Electron detachment of H^- in collision with Ne^{4+} and Ar^{4+} ions

J. T. Lin
Department of Electrophysics, National Chiao-Tung University, Hsin-Chu, Taiwan 30050

T. F. Jiang
Institute of Physics, National Chiao-Tung University, Hsin-Chu, Taiwan 30050

J. Y. Kuang and C. D. Lin
Department of Physics, Kansas State University, Manhattan, Kansas 66506

(Received 17 April 1997)

Total-electron detachment cross sections for H^- colliding with multiply charged Ne^{4+} and Ar^{4+} ions are calculated using the two-center atomic-orbital close-coupling expansion method in the center-of-mass energy range of 4–200 keV. The calculation shows that there is no core effect, and that electron capture only plays a minor role for energies above 20 keV. At 50 keV, where electron capture is not important, the single-center atomic-orbital expansion method was used to calculate the detachment cross sections for incident charges $q=1-8$. The present calculations are shown to be in good agreement with experimental data. [S1050-2947(97)09909-5]

PACS number(s): 34.50.Dy, 34.50.Fa, 34.10.+x, 34.70.+e

I. INTRODUCTION

The neutralization of H^- ions with multiply charged ions was reported by Melchert *et al.* [1] for Ne^{q+} $(q\leqslant 4)$ and $Xe^{q+}(q\leqslant 8)$ ions at center-of-mass energies from 4 to 200 keV. These experiments were carried out in conjunction with possible applications in magnetic-fusion-related neutral beam injection. Furthermore, the dependence of electron detachment and/or electron capture of the loosely bound electron of the H^- ion by the strong long-range Coulomb force is of intrinsic interest. Experimentally, only neutral hydrogen atoms were detected so far; thus the relative importance of electron detachment vs electron-capture processes has not been determined.

There have been a few theoretical calculations carried out for the above collision systems. The calculation presented in Melchert *et al.* treated a detachment process analogous to the Keldysh theory of multiphoton ionization. Since the detachment occurs at large internuclear separations, the electric field exerted by the multiply charged ions can be approximated by an electric dipole, thus the detachment of the active electron in H^- is similar to the multiphoton detachment process. Since the unbound state in this case has an analytical solution called the Volkov state, the calculation of detachment using this model is quite attractive. Calculations based on this simple model did predict cross sections in good agreement with experiments; see Melchert *et al.* [1].

Another calculation for the detachment cross section was carried out by Cherkani *et al.* [2]. This group used a method very similar to the single-center atomic-orbital expansion method to solve the time-dependent electronic wave function of the active electron in H^-. However, they did not use actual eigenstates of the target for the continuum electron. Instead, for each partial wave, only one basis function is used and rotational coupling has been neglected. Again they were able to obtain results in reasonable agreement with experimental data at higher energies but the deviation at lower energies is not small.

In this paper we used the two-center atomic-orbital expansion method to calculate the electron detachment and electron-capture cross sections for collisions between H^- and multiply charged ions. Our goal is not only to obtain cross sections which can be compared to the measurements of Melchert *et al.* [1] , but also to examine the validity of the approximations used in the two calculations mentioned above. In particular, we want to examine at what energies the electron capture processes can be neglected, and if the detachment cross sections are indeed independent of the ionic species used, i.e., only the charge of the ions used is important. Both approximations were used implicitly in the aforementioned calculations. In Sec. II we briefly state the theoretical model and the parameters used. The results and comparison with experiment and other calculations are addressed in Sec. III.

II. THEORETICAL MODEL

We used the standard close-coupling method to expand the time-dependent electronic wave function in terms of atomic orbitals of the two collision centers. The method was fully described in the literature [3,4]. The collision system is further approximated as a one-electron problem, where the H^- ion is treated as an one-electron ''atom'' in a model potential. Similarly each of the projectile ions Ne^{4+} or Ar^{4+} is also described by a model potential such that the energy levels of the first few subshells of the Ne^{3+} and Ar^{3+} ions are close to the experimental values.

