

High-resolution experiments and B -spline R -matrix calculations for elastic electron scattering from krypton

O. Zatsarinny,¹ K. Bartschat,¹ and M. Allan²

¹*Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA*

²*Department of Chemistry, University of Fribourg, CH-1700 Fribourg, Switzerland*

In a joint experimental and theoretical effort, we carried out a detailed study of elastic electron scattering from Kr atoms. Absolute angle-differential cross sections for elastic electron scattering were measured over the energy range 0.3–9.8 eV with an energy width of about 13 meV at scattering angles between 0° and 180°. Excellent agreement is obtained between our experimental data and predictions from a fully relativistic Dirac B -spline R -matrix (close-coupling) model that accounts for the atomic dipole polarizability through a specially designed pseudostate.

I. INTRODUCTION

Electron scattering from the noble gases is an important problem in the field of atomic collisions. Numerous experimental and theoretical studies have been performed over many decades, both for fundamental and practical reasons. The detailed study of the many near-threshold resonance features [1] has proven to be very challenging to both experiment and theory alike and is valuable in the sense that it represents a sensitive test of the quality of new theoretical models. A reliable knowledge of absolute elastic cross sections for rare gases is very important for applications in plasma and discharge physics.

In a recent paper [2], we reported the results of a joint experimental and theoretical study of electron scattering from Kr atoms in the vicinity of the low-lying $\text{Kr}^-(4p^55s^2)$ Feshbach resonances. Very satisfactory agreement between the experimental data and results from a fully relativistic Dirac-based B -spline R -matrix (DBSR) close-coupling calculation was obtained for the resonance features, particularly in elastic scattering. As one might have expected, it was very important to properly account for the dipole polarizability of the target, which was achieved by adding a specially designed pseudostate to the close-coupling expansion containing the lowest 31 physical target states of Kr as well.

The present work was motivated by the desire to test our theoretical model in more detail over extended energy and angular ranges. Experimentally, it has become possible to scan the entire angular region 0°–180°, with an energy resolution of better than 15 meV. For elastic scattering in particular, there are a number of previous experimental data and theoretical predictions available for comparison (see, for example, the recent paper by Linert *et al.* [3] and references therein). Consequently, this problem seemed to be an excellent testing ground to benchmark the reliability of our model.

This paper is organized as follows: In Sec. II we briefly describe the apparatus that was used to carry out the measurements. Section III then summarizes the numerical method employed in the calculation. In Sec. IV we present a comparison of our theoretical predictions with a number of experimental data from other groups as well as measurements carried out particularly for the present project. Both angular

scans at fixed energy and energy scans at a fixed scattering angle will be presented. We conclude with a brief summary.

II. EXPERIMENT

Electrons emitted from a hot filament were energy selected by a double-hemispherical monochromator and focused onto an effusive beam target, introduced by a 0.25-mm nozzle kept at about 30 °C. A double-hemispherical analyzer for detection of elastically or inelastically scattered electrons ensured background-free signals [4]. Absolute cross sections were determined by comparison against He using a relative-flow method [5]. A specially designed magnetic angle changer allowed for measurements up to a 180° scattering angle [6]. The angular acceptance was limited to $\pm 1.5^\circ$ at 10 eV, with an estimated uncertainty in the angular position of $\pm 2^\circ$. The angular acceptance increases with decreasing energy approximately as $E^{-1/2}$, down to an energy of about 1 eV, where it reaches about $\pm 5^\circ$. It remains approximately constant below that. Procedures for ensuring reliable cross sections were described in detail elsewhere [7,8]. The confidence limit (two standard deviations) for the absolute cross sections is generally about $\pm 15\%$, although it degrades to about $\pm 25\%$ at energies below 1 eV. The incident electron resolution was ≈ 13 meV at a beam current of ≈ 400 pA.

III. THEORY

In our recent calculation [2], we supplemented the lowest 31 physical states in the close-coupling expansion by a pseudostate that accounted for the otherwise missing portion of the dipole polarizability of the ground state due to coupling to higher-lying discrete Rydberg states as well as the ionization continuum. Since the present calculation was targeted specifically toward elastic scattering, we simplified the procedure dramatically in the current DBSR_pol model. The basic idea is the generalization of the nonrelativistic two-state (ground state plus one pseudostate) approach employed by Bell *et al.* [9] to a fully relativistic framework.

