01 Jan 2003

Perturbative and Nonperturbative Calculations of Electron-Hydrogen Ionization

Stephenie J. Jones

Don H. Madison
Missouri University of Science and Technology, madison@mst.edu

Mark D. Baertschy

Perturbative and nonperturbative calculations of electron-hydrogen ionization

S. Jones and D. H. Madison
Laboratory for Atomic, Molecular and Optical Research, Physics Department, University of Missouri–Rolla, Rolla, Missouri 65409-0640

M. Baertschy
Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado 80309-0440
(Received 3 August 2002; revised manuscript received 21 October 2002; published 10 January 2003)

We compare calculations of the fully differential cross section for ionization of atomic hydrogen by electron impact using two different theories—the perturbative CDW-EIS (continuum distorted wave with eikonal initial state) approximation and the nonperturbative ECS (exterior complex scaling) method. For this comparison, we chose an impact energy of 54.4 eV, since this is near the lowest energy that our perturbative approach would be applicable and near the highest energy that can be tackled by the ECS method with our present computational resources. For the case of equal-energy outgoing electrons investigated here, the two theories predict nearly identical results except that CDW-EIS underestimates the ECS values nearly uniformly by about 30%. Interestingly, when initial-state projectile-target interactions are neglected by replacing the eikonal initial state with the unperturbed initial state (the approximation of Brauner, Briggs, and Klar [J. Phys. B **22**, 2265 (1989)]), the cross section oscillates by $\pm 50\%$ about the ECS values.

DOI: 10.1103/PhysRevA.67.012703 PACS number(s): 34.80.Dp, 34.10.+x, 03.65.Nk

I. INTRODUCTION

Two of the most successful theories of electron-hydrogen ionization in recent years have been the nonperturbative ECS (exterior complex scaling) method of Baertschy, Rescigno, and McCurdy [1] for low impact energies and the perturbative CDW-EIS (continuum distorted wave with eikonal initial state) approximation of Jones and Madison [2–4] for intermediate energies. Although perturbation theory is appropriate for intermediate-to-high energies, nonperturbative methods are valid, in principle, at any energy. In practice, it is very difficult to obtain convergence for impact energies above 50 eV in the ECS method simply because of the large number of contributing partial waves. This is not a major problem, however, since 50 eV is just about where perturbative methods, in particular CDW-EIS, become applicable.

In this paper, numerically accurate ($\pm 2\%$), fully differential CDW-EIS cross sections for unpolarized 54.4-eV incident electrons are compared with ECS results converged to $\pm 10\%$. The fully differential cross section provides the most stringent test of theory since the momenta of all three collision fragments (scattered electron, ejected electron, and recoil ion) are fully determined. While it would also be helpful to compare CDW-EIS and ECS for less differential and integrated (total) ionization cross sections, such a comparison is not presently feasible, since each outcome of the collision process requires a separate six-dimensional numerical quadrature in our CDW-EIS calculations and a much larger ECS calculation would be needed to obtain convergence for highly asymmetric energy sharing. Atomic units (a.u.) are used throughout this work except where stated otherwise and we take the mass of the target nucleus to be infinite.

II. THEORY

We consider an incident electron with momentum $\mathbf{k}_0$ ionizing a target hydrogen atom. The fully differential cross section is given by [5]

$$\frac{d^5\sigma}{d\hat{\mathbf{k}}_1 d\hat{\mathbf{k}}_2 dE_2} = (2\pi)^4 \frac{k_1 k_2}{k_0} |T_{fi}|^2, \tag{1}$$

where $\mathbf{k}_1 = k_1 \hat{\mathbf{k}}_1$ and $\mathbf{k}_2 = k_2 \hat{\mathbf{k}}_2$ are the momenta of the two final-state electrons and $E_2 = k_2^2/2$. [In Eq. (1), we have assumed that continuum waves are normalized to a δ function in momentum space.] A general "two-potential" expression for the transition amplitude T_{fi} in Eq. (1) has been given by Gell-Mann and Goldberger [6],

$$T_{fi} = \langle \chi_f^- | (H-E)^\dagger | \chi_i^+ \rangle + \langle \chi_f^- | H - H^\dagger | \beta_i \rangle. \tag{2}$$

