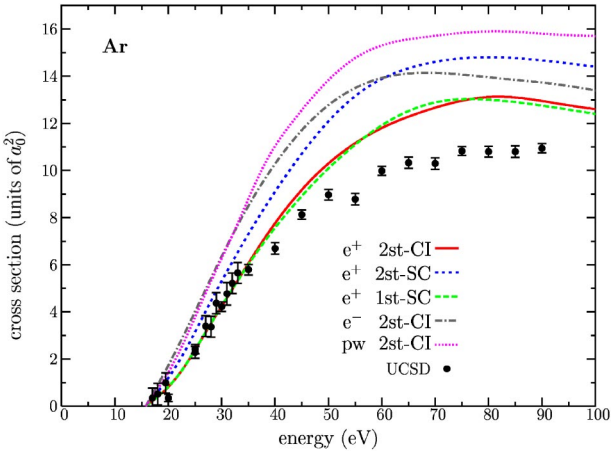


FIG. 4. Direct ionization cross sections for Ar(3*p*) and Ar(3*s*) combined by positron and electron impact, as obtained in various methods described in the text. The experimental data are those of Marler *et al.* [1].

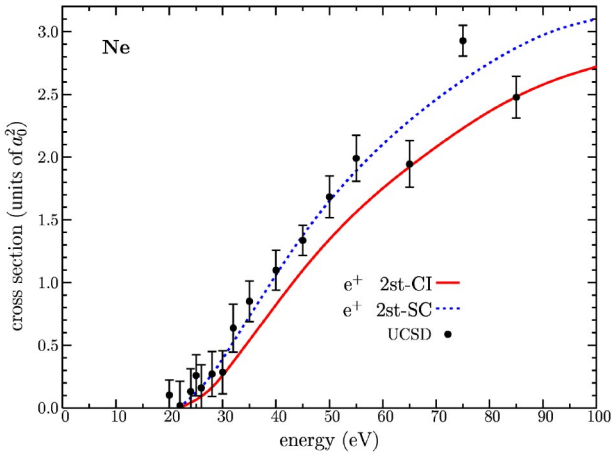


FIG. 5. Direct ionization cross sections for Ne(2*p*) and Ne(2*s*) combined by positron impact, as obtained in the DW-2st-CI and DW-2st-SC methods. The experimental data are those of Marler *et al.* [1].

## III. RESULTS AND DISCUSSION

Figure 1 displays the SDCS for direct ionization of Ar(3*p*) by positron and electron impact, as obtained in the hybrid distorted-wave plus two-state close-coupling method described above. The results for an incident projectile energy of 68 eV show indeed the decrease of the SDCS with increasing energy loss. In this case, the total cross section for electron-impact ionization is obtained by integrating the energy loss from threshold ($\approx$15.8 eV) to $\approx$41.9 eV, corresponding to half the excess energy to be shared between the two outgoing electrons. For positron-impact ionization, the SDCS is extrapolated (linearly) to the maximum energy loss of 68 eV. Note that the SDCS for positron impact is predicted to be significantly smaller than for electron impact, but the larger integration range makes up for some of the difference and leads to rather similar results for the total ionization

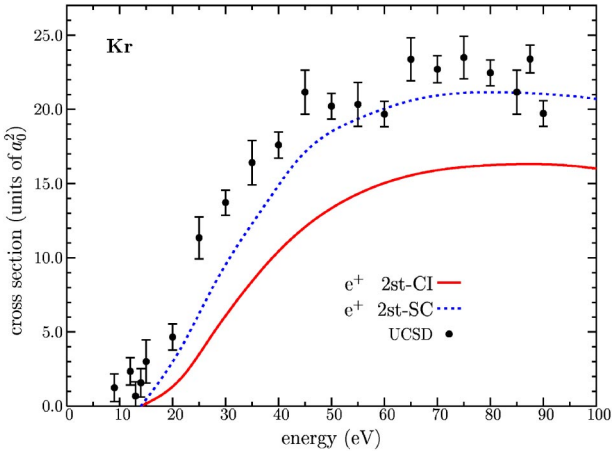


FIG. 6. Direct ionization cross sections for Kr(4*p*) and Kr(4*s*) combined by positron impact, as obtained in the DW-2st-CI and DW-2st-SC methods. The experimental data are those of Marler *et al.* [1].