For H^-, the model potential is taken to be the Yukawa potential $V(r)=-\exp(-Z_3 r)/r$ with $Z_3=0.8817$. This potential gives a bound state at -0.02755 a.u. which is very close to the experimental binding energy of H^- at -0.02756 a.u. This potential was used in other previous studies involving H^- as the target [5,6]. For the multiply charged ions the

TABLE I. Model potential representation of bound and pseudostates of H^-. The model potential is taken to be of the form $V(r)=-(1/r)\exp(-0.8817r)$. The eigenstates are obtained by using even-tempered basic functions $r^{\ell}\exp(-\xi\gamma)$, where $\xi=\alpha\beta^{\kappa}$ ($\kappa=1,2,\ldots$). The parameters α and β and the resulting eigenvalues (in a.u.) are given.

	$\ell=0$	$\ell=1$	$\ell=2$	$\ell=3$	$\ell=4$	$\ell=5$
α	0.110	0.150	0.200	0.295	0.100	0.100
β	2.080	1.910	1.666	1.100	1.420	1.600
E_n	−0.027 55	0.024 12	0.035 39	0.020 62	0.005 98	0.009 65
	0.024 23	0.123 76	0.151 71	0.058 69	0.017 08	0.029 99
	0.228 44	0.521 16	0.619 20	0.147 75	0.042 75	0.083 88
	1.645 38			0.413 56	0.106 98	0.234 51
					0.304 03	0.724 67

potentials were fitted to the form

$$V(r)=\frac{-Z_0}{r}+\frac{(Z_1+Z_2r)\exp(-Z_3r)}{r}, \tag{1}$$

where the parameters for Ne^{3+} and Ar^{3+} ions are given in Table II. We used the recently developed close-coupling code, where each atomic orbital is expanded in terms of even-tempered basis functions [7]

$$\chi_{klm}(\mathbf{r})=N_l(\zeta_k)e^{-\zeta_k r}\mathcal{Y}_{lm}(\mathbf{r}), \quad \mathcal{Y}_{lm}(\mathbf{r})=r^l Y_{lm}(\hat{\mathbf{r}}), \tag{2}$$

where $N_l(\zeta_k)$ is a normalization constant, and the orbital exponents ζ_k are taken to form a geometric sequence

$$\zeta_k=\alpha\beta^k, \quad k=1,2,\ldots,N. \tag{3}$$

The parameters α and β used for each partial wave are listed in Table I for H^-, where the calculated eigenenergies are also tabulated. Since H^- has only one bound state, the remaining states which have positive energies are pseudostates representing approximately the continuum states of the electron-hydrogen collision system. The probabilities for populating these pseudostates are interpreted as electron detachment probabilities.

TABLE II. Binding energies of Ne^{3+} and Ar^{3+} ions calculated in the model potential $V(r)=-(Z_0/r)+(Z_1+Z_2r)(1/r)\exp(-Z_3r)$ using even-tempered basic functions (with parameters α and β). The calculated and experimental binding energies [8] are given in a.u.

	Ne^{3+}				Ar^{3+}		
Z_0	4.0				4.0		
Z_1	−6.0				−14.0		
Z_2	−0.5				−0.7153		
Z_3	2.97				2.73		
$n\ell$	E_{theory}	E_{exp}	(α/β)	$n\ell$	E_{theory}	E_{exp}	(α/β)
3s	−1.3652	−1.3700	0.080	4s	−1.0246	−1.0246	0.080
4s	−0.6727	−0.6716	1.700	5s	−0.5219		1.881
5s	−0.3922	−0.4079		6s	−0.2991		
6s	−0.2510	−0.1334		7s	−0.1841		
2p	−3.5717	−3.5716	0.090	3p	−2.1972	−2.1972	0.094
3p	−1.1812	−1.1823	1.917	4p	−0.8843	−0.8798	1.800
4p	−0.6085	−0.6188		5p	−0.4913		
5p	−0.3529			6p	−0.3015		
6p	−0.1911			7p	−0.1735		
3d	−0.9164	−0.9131	0.200	3d	−1.0898	−1.1050	0.500
4d	−0.4508	−0.4255	2.754	4d	−0.5852		1.260
5d	−0.1972	−0.1971		5d	−0.3620		
4f	−0.4993		0.183	4f	−0.4996		0.277
5f	−0.3146		1.711	5f	−0.3200		1.299