Consequently, the DBSR_pol model only included the $4s^24p^6$ ground state with total electronic angular momentum $J = 0$ and a single pseudostate $|\psi_p\rangle$ with $J = 1$ constructed from the configurations $4s^24p^5\bar{5}s$, $4s^24p^5\bar{4}d$, and $4s4p^6\bar{5}p$,

respectively. This pseudostate, and the corresponding pseudo-orbitals $5s$, $5p$, and $4d$, can be defined by the requirement that the static dipole polarizability of the atomic state $|\psi_0\rangle$ be expressed as

$$\alpha = 2 \frac{|\langle \psi_0 | D^{(1)} | \psi_p \rangle|^2}{E_p - E_0}, \quad (1)$$

where $D^{(1)}$ is the dipole operator and E_0 and E_p are the total energies of the ground state and the polarized pseudostate, respectively. As shown by Burke and Mitchell [10], $|\psi_p\rangle$ is a normalized solution of the equation

$$(H - E_0)|\psi_p\rangle = D^{(1)}|\psi_0\rangle, \quad (2)$$

with energy

$$E_p = \langle \psi_p | H_{\text{at}} | \psi_p \rangle, \quad (3)$$

where H_{at} is the target Hamiltonian.

As shown below, polarized pseudostates allow for very accurate descriptions of low-energy pseudo elastic scattering, based on first principles without using semiempirical polarization potentials. Our pseudostate yielded a dipole polarizability of $17.3 a_0^3$, where $a_0 = 0.529 \times 10^{-10}$ m is the Bohr radius. This is in very good agreement with the most recent recommended value of $17.075 a_0^3$ [11,12].

We then used the recently developed DBSR program [13] to solve the $(N+1)$ -electron collision problem. The essential idea is to expand the basis of continuum orbitals used to describe the projectile electron inside the R -matrix box, i.e., the region where the problem is most complicated due to the highly correlated motion of $N+1$ electrons, also in terms of a B -spline basis. A semiexponential grid for the B -spline knot sequence was set up to cover the inner region up to the R -matrix radius a . We used the same grid for the structure and the collision calculations. For $a = 50 a_0$, we employed 111 splines. A tight knot distribution near the origin was necessary to incorporate a finite-size nuclear model with a Fermi potential.

We calculated partial-wave contributions up to $J = 51/2$ numerically. This high limit on J guaranteed convergence of the results at all energies considered in this paper, thereby avoiding unphysical structures in the calculated angle-differential cross sections (DCS). The cross sections of interest were then obtained in the same way as in the standard R -matrix approach. We employed an updated version [14] of the flexible asymptotic R -matrix (FARM) package by Burke and Noble [15] to solve the problem in the asymptotic region and to obtain the transition matrix elements of interest. After transforming the latter from the present jj -coupling to the jlK -coupling scheme and also accounting for the appropriate phase convention of the reduced matrix elements, we employed the program MJK of Grum-Grzhimailo [16] to calculate the results shown below.

IV. RESULTS AND DISCUSSION

Figure 1 shows results for the differential cross section for elastic e -Kr scattering at incident electron energies of 5, 7.5, and 10 eV. Various experimental data sets [3,17–19] are compared to angular distributions from the DBSR_pol