Here χ_f^- is a wave function for the final-state satisfying appropriate incoming-wave $(-)$ boundary conditions, χ_i^+ is a wave function for the initial-state satisfying proper outgoing-wave $(+)$ boundary conditions, and

$$\beta_i = (2\pi)^{-3/2} \exp(i\mathbf{k}_0 \cdot \mathbf{r}_1) \psi_i(\mathbf{r}_2) \tag{3}$$

is the initial asymptotic state, where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of the electrons relative to the target ion and ψ_i is the wave function of the target hydrogen atom. The Hamiltonian of the system is

$$H = -\frac{1}{2}\nabla_{\mathbf{r}_1}^2 - \frac{1}{2}\nabla_{\mathbf{r}_2}^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}}$$

and

$$E = \frac{1}{2}k_0^2 + \epsilon_i = \frac{1}{2}k_1^2 + \frac{1}{2}k_2^2$$

is the total energy, where $r_{12} = |\mathbf{r}_{12}|$, $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$, and ϵ_i is the binding energy of the atom. In Eq. (2), the adjoint of an operator O, $O^\dagger$, means that it operates to the left. The expression for T_{fi} (2) is exact if χ_i^+ and (or) χ_f^- is exact.

In the ECS method of Baertschy, Rescigno, and McCurdy [1], no approximations other than numerical are made to obtain χ_i^+, a product of two Coulomb waves is used for χ_f^-, and the second term on the right-hand side of Eq. (2) vanishes. In the CDW-EIS approximation of Jones and Madison [2–4], χ_i^+ is an eikonal approximation to the exact wave function, χ_f^- is the product of *three* Coulomb waves, and the second term on the right-hand side of Eq. (2) is comparable in magnitude to the first [4]. Electron exchange is fully included in both theories. In the ECS method, χ_i^+ is explicitly antisymmetrized. In the CDW-EIS approximation, an exchange amplitude is calculated by interchanging the momenta of the two final-state electrons. This is the first time that projectile exchange has been included in a CDW-EIS calculation. In previous applications of CDW-EIS, Jones and Madison [2–4] considered only asymmetric energies and (or) small projectile scattering angles where exchange was not important.

A. CDW-EIS approximation

The CDW-EIS approximation has been discussed in full detail by Jones and Madison [3]. Here we mention just the main points. For the initial-state wave function χ_i^+ in Eq. (2) we make the eikonal approximation [7–9]

$$\chi_i^+ = (2\pi)^{-3/2}\exp(i\mathbf{k}_0\cdot\mathbf{r}_1)\psi_i(\mathbf{r}_2) \times\exp\left[-\frac{i}{k_0}\ln\left(\frac{k_0 r_1-\mathbf{k}_0\cdot\mathbf{r}_1}{k_0 r_{12}-\mathbf{k}_0\cdot\mathbf{r}_{12}}\right)\right] \quad (4)$$

and for the final-state wave function χ_f^- we use the CDW (3C) wave function [9–13]

$$\chi_f^- = (2\pi)^{-3}\exp(i\mathbf{k}_1\cdot\mathbf{r}_1+i\mathbf{k}_2\cdot\mathbf{r}_2)C^-(-1/k_2,\mathbf{k}_2,\mathbf{r}_2) \times C^-(-1/k_1,\mathbf{k}_1,\mathbf{r}_1)C^-(\mu/k_{12},\mathbf{k}_{12},\mathbf{r}_{12}). \quad (5)$$

Here $\mathbf{k}_{12}=\mu(\mathbf{k}_1-\mathbf{k}_2)$, where $\mu=1/2$ is the reduced mass of two electrons. Distortion effects of the Coulomb potential are contained in the function

$$C^-(\eta,\mathbf{k},\mathbf{r}) = N(\eta)\,{}_1F_1(i\eta,1;-ikr-i\mathbf{k}\cdot\mathbf{r}).$$

Here ${}_1F_1$ is the confluent hypergeometric function and $N(\eta)=\Gamma(1-i\eta)\exp(-\pi\eta/2)$, where Γ is the γ function. The transition amplitude (2) is evaluated using six-dimensional numerical quadrature [14].