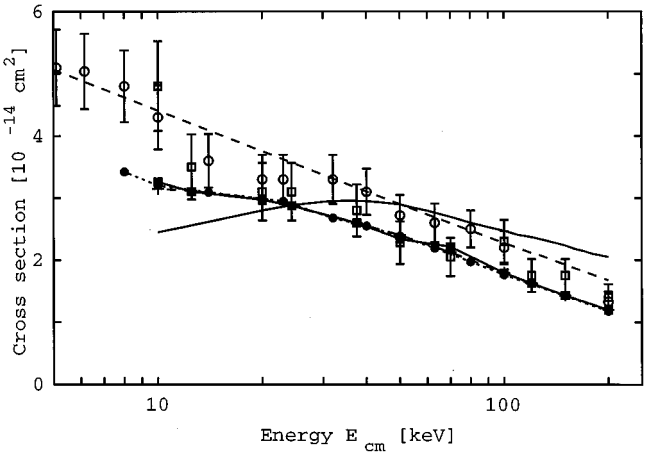

FIG. 1. Total electron-loss cross sections for $X^{4+}+H^-$ as a function of the center-of-mass energy. Experimental results: $X=$Ne, open squares; $X=$Ar, open circles. Theoretical calculations: present results are given by symbols connected by lines, with solid squares for Ne and solid circles for Ar, and the dotted lines on top of the solid line is for X, a bare ion with $q=4$. The dashed lines are from the Keldysh-Volkov theory of Melchert *et al.* [1], and the thin line is from Cherkani *et al.* [2].

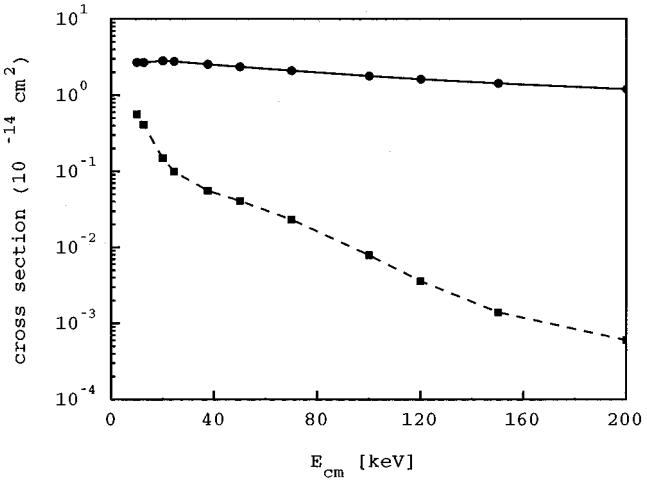

FIG. 2. True electron detachment cross sections and electron-capture cross sections for $X^{4+}+H^-$ collisions as a function of the center-of-mass energy. Solid circles: true detachment cross sections and solid squares: capture cross sections.

In Table II we also show the parameters α and β used for each partial wave for Ne^{3+} and Ar^{3+} ions, and the resulting calculated binding energies for the first few excited states. The binding energies are compared to the experimental values [8] to show the accuracy of the model potential used.

After the model potentials and the basis functions are decided, we then carry out the two-center close-coupling expansion to solve for electron capture and electron detachment probabilities for each impact parameter assuming straight-line trajectories. The probabilities are then integrated over impact parameters to obtain total electron-capture and detachment cross sections. Since the experiment of Melchert *et al.* only measured the total yield of neutral H atoms after the collision, the true detachment and the electron-capture cross sections are added together in order to compare with experimental total electron-loss cross sections.

III. RESULTS AND DISCUSSION

In Fig. 1 we show the comparison between the calculated and the experimental electron-loss cross sections for Ne^{4+} on H^- and Ar^{4+} on H^- collisions in the center-of-mass energy range of 4–200 keV. The experimental results for the two systems show small differences, but the results from the present calculation give essentially identical cross sections, indicating that there is no core effect. We also performed calculations assuming that the projectile is a bare ion with charge $q=4$ (shown as dotted lines on top of the solid line in Fig. 1), and obtained identical total electron-loss cross sections. Thus there is no evidence that the total electron-loss cross section depends on the core of the ion. Since the cross section is dominated by contributions from large impact parameters, the lack of dependence on the core is not surprising.