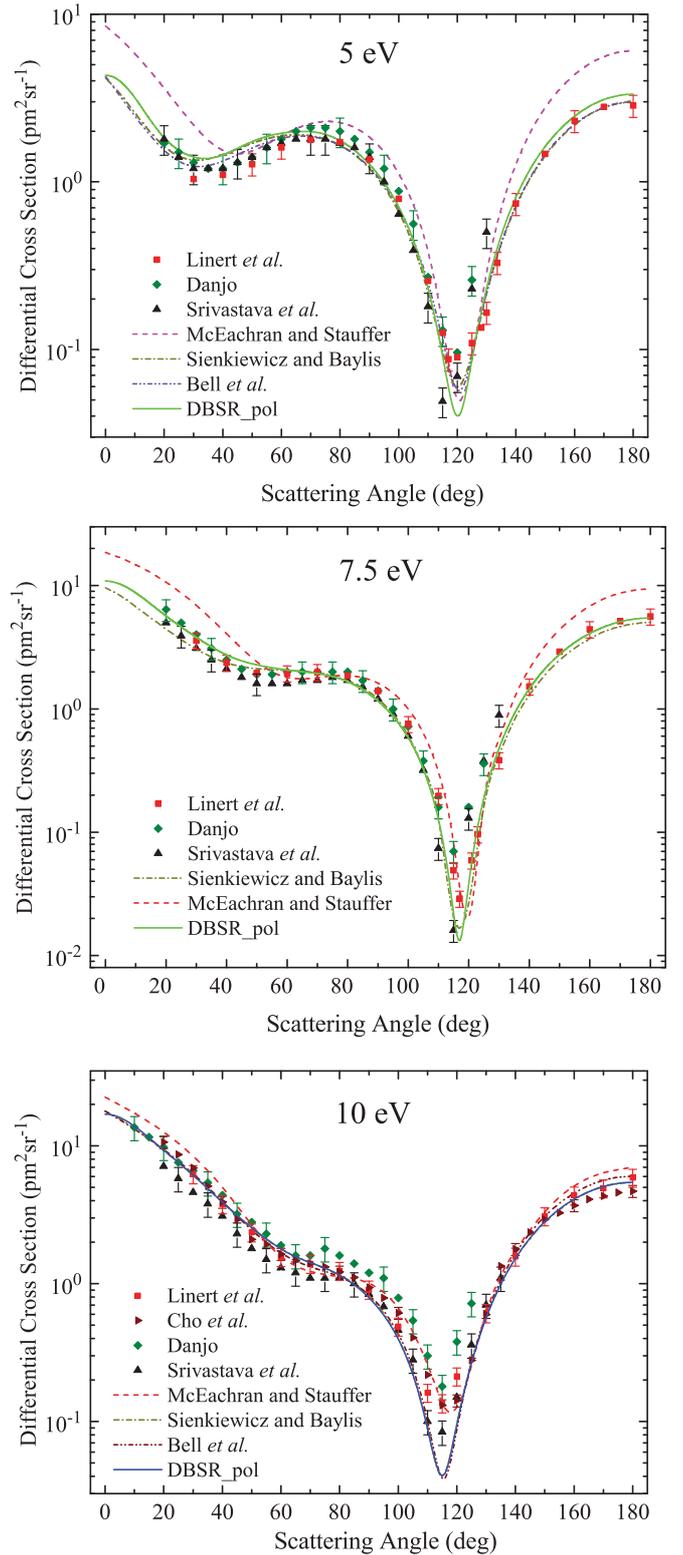


FIG. 1. (Color online) Differential cross section for elastic e -Kr scattering at electron energies of 5, 7.5, and 10 eV. The experimental data of Srivastava *et al.* [17], Danjo [18], Cho *et al.* [19] (10 eV only), and Linert *et al.* [3] are compared to angular distributions obtained with the DBSR_pol model and those from earlier calculations by Bell *et al.* [9] (5 and 10 eV only), Sienkiewicz and Baylis [20], and McEachran and Stauffer [21].

model and those from earlier calculations by Bell *et al.* [9], Sienkiewicz and Baylis [20], and McEachran and Stauffer [21]. These calculations (even more can be found in [3]) are representatives of a nonrelativistic model [9] with a single pseudostate to account for the atomic dipole polarizability (i.e., a nonrelativistic forerunner of the current DBSR_pol model) and fully relativistic calculations in which this dipole polarizability was accounted for by way of an optical potential [20] or in the polarized-orbital approach [21]. There is excellent agreement between the DBSR_pol predictions and experiment as well as the other theoretical results, except for the polarized-orbital predictions of McEachran and Stauffer [21], which seem to overestimate the DCS in the forward and backward directions. More recent calculations by McEachran [22] reduce the overestimate to some extent, but without remedying the problem completely

Figure 2 shows the experimental data generated in the current project and compared to the DBSR_pol predictions. The agreement is again very satisfactory, even though there seems to be a small shift in the position of the minima between the current measurements and the DBSR_pol results. The experiment has a weakness of a “blind spot” around 160° at low energies. Such blind spots are caused by the incident electron beam being deflected by the magnetic angle changer. It is then no longer collected in the “beam dump” but, instead, hits a nearby electrode and causes a large background. The problem