B. ECS method

In the ECS method the radial functions in an angular momentum expansion of χ_i^+ are calculated on a numerical grid using complex scaling outside of some distance to simplify the scattering boundary conditions [15]. For the present calculations we include components for total angular momentum up to $L=12$ and the wave function is calculated out to a distance of 80 a_0. The ionization amplitude is obtained by calculating *T*-matrix elements, as in the first term of Eq. (2), using products of two Coulomb waves [1]. We estimate the accuracy of the calculated cross section for equal-energy outgoing electrons to be between 5% and 10% depending on the geometry. To converge the cross section for asymmetric energies we will need to include additional angular momentum components. Based on our studies of the energy differential cross section [1] we believe that converging the cross section for highly asymmetric energy sharing will require angular momentum components up to $L=40$.

III. RESULTS AND DISCUSSION

We investigate the fully differential cross section for ionization of atomic hydrogen by the impact of 54.4-eV electrons. We confine our attention to the case where both outgoing electrons are emitted in a plane containing $\mathbf{k}_0$ (the scattering plane), with scattering angles θ_1 and θ_2 relative to $\mathbf{k}_0$. For impact energies of 54.4 eV and higher, interest has focused on the case where the projectile transfers only a small amount of energy and momentum to the target, since this is the dominant mode of ionization for intermediate and higher energies.

Here we are interested in the smaller cross sections that result when the two final-state electrons have the same energy (unfortunately, no measurements are available for comparison with theory in this case). Such cross sections provide important information on the collision dynamics and provide a severe test of theoretical models. In fact, different angular arrangements for the two outgoing electrons tend to isolate different dynamical effects [16].

A. Constant θ_{12} geometry

The constant θ_{12} geometry, where the angle θ_{12} between the two electrons is held fixed while θ_1 and θ_2 are rotated simultaneously, is not as sensitive as other geometries to the final-state electron-electron interaction, which allows other higher-order effects to be clearly seen [16]. In this geometry, the physical cross section for unpolarized incident electrons is symmetric about $\theta_1=\theta_{12}/2$ (no matter how high the collision energy is, electron exchange must be included to preserve this symmetry). To exploit this symmetry, we plot the cross section from $\theta_1=\theta_{12}/2-\pi$ to $\theta_1=\theta_{12}/2+\pi$.

Our results for $\theta_{12}=90°$, 120°, and 180° are shown in Fig. 1. To facilitate comparison of the theories, we scaled CDW-EIS to ECS. The scale factor, given in the figure, is just the ratio of CDW-EIS to ECS at the angle where the largest ECS cross section occurs. For the three different values of θ_{12}, the three scaling factors for CDW-EIS can be written as $0.71\pm0.06(\pm8\%)$, since they range from 0.65 to 0.77, with a median value of 0.71. Although the overall magnitude of CDW-EIS is 29% smaller than ECS, the $\pm8\%$ range for the internormalization of different θ_{12} data sets is consistent with the $\pm10\%$ numerical uncertainty of the ECS results.

Results of the 3C approximation (scaled to ECS) are also shown. The 3C approximation uses the CDW (3C) wave function (5) for the final state, but approximates the initial-state wave function χ_i^+ by the unperturbed state β_i (3). Since CDW-EIS contains projectile-target correlation in the initial-state wave function, while 3C does not, comparison of