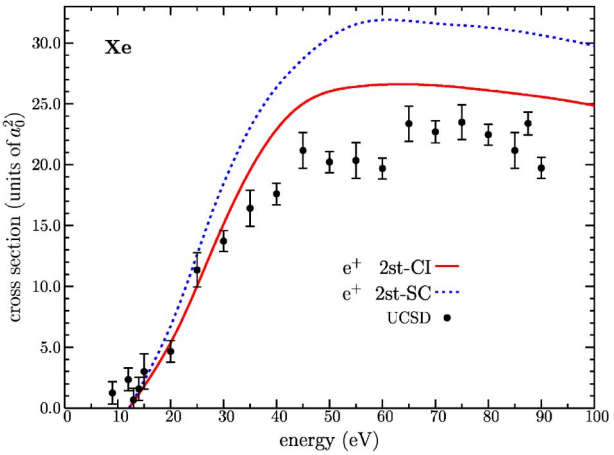


FIG. 7. Direct ionization cross sections for Xe($5p$) and Xe($5s$) combined by positron impact, as obtained in the DW-2st-CI and DW-2st-SC methods. The experimental data are those of Marler *et al.* [1].

cross section by electron and positron impact (see Fig. 3).

Note the Rydberg resonances that are predicted below the ionization threshold of the $Ar^+(3s3p^6)^2S$ final ionic state with a threshold energy loss of ≈29.4 eV. However, these resonances are too narrow to have a substantial effect on the total ionization cross section after integrating over all energy losses. The structure seen around an energy loss between 42 eV and 43 eV is actually a pseudostructure. It originates from the fact that not all target states that could be constructed from the individual configurations were actually included in the close-coupling plus correlation expansion of the ejected-electron–residual-ion collision problem.

Figure 2 exhibits predictions from the same model for generating $Ar^+$ in the excited $(3s3p^6)^2S$ final ionic state. Interestingly, the size of the SDCS is only two to three times smaller than the SDCS for creating a $3p$ hole, but the smaller integration range leads to a nearly negligible total cross section for $3s$ ionization at incident energies below 100 eV. The individual $3p$ and $3s$ total ionization cross sections for electron and positron impact are shown in Fig. 3.

Figure 4 presents our combined cross sections for direct ionization of Ar($3p$) plus Ar($3s$) by electron and positron impact. For positron impact, we also show the results for the cases when only the $(3s^23p^5)^2P^o$ state is included in the close-coupling expansion and when single-configuration (SC) descriptions of the initial bound state and the final ionic state are used. Finally, we show what happens when the distortion potential for the projectile is set to zero, i.e., the distorted wave is replaced by a plane wave (pw). As can be seen from the figure, the sensitivity of the theoretical results is quite limited. This lack of sensitivity likely explains why the present predictions, as well as those of purely perturbative models [2,3], are all in reasonable agreement with the experimental data of Marler *et al.* [1]. We refer to the latter work for a more detailed comparison with other theoretical and experimental datasets.

Figures 5–7 present our results for the Ne, Kr, and Xe targets. As a general trend, using multiconfiguration interaction descriptions of the initial bound state and the final ionic target states lowers the theoretical results, presumably since the ionization potential in the structure model increases. However, this better computational model does not necessarily yield better agreement with the experiment data. For Ne and Kr, the predictions from the single-configuration models are in nice agreement with the data of Marler *et al.* [1], and hence improving the target structure actually worsens the agreement between theory and experiment. For the Xe target, similar to the Ar case, the decrease in the predicted direct ionization cross section by the CI model brings the results into closer agreement with experiment, but the theoretical results are still systematically too large.

## IV. SUMMARY AND CONCLUSIONS

We used a hybrid distorted-wave plus close-coupling expansion to calculate cross sections for direct ionization of the heavy noble gases. Results from various computational models, distinguished mostly by the quality of the atomic and ionic wave functions used, were compared with each other and with recent experimental data. Overall, satisfactory but certainly not perfect agreement was achieved with both experiment and results from purely perturbative methods. Due to the apparent lack of sensitivity of the results for total ionization cross sections to the details of the numerical model, it seems necessary to compare theory and experiment at a more differential (angle-resolved and/or energy-resolved) level before more definite conclusions about the quality of a computational approach can be drawn.

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