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Electron Capture Cross Sections in $N^{4+}+H$ Collisions

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We present total electron capture cross sections for collisions of N^{4+} ions with atomic hydrogen in the energy range of 30-3500 eV/u calculated with the two-center atomic orbital close-coupling expansion method in a quasi-one-electron model. Various basis sets have been used to check the convergence of the calculation and the results are shown to be in general agreement with existing experimental and theoretical data. However, the small structures observed and predicted by different theories below 100 eV/u are not reproduced in the present calculation.

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I. Introduction

The capture of a single electron often is the dominant inelastic process in collisions of multiply charged ions with neutral atoms in the low and intermediate energy regime. Because of its relevance to processes in astrophysical and thermonuclear plasmas, the determination of single electron capture cross sections from atomic hydrogen by multicharged nitrogen ions continues to receive considerable attention [1] in recent years. Using the merged-beam technique, Huq et al. [2] obtained the absolute total cross sections for single electron capture in the energy range of l-400 eV/u, while Folkerts et al. [3] obtained relative cross sections in the energy range of l-300 eV/u. Furthermore, McCullough *et al.* [10] first measured state-selective cross sections using translational energy spectroscopy (TES) in the energy range of 250-1600 eV/u. To resolve electron capture to singlet and triplet states separately, Bliek *et al.* [9] used photon emission spectroscopy (PES) to obtain state-selective cross sections in the energy range of 1-4 keV/u.

On the theoretical side, Bultler *et al.* [4] used the two-state Landau-Zener approximation to study this system. Within the framework of the molecular orbital (MO) model, this system has been studied quantum mechanically by Feickert *et al.* [5], Shimakura *et al.* [6], Folkerts *et al.* [3], and Zygelman *et al.* [7,8]. Feickert *et al.* [5] studied this system with the so-called improved virtual orbital approach at lower energies while Zygelman et *al.* [7,8] performed calculations using *ab initio* adiabatic potentials and radial couplings, but the rotational coupling was neglected and electron translation factors were ignored. Shimakura *et al.* [6] used a semiclassical method including electron translation factors for collision energies from 10 eV up to several keV. Using the same molecular model, the cross

sections have been calculated down to the lower energies by treating the motion of the heavy particles quantum mechanically. The results were reported by Folkerts *et al.*[3] for energies from a few tenths of one eV. The recent MO results of Zygelman *et al.* [8] and Folkerts et al. [3] are generally in qualitative agreement with the available experimental results, however there are significant differences between the two calculations.

With the advent of faster computers, large set of basis functions have been employed in recent MO calculations and the results are expected to be relatively reliable. It is surprising that there is still nonnegligible discrepancy in the 0.01 - 1 keV/u energy region between the various MO calculations and the experimental results. To investigate the origin of the discrepancy we undertook a new calculation using the two-center atomic orbital (AO) close coupling expansion method within the quasi-one electron model. This model is expected to be adequate since contribution from the dominant two-electron processes in all the energy region considered is no more than 10% [2,6,8,9,10,11,12]. This work is to provide results from the AO calculation to discriminate the difference between the various MO calculations and the experimental results.

We have found that our results are in general agreement with experiments above 100 eV/u. For energies below 80 eV/u simple estimate indicates that accounting for the curved trajectories can affect the calculated total cross section. When the trajectory effect is considered we were able to obtain total electron capture cross sections in better agreement with the data of Huq *et al.* [2] and of Folkerts *et al.* [3]. Our low energy results are also in reasonable agreement with the MO calculations of Folkerts et al. [3]. However, as we will show later, the agreement among the various experiments and theories are only qualitative. In the low energy region, precise experimental data are still needed to unravel the limitation of the various theoretical models.

The theoretical method used in this calculation is essentially the same as the recent one used in Tseng and Lin [13]. In Section II we describe the model potential and the basis functions used in the calculation. The results are shown and analyzed in Section III. A short summary is given in Section IV.