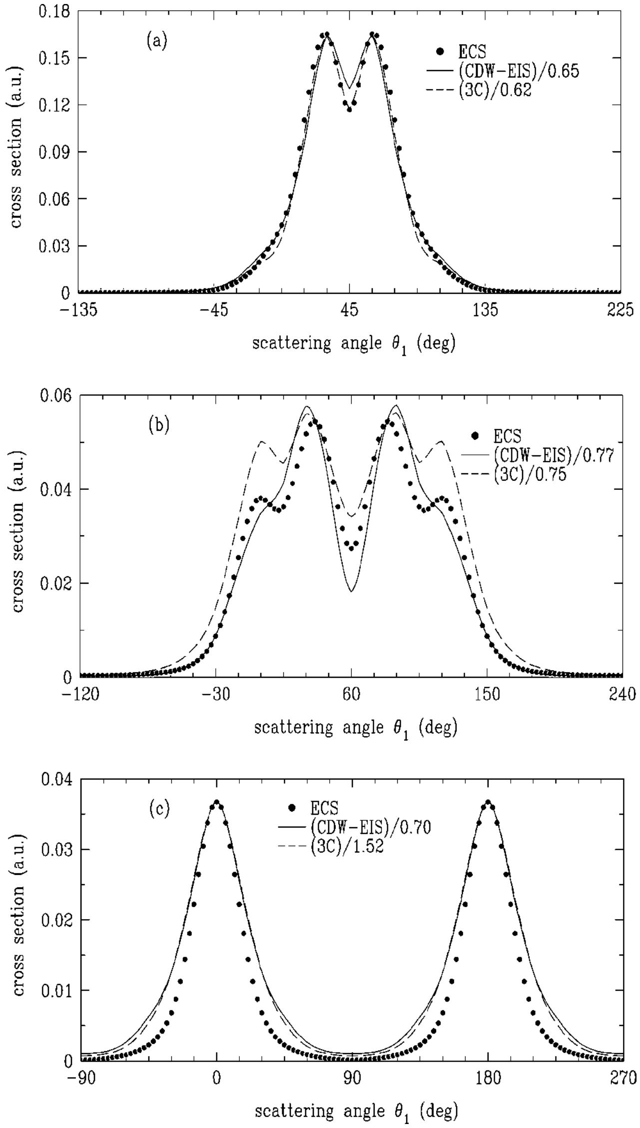

FIG. 1. Scattering-plane fully differential cross section for 54.4-eV electron-impact ionization of atomic hydrogen, H$(1s)$. The two final-state electrons have the same energy (20.4 eV) and their scattering angles θ_1 and θ_2 are measured in the same sense relative to the incident electron direction. Here the angle $\theta_{12}=\theta_1-\theta_2$ is fixed at (a) 90°, (b) 120°, or (c) 180°.

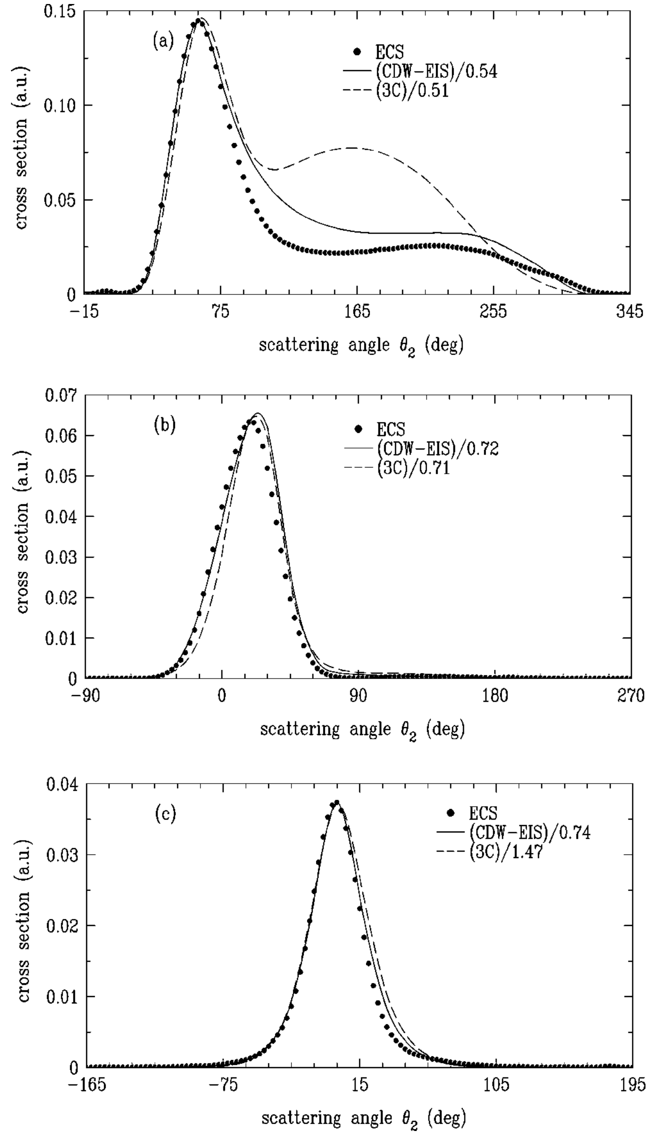

FIG. 2. Same as Fig. 1 except that here the angle θ_1 is fixed at (a) $-15°$, (b) $-90°$, or (c) $-165°$.