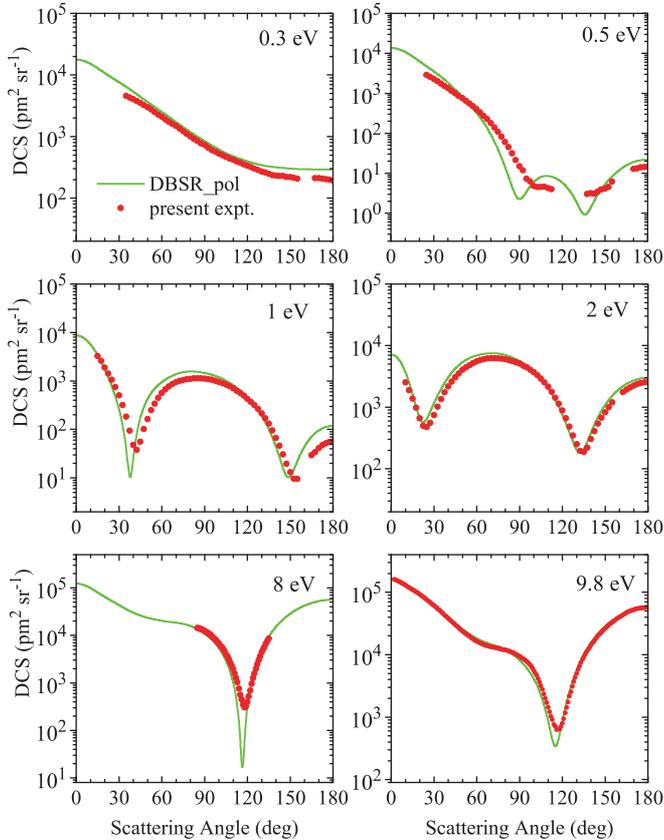


FIG. 2. (Color online) Differential cross section for elastic e -Kr scattering at electron energies between 0.3 and 9.8 eV as a function of the scattering angle.

is most severe at 0.5 eV in Fig. 2 because the cross section is extremely small there (only a few pm^2/sr). The measurement then becomes highly sensitive to even a very small background, and a second “blind spot” appears around 120° – 130° . A second weakness of the experiment is the increasing acceptance angle at low energies, which makes it difficult to separate elastically scattered electrons from unscattered electrons at low energies and near-forward angles. Small-angle data are thus missing at low energies.

The largest discrepancies appear at the very low energy of 0.5 eV, where the theory predicts two minima, like at 1 eV, but closer together. In particular, the lower minimum is predicted to shift dramatically, from about 40° at 1 eV to about 90° at 0.5 eV. The experiment suggests that the lower minimum shifts slightly more than predicted, to about 100° , so that the two minima are even closer together than predicted by theory and coalesce into a nearly flat section between 100°

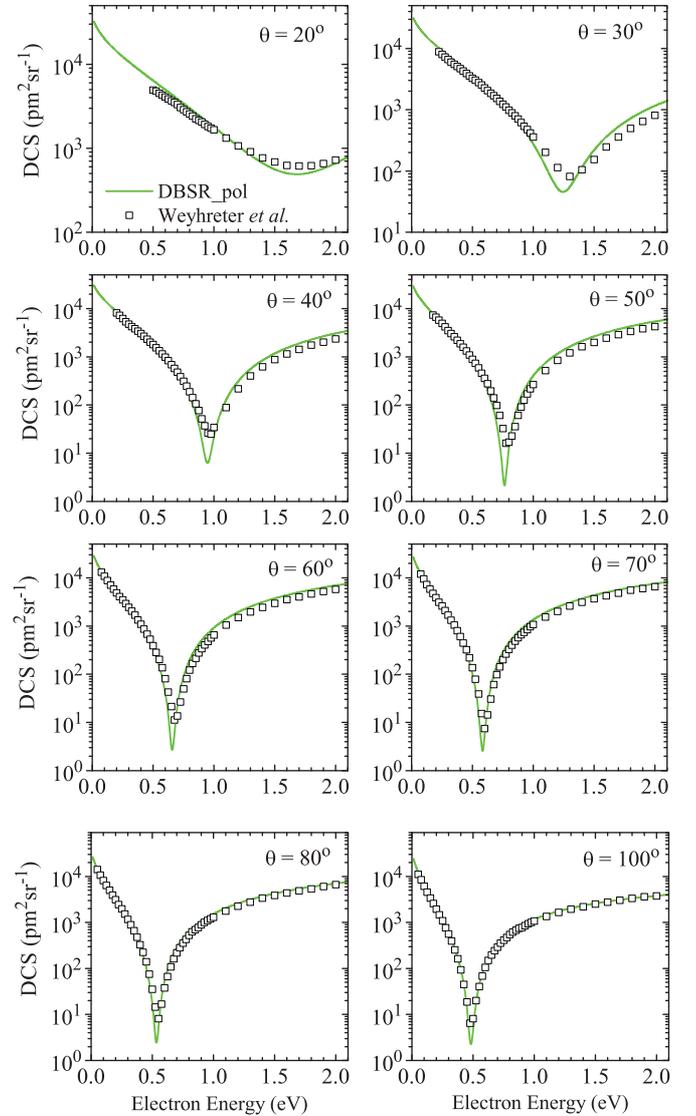


FIG. 3. (Color online) Differential cross section for elastic e -Kr scattering at angles between 20° and 100° as a function of the projectile energy. The experimental data of Weyhreter *et al.* [23] are compared with the present DBSR_pol predictions.