II. Theoretical method

We used the semiclassical impact parameter approximation where the projectile is moving along a straight-line trajectory for each impact parameter b. The time-dependent electronic wave function $\Psi(\mathbf{r},t)$ is expanded in terms of bound atomic orbitals plus pseudostates on the two collision centers with the plane-wave electronic translational factors

$$\Psi(\mathbf{r},t) = \sum_i a_i(t)\phi_i^A(\mathbf{r},t) \text{ t } \sum_3 b_j(t)\phi_j^B(\mathbf{r},t) \text{ t } \sum_k c_k(t)\phi_k^C(\mathbf{r},t)$$

where the set of atomic states $\{\phi_i^A(\mathbf{r},t)\}$ and $\{\phi_j^B(\mathbf{r},t)\}$ are bound states of projectile or target, respectively, and the set of pseudostates $\{\phi_k^C(\mathbf{r},t)\}$ need not be associated with a specific center (either projectile or target.). The atomic states used in the present work are generated from the even-tempered basis set of Kuang *et al.* [14]. The transition amplitudes $\{a_i,b_j,c_k\}$ are obtained through the standard procedure (see Brankin et *al.* [15]) by solving the first order coupled ordinary differential equations with the proper initial condition. The parameters in the model potential for the interaction between the electron and N^{4+} are

TABLE I. Comparison of calculated and experimental energy levels of N^{3+} (in atomic units).

bound state	present work	experiment
3s	-1.11178	-1.1150
4s	-0.59987	-0.5912
3P	-0.99830	-0.9992
4P	-0.54962	-0.5485
3d	-0.92124	-0.9231
4d	-0.51628	-0.5133
4*f*	-0.48799	-0.4871

determined by requiring that the bound excited state energies of the N^{3+} ion be accurately reproduced. The predicted binding energies from the model potential are compared to the experimental values in Table I where the experimental energies are taken to be the statistical average of singlet and triplet states of $N^{3+}(1s^2\ 2s\ n\ell)$.

In this study we employed several sets of basis functions, but only those from two sets will be shown. In the 10-3500eV/u collision energy range, electron capture to the 3d state of N^{3+} is the dominant process, with a less significant capture to 3s and 3p states, and very minor contribution from capture to the $n=4$ states. In the first basis set we include the $n=3$ and $n=4$ atomic states of the N^{3+} ion and the n=l and $n=2$ atomic states of the H atom. The expansion of the wavefunction in terms of these atomic orbitals is expected to be adequate since electron capture for the $N^{4+}+H$ system occurs mostly at large impact parameters between $b=4$ and $b=8$. However, in view of the nonnegligible contribution from the region between $b=2$ and $b=4$, we decided to perform a number of calculations with larger basis set. We include ℓ = 0, 1, 2 and 3 states on the N^{4+} center and for each ℓ, there are a few pseudostates in addition to the bound states included in the first set. It is expected that the pseudostates included would provide a better flexibility for representing the time dependent wavefunction at small internuclear separations [16]. Altogether, there are 35 and 66 states on the N^{4+} center in the first and second set, respectively, together with the four states on the H center. As we shall show in the next section, the probabilities calculated differ only at small impact parameters and the resulting electron capture cross sections from the two calculations agree to within a few percents. We have also performed calculations using different pseudostates generated from different primitive basis functions but obtained essentially the same electron capture cross sections. Thus we believe that the results reported below are converged to a few percents within the model adopted.

To account for the deflection of the projectile for collisions at low energies where the straight-line trajectory approximation is not valid, we use the same model which was used previously in the calculation of electron capture cross section for the $C^{4+}+H$ system [13]. In this model the distance of closest approach r_c was obtained by assuming that the

internuclear potential is due to the Coulomb repulsion between N^{3+} and H^{+} for each impact parameter b. Since the incoming path is between the neutral H and the N^{4+} ion, the trajectory in the incoming part is essentially a straight line, thus the distance of closest approach is set to be $b+(r_c-b)/2$, assuming that the incoming path is a straight line trajectory and the outgoing part is a repulsive Coulomb trajectory. We then interpret the probability for electron capture at impact parameter b in the straight line trajectory calculation to be the electron capture probability for a curved trajectory which has the distance of closest approach given by $b+(r_c-b)/2$. The above assumption implies that the electron capture probabilities will be suppressed by the repulsive Coulomb interaction in the lower energy region.