CDW-EIS with 3C elucidates the role of initial-state correlation. The most interesting observation concerning Fig. 1 is that the scaling factors for 3C vary greatly—from 0.62 for $\theta_{12}=90°$ to 1.52 for $\theta_{12}=180°$. That is, 3C is 38% *smaller* than ECS for $\theta_{12}=90°$, but 52% *larger* than ECS for $\theta_{12}=180°$. Obviously, the internormalization of different θ_{12} data sets in the 3C approximation is *not* consistent with the ECS results.

B. Fixed θ_1 geometry

Another common geometrical arrangement for the two outgoing electrons, considered in Fig. 2, is to fix θ_1 and rotate θ_2. It is seen from Fig. 2 that CDW-EIS and ECS predict similar results for this geometry (except for the overall scale, as already noted). On the other hand, the 3C theory predicts a much larger secondary structure than ECS for $\theta_1=-15°$. Note also that the scale factors for 3C vary greatly once again. Both of these problems are corrected in large part by including projectile-target interactions in the initial state.

In this geometry, calculations omitting exchange (not shown) reveal that the role of electron exchange varies greatly for different fixed values of θ_1. For $\theta_1=-15°$, exchange effects are relatively weak (less than 20%). Thus the cross section in Fig. 2(a) corresponds primarily to the ejection of the atomic electron at the angle θ_2 and the projectile scattering to $\theta_1=-15°$. In contrast, for $\theta_1=-165°$, the *exchange* amplitude dominates—the peak in the cross section for $\theta_2\approx 0°$ [see Fig. 2(c)] can be ascribed primarily to the

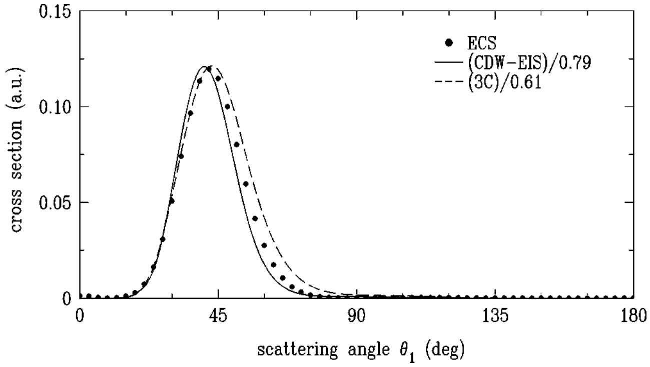

FIG. 3. Same as Fig. 1 except that here $\theta_1 = -\theta_2$.

projectile scattering in the forward direction and the atomic electron being ejected at $\theta_1 = -165°$.

C. Coplanar symmetric geometry

In Fig. 3, we compare ECS, CDW-EIS, and 3C results in coplanar symmetric geometry. In this geometry, the two equal-energy final-state electrons have equal and opposite scattering angles relative to $\mathbf{k}_0$ (as a result, the direct and exchange amplitudes are identical). In contrast to the constant θ_{12} geometry, the coplanar symmetric geometry is very sensitive to the final-state interaction between the two electrons. Good agreement is found between all three theories for the shape of the cross section, but CDW-EIS is about 20% smaller than ECS and 3C is nearly 40% smaller than ECS. Including correlation in the initial state thus removes about half of the overall difference between 3C and ECS.

D. Discussion

It should come as no surprise that CDW-EIS underestimates the true cross section, which we assume to be given by ECS to 10%. The catastrophic failure of the 3C approximation as the ionization threshold is approached is well documented and applies equally well to CDW-EIS. Multiplying the unperturbed initial-state wave function by an eikonal phase factor [Eq. (4)] cannot possibly compensate for the exponentially decaying electron-electron normalization factor in the CDW (3C) wave function (5).

Nevertheless, it is naive to assume that the normalization of the 3C wave function is the *cause* of the problem, since it has been shown that the 3C wave function is properly normalized [17]. We believe that the failure of the 3C approximation for vanishing total energy results from the very nature of the approximation—each two-body subsystem evolves independently of the others with fixed final asymptotic relative momentum. The exact scattering wave function developed from the final state of three continuum charged particles would allow for energy and momentum exchange between these subsystems. For example, all three particles might remain in the continuum, but their relative momenta could change. In addition, either electron could combine with the H^+ ion to form a bound state. We believe that it is the neglect of these open channels, and not the normalization, that leads to the failure of the 3C approximation close to threshold.