We also show results from the calculation presented in Melchert *et al.* [1] and the results of Cherkani *et al.* [2] in Fig. 1. The energy dependence from the calculation of Cherkani *et al.* [2] is different from the experimental data. The theoretical results of Melchert *et al.* [1] are in good agreement with their Ar^{4+} data, but ours are in better agreement with their Ne^{4+} data. As explained above, we do expect the experimental results for the two collision systems to be essentially identical. Thus the scattering between the experimental data for the two systems is a measure of the accuracy of the data. It should be pointed out that the Keldysh-Volkov theory used in the paper of Melchert *et al.* treats the electron-projectile interaction only to the dipole term, while the present method includes this interaction to all order.

In Fig. 2 we compare the relative magnitude of the true detachment cross section with the electron-capture cross section. Since the core plays no role, we show only results from calculations for collisions between a bare ion with charge $q=4$ with H^-. We note that in the covered energy region, electron capture plays a very minor role (less than 1%) until the collision energy is below 20 keV in the center-of-mass frame. Since electron capture plays only a minor role at higher energies, we can study electron detachment cross sections of H^- by various ions using the single-centered atomic-orbital expansion method. In Fig. 3 we show the electron detachment cross sections by bare ions with charge $q=1-8$ in the center-of-mass energy of 50 keV. The calculated results are compared to the measurement of Melchert *et al.* The agreement with experiment is very satisfactory except for $q=1$. For $q=1$ where the experiment was carried out using Ne^+ ions we found that the experimental data are reproduced if the Ne^+ ion is described by a model potential in a one-center atomic-orbital calculation. For incident ions with higher q, the effect of the core is not visible.

To understand the origin of the q dependence shown in Fig. 3 we examine the impact parameter dependence of the detachment probabilities for $q=1$, 4, and 8 at a center-of-mass energy of 50 keV. In Fig. 4(a) we note that the detachment probabilities are near unity at small impact parameters, and drop to zero with a long ''tail'' at large impact parameters. This is characteristic of collisions with negative ions,

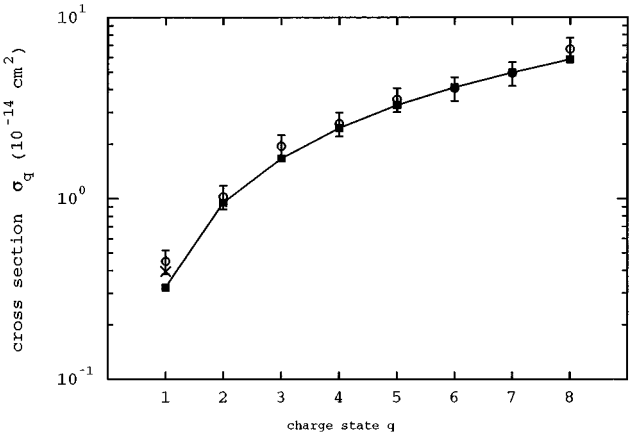

FIG. 3. Cross sections σ_q for detachment of H^-, by bare ions with charge $q=1-8$ at a center-of-mass energy of 50 keV. The calculated results are given in solid squares connected by a line to guide the eye. The experimental data are from Melchert *et al.* [1]. For $q=1$ the discrepancy is removed if the calculation is performed using Ne^+ ions (shown by a cross), which were used by the experimentalists. The core effect becomes negligible for higher charges.

where the electron can be detached even at very large distances. From Fig. 4(a) we see that the increase of detachment cross sections with q is mainly due to the increase in the range of impact parameters where detachment can occur.

We next examine the nature of the continuum electron distribution in the detachment of H^- by multiply charged ions at 50 keV in the center-of-mass energy. In particular, we are interested in the angular momentum distribution of the continuum electrons with respect to the target center. If the detachment is a perturbative process, then the dipole term of the projectile-electron interaction will populate mostly the $l=1$ continuum electrons. For multiply charged incident ions where the detachment occurs at very large distances, we may expect large contributions from high angular momentum continuum electrons. In Fig. 4(b) we present the normalized l distribution of the continuum electrons for incident ions with charge $q=1-8$ at 50 keV. Clearly for $q=1$ the $l=1$ component is indeed dominant, with some contributions from $l=0$ and 2. For $q=4$ even $l=4$ already contribute to about 10%. For even higher $q=8$, while $l=1$ is still the highest component, contributions from other higher partial waves become comparable. In fact, we are not sure that the l distribution for the higher q presented here is correct. For the total detachment cross section, on the other hand, we do expect that the calculation is adequate.