III. Results and discussion

We have calculated electron capture cross sections using the two basis sets described in the previous section. The electron capture probabilities oscillate rapidly with impact parameters in the low energy region. We checked to make sure that the calculations were performed with sufficient dense mesh points in obtaining the total cross section.

In Table 11(a) we present the calculated total electron capture cross sections and partial cross sections to individual 3s, 3p, and 3d states. These results were obtained with the first basis set. At energies below 0.1 keV/u, we begin to see the difference originating from the curved trajectories calculated within the present model. In Table II(b), the cross sections for the hydrogen and deuterium targets calculated using curved trajectories are shown. The D target results are about 3-8% higher than the H target. Trajectory effect was found to be negligible above 0.1 keV/u.

In Fig. 1 we compare the total electron capture cross sections in the lo-3500 eV/u region obtained from different theoretical calculations with the experiment data of Huq et al. [2] and of Folkerts et al. [3]. Besides the present calculation, we also show the recent MO results of Shimakura *et al.* [6] and Zygelman *et al.* [8]. The results of Zygelman *et al.* [8] are much smaller than ours but ours are in good agreement with the results of Shimakura *et al.* [6] in the whole energy region. All the theoretical results show some minor structures at slightly lower energies than the dip reported by Folkerts *et al.* [3] at around 100 eV/u. The present AO results below 100 eV/u are those calculated including corrections due to the curved trajectories. Except for the discrepancy in the fine details, they are in good agreement with the data of Huq et al. [2] and of Folkerts *et* al. [3] in the energy region below 1 keV/u.

In Fig. 1 we also compare the calculated cross sections obtained for the deuterium target with the available experimental data. Our results are in agreement with the results of Seim *et al.* [11] and of Crandall et *al.* [12], but are somewhat higher than the recent result of Bliek *et al.* [9] above 1 keV/u. According to our model the trajectory effect makes only negligible difference (about 3-8%) for the two cross sections at energies above 35 eV/u. The isotope dependence occurs at much lower energies for the N^{4+} on H system than for the C^{4+} on H system [13] since for the former electron capture occurs at larger impact parameters.

TABLE II. (a). Cross sections (in 10^{-16} cm^2) for electron capture to $N^{3+}(n\ell)$ subshells $(\sigma_{n\ell})$ and to all states (σ_{tot}) in $N^{4+}+H$ collisions from the present calculations. a(b) stands for $a\times10^b$.

	Straight-line				Curved trajectory			
E(keV/u)	σ_{3s}	σ_{3p}	σ_{3d}	σ_{tot}	σ_{3s}	σ_{3p}	σ_{3d}	σ_{tot}
0.03	0.01	0.95	31.66	33.48	0.76(-3)	0.57	25.24	26.66
0.06	0.05	2.87	29.42	33.49	2.35(-2)	2.39	26.13	28.73
0.08	0.07	4.42	30.01	34.69	0.05	3.76	27.47	31.46
0.10	0.15	5.06	31.13	36.61	0.11	4.52	29.10	33.98
0.20	0.65	11.03	26.32	38.43	0.51	10.49	25.61	37.04
0.50	1.62	19.26	14.64	36.55	1.60	19.10	14.40	36.13
1.00	3.78	22.44	6.77	34.79	3.75	22.30	6.72	34.57
2.00	6.13	17.24	5.75	31.41	6.11	17.19	5.72	31.32
3.00	6.86	13.16	6.51	29.55	6.85	13.13	6.49	29.49
3.50	7.15	11.59	6.51	28.64	7.14	11.57	6.49	28.59

TABLE II. (b). Total cross sections σ_{tot} (in 10^{-16} cm^2) for electron capture in collisions of N^{4+} with H and D target from the present calculations using curved trajectories.