To compensate for the neglect of these channels in the final-state wave function, a theory would have to include all excitation and ionization channels in the initial-state wave function. It is clear, however, that the eikonal approximation (or any other perturbative approximation) fails to do this. For low collision energies, especially close to threshold, a nonperturbative method such as ECS must be used to obtain systematically converged results, since summing a perturbation series to all contributing orders is generally not practical for low energies.

Finally, we note that the difference between the exact and 3C wave functions, which represents coupling to an infinite number of channels, *is* included to first order in perturbation theory in the CDW-EIS approximation through the $(H-E)^\dagger$ term in Eq. (2). [In the 3C approximation, this effect is not included even to first order, since the $(H-E)^\dagger$ term is canceled exactly by a piece of the second term in Eq. (2).] For collision energies close to threshold, however, this coupling is much too large to be treated as a perturbation and this is why the CDW-EIS approximation is applicable only to relatively fast ionizing collisions.

IV. CONCLUSION

Significant progress in the theoretical treatment of electron-impact ionization of hydrogen atoms has been made since the definitive paper by Brauner, Briggs, and Klar [13]. Exterior complex scaling [1] and convergent close coupling [18] methods now effectively solve this three-body problem down to impact energies a few eV above threshold, at least for equal-energy outgoing electrons where absolute measurements are available for low impact energies and where theory and experiment are in spectacular agreement. On the other hand, the perturbative 3C [13] and CDW-EIS [2] approximations have led to keen insights into three-body dynamics at intermediate energies.

Here we compared perturbative CDW-EIS and nonperturbative ECS calculations for ionization of atomic hydrogen by 54.4-eV electrons. We considered the fully differential cross section for the case where both outgoing electrons have the same energy. We found that the two very different theories predict similar results, but differ in overall magnitude by about 30%. On the other hand, comparison of 3C with ECS exposed a serious relative normalization problem of the 3C theory. This problem is corrected by CDW-EIS; that is, by also including projectile-target interactions in the initial state. We hope that the present work stimulates experimental and further theoretical investigations of the collision geometries considered here.

ACKNOWLEDGMENTS

This work was supported by the NSF under Grant No. PHY-0070872 and by the U.S. Department of Energy, Office of Science.

[1] M. Baertschy, T.N. Rescigno, and C.W. McCurdy, Phys. Rev. A **64**, 022709 (2001).
[2] S. Jones and D.H. Madison, Phys. Rev. Lett. **81**, 2886 (1998).
[3] S. Jones and D.H. Madison, Phys. Rev. A **62**, 042701 (2000).
[4] S. Jones and D.H. Madison, Phys. Rev. A **65**, 052727 (2002).
[5] H.A. Bethe, Ann. Phys. (Leipzig) **5**, 325 (1930).
[6] M. Gell-Mann and M.L. Goldberger, Phys. Rev. **91**, 398 (1953).
[7] R.J. Glauber, in *Lectures in Theoretical Physics*, edited by W.E. Brittin and L.G. Dunham (Interscience, New York, 1959), Vol. 1, p. 315.
[8] J.H. McGuire, Phys. Rev. A **26**, 143 (1982), and references therein.
[9] D.S.F. Crothers and J.F. McCann, J. Phys. B **16**, 3229 (1983).
[10] L. Rosenberg, Phys. Rev. D **8**, 1833 (1973).
[11] Dž Belkić, J. Phys. B **11**, 3529 (1978).
[12] C.R. Garibotti and J.E. Miraglia, Phys. Rev. A **21**, 572 (1980).
[13] M. Brauner, J.S. Briggs, and H. Klar, J. Phys. B **22**, 2265 (1989).
[14] S. Jones, D.H. Madison, and D.A. Konovalov, Phys. Rev. A **55**, 444 (1997).
[15] M. Baertschy, T.N. Rescigno, W.A. Isaacs, X. Li, and C.W. McCurdy, Phys. Rev. A **63**, 022712 (2001).
[16] T. Rösel, J. Röder, L. Frost, K. Jung, H. Ehrhardt, S. Jones, and D.H. Madison, Phys. Rev. A **46**, 2539 (1992).
[17] M. Brauner, J.S. Briggs, H. Klar, J.T. Broad, T. Rösel, K. Jung, and H. Ehrhardt, J. Phys. B **24**, 657 (1991).
[18] I. Bray (private communication).