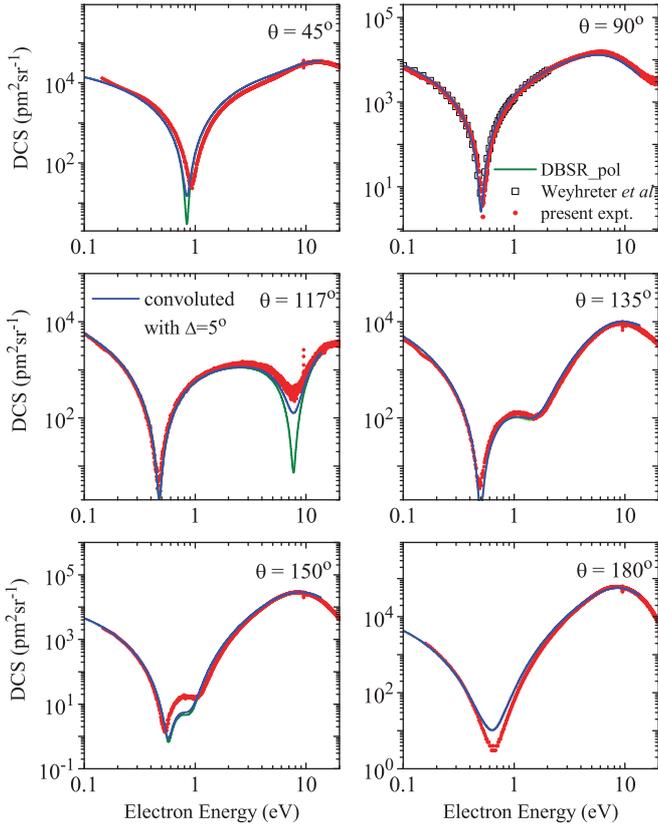


FIG. 4. (Color online) Differential cross section for elastic e -Kr scattering at angles between 45° and 180° as a function of the projectile energy. Our experimental data are compared with the present DBSR_pol predictions. For $\theta = 90^\circ$, we also show the experimental data of Weyhreter *et al.* [23]. The line with the shallower minima represents the calculation after convoluting the results with an angular resolution of 5° (FWHM). The structure just below 10 eV is due to the $(4p5^5s^2)^2P_{3/2}$ Feshbach resonance.

and 140° . The visibility of two distinct minima is decreased by the increased instrumental acceptance angle at small energies. In judging the data at 0.5 eV, it must also be kept in mind that it is, at scattering angles above about 60° , nearly exactly at the bottom of the Ramsauer-Townsend minimum (see Figs. 3 and 4), thereby bringing together the two complications of very small cross sections and a very strong sensitivity on the electron energy.

Finally, Figs. 3 and 4 display the energy-dependent differential cross sections for elastic electron scattering from Kr for a number of fixed angles as a function of energy. The characteristic feature in the energy-dependent DCS is related to the well-known Ramsauer-Townsend minimum, which is caused by the phase shift of the s -wave going through zero. In elastic electron scattering from Kr, it is found at 0.72 eV in the total cross section. In the DCS, however, interference effects with other partial waves cause a dependence of the position and the depth of this minimum on the scattering angle, as seen in Figs. 3 and 4. Furthermore, we see a second minimum in Fig. 4 for the scattering angles of 117° and above. That second minimum is at about 8 eV at 117° (see the 8 eV panel in Fig. 2

for the angular dependence at this point) and then shifts to lower energies with increasing angle, to reach 1 eV at 150° . At 180° the two minima appear to merge into one broader minimum at 0.6 eV. It is tempting to seek a simple explanation of the second minimum, similar to that for the Ramsauer-Townsend minimum but caused by the phase shift of the p -wave going through zero. Our analysis shows, however, that this minimum is not related to the phase shift of any particular partial wave crossing zero. As for the minima in the angle-differential DCSs for a fixed collision energy, they are caused by the interference of several partial waves with nonzero phase shifts.