E(keV/u)	Straight-line	D	H
0.03	33.48	28.55	26.66
0.05	33.51	29.94	28.94
0.06	33.49	29.65	28.73
0.07	33.11	30.62	29.81
0.08	34.68	32.28	31.46
0.10	36.61	34.60	33.98

To show that the reported calculated cross sections are essentially converged we depict the impact parameter dependence of bP(b) for electron capture to the 3p state at 300 eV/u in Fig. 2(a) and to 3d state at 200 eV/u in Fig. 2(b). The calculations were performed using the two different basis sets explained in the last section. Clearly the results are essentially independent of the basis set used to better than a few percents. We have also checked

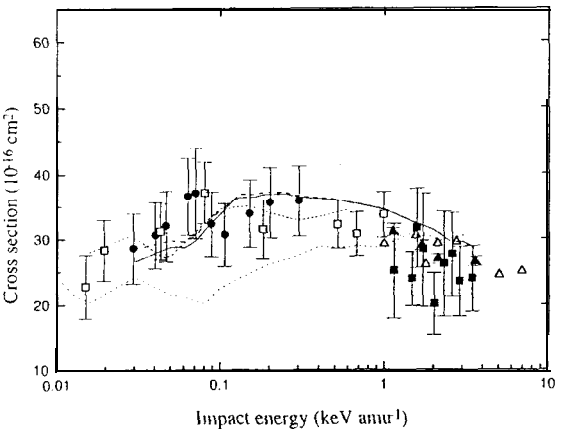

FIG. 1. Comparison of total electron capture cross sections for N^{4+} on H and N^{4+} on D collisions. Theoretical results: Present, solid line (H target), long dashed lines (D target); dashed lines, Shimakura *et* al. [6]; dotted line, Zygelman *et* al. [8]. Experimental results: Huq et al. [2] (open squares), Folkerts *et* al. [3] (solid circles), Crandall *et* al. [12] (open triangles), of Seim *et* al. [11] (solid triangles), and Bliek *et* al [9] (solid squares).

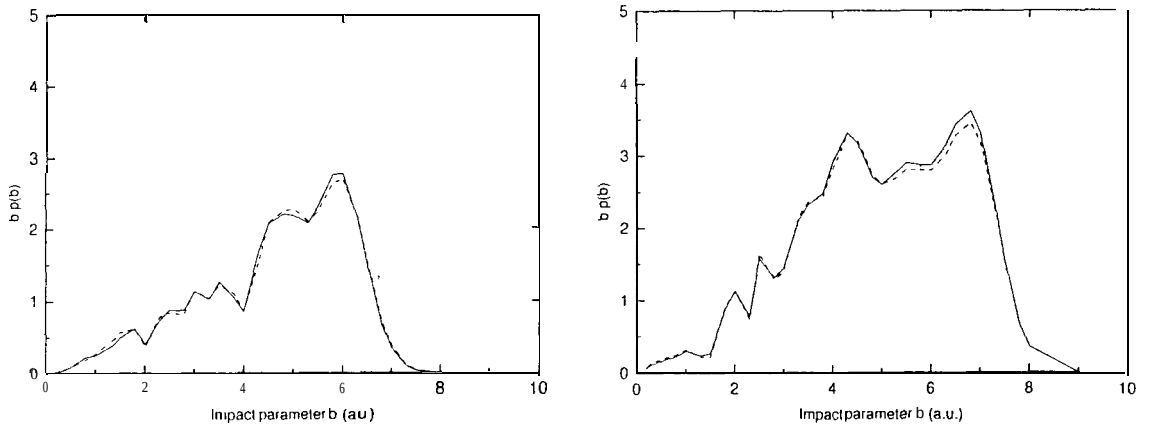

FIG. 2. (a) Impact parameter dependence of bP (b) for electron capture to (a) 3p state at impact energy of 0.3 keV/u and (b) 3d state at 0.2 keV/u calculated with two different basis sets as explained in the text. The solid line is from the large basis set calculation and the dashed one from the small basis set calculation.

the calculations using other basis functions and found essentially identical results. We thus believe that the results are converged. It