IV. CONCLUSIONS

In this paper we showed that electron detachment of negative ions by multiply charged ions can be easily calculated

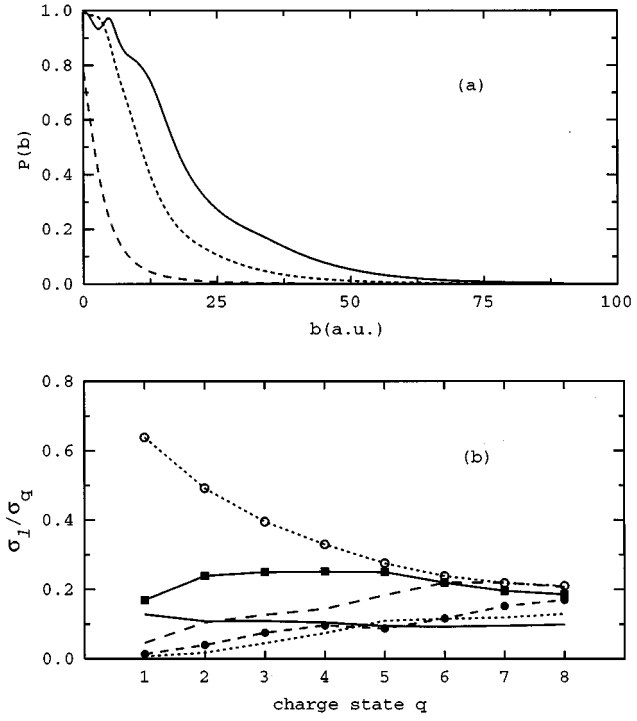

FIG. 4. (a) The detachment probabilities $P(b)$ vs impact parameters b for incident ions with $q=1$ (dashed lines), $q=4$ (dotted lines), and $q=8$ (solid line). The collision energy is at 50 keV. (b) The normalized l-distribution cross sections σ_l/σ_q of the detached electron vs q of the incident ion. The symbols: $l=0$, (solid line), 1 (open circles), 2 (solid squares), 3 (dashed lines), 4 (solid circles), and 5 (dotted lines). The target is the H^- ion.

using the two-center atomic-orbital expansion method. The inclusion of basis functions with high angular momentum is important for such collisions but they can be easily performed with present-day workstations or Pentium-based PC's. We showed that the electron-loss cross sections measured by Melchert *et al.* [1] for Ne^{4+} and Ar^{4+} on H^- are in agreement with the present calculation. We also examined the validity of the Keldysh-Volkov theory for such collisions. We conclude that the total-electron detachment cross sections can be obtained accurately using the existing two-center close-coupling method which has been widely applied to ion-atom collisions.

ACKNOWLEDGMENTS

This work was supported in part by the National Research Council of Taiwan under Contract No. NSC86-2112-M009-011. C.D.L. was supported in part by the U.S. Department of Energy, Office of Energy Research, Division of Chemical Sciences. This work was also supported by a U.S.-Taiwan collaborative research grant.

[1]

[1] F. Melchert, M. Benner, S. Krüdener, R. Schulze, S. Meuser, K. Huber, E. Salzborn, D. B. Uskov, and L. P. Presnyakov, Phys. Rev. Lett. **74**, 888 (1995).
[2] M. H. Cherkani, D. Fussen, M. I. Chibisov, and F. Bouillard, Phys. Rev. A **54**, 1445 (1996).
[3] W. Fritsch and C. D. Lin, Phys. Rep. **202**, 1 (1991).
[4] B. H. Bransden and M. R. C. McDowell, *Charge Exchange and the Theory of Ion-atom Collisions* (Clarendon, Oxford 1991).
[5] J. T. Lin, T. F. Jiang, and C. D. Lin, J. Phys. B **29**, 6175 (1996).
[6] A. M. Ermolaev, J. Phys. B **25**, 3133 (1992).
[7] J. Y. Kuang and C. D. Lin, J. Phys. B **29**, 1207 (1996).
[8] C. E. Moore, *Atomic Energy Levels*, NBS Circular No 467 (U.S. Gov't Printing Office, Washington, D.C., 19xx), Vol. 1.