The influence of the finite angular resolution on the measured depth of the minimum DCS is such that the apparent cross section in the very narrow minima is raised when the theoretical DCS, calculated by the DBSR_pol method, is convoluted with a Gaussian angular resolution profile with a full width at half maximum (FWHM) of 5° . This convolution substantially improves the agreement at 45° and 0.9 eV in Fig. 4, where the instrumental angular profile is expected to be about 5° . On the other hand, the observed differences in the apparent cross sections close to the minima at 8 eV and 117° and 0.7 eV and 180° are too large to be accounted for solely by angular resolution effects. The discrepancy between experiment and theory between 0.6 and 1 eV at 150° is, in part, explainable by the strong dependence of the cross section on the scattering angle, as seen from the 1 eV panel in Fig. 2.

V. CONCLUSIONS

We have presented results from a joint experimental and theoretical study of elastic electron scattering from Kr in the energy range 0.3 – 10 eV. The computational model, DBSR_pol, included only two states, namely, the ground state and a dipole-polarized pseudostate that yields a dipole polarizability of $17.3 a_0^3$. Based on the excellent agreement with a variety of measurements, this relatively simple, but still fully relativistic and *ab initio*, model appears to be sufficient for an accurate description of low-energy elastic scattering, reproducing most of both the energy and angle dependence of the DCS. In the near future, we will use this model for the other heavy noble gases Ne, Ar, and Xe. In particular, we plan to calculate angle-integrated elastic as well as momentum transfer cross sections. The latter are critical ingredients to simulate energy transport phenomena in plasmas.

ACKNOWLEDGMENTS

We thank H. Hotop for encouraging us to carry out this work and for many stimulating discussions and M. Zubek for making the data and graphic files of Ref. [3] available in electronic form. This work was supported by the United States National Science Foundation under Grants No. PHY-0757755, No. PHY-0903818, and the TeraGrid allocation TG-PHY090031, and by the Swiss National Science Foundation (Project No. 200020-131962).

- [1] S. J. Buckman and C. W. Clark, *Rev. Mod. Phys.* **66**, 539 (1994).
- [2] T. H. Hoffmann, M.-W. Ruf, H. Hotop, O. Zatsarinny, K. Bartschat, and M. Allan, *J. Phys. B* **43**, 085206 (2010).
- [3] I. Linert, B. Mielewska, G. C. King, and M. Zubek, *Phys. Rev. A* **81**, 012706 (2010).
- [4] M. Allan, *J. Phys. B* **25**, 1559 (1992).
- [5] J. C. Nickel, P. W. Zetner, G. Shen, and S. Trajmar, *J. Phys. E* **22**, 730 (1989).
- [6] M. Allan, *J. Phys. B* **33**, L215 (2000).
- [7] M. Allan, *J. Phys. B* **38**, 3655 (2005).
- [8] M. Allan, *J. Phys. B* **40**, 3531 (2007).
- [9] K. L. Bell, K. A. Berrington, and A. Hibbert, *J. Phys. B* **21**, 4205 (1988).
- [10] P. G. Burke and J. F. B. Mitchell, *J. Phys. B* **7**, 665 (1974).
- [11] U. Holm and K. Kerl, *Mol. Phys.* **69**, 803 (1990).
- [12] [<http://ctcp.massey.ac.nz/dipole-polarizabilities>].
- [13] O. Zatsarinny and K. Bartschat, *Phys. Rev. A* **77**, 062701 (2008).
- [14] C. J. Noble (private communication, 2008).
- [15] V. M. Burke and C. J. Noble, *Comput. Phys. Commun.* **85**, 471 (1995).
- [16] A. N. Grum-Grzhimailo, *Comput. Phys. Commun.* **152**, 101 (2003).
- [17] S. K. Srivastava, H. Tanaka, A. Chutjian, and S. Trajmar, *Phys. Rev. A* **23**, 2156 (1981).
- [18] A. Danjo, *J. Phys. B* **21**, 3759 (1988).
- [19] H. Cho, R. J. Gulley, and S. J. Buckman, *J. Korean Phys. Soc.* **42**, 71 (2003).
- [20] J. E. Sienkiewicz and W. E. Baylis, *J. Phys. B* **24**, 1739 (1991).
- [21] R. P. McEachran and A. D. Stauffer, *J. Phys. B* **36**, 3977 (2003).
- [22] R. P. McEachran (unpublished), as discussed in Ref. [3].
- [23] M. Weyhreter, B. Barzik, A. Mann, and F. Linder, *Z. Phys. D* **7**, 333 (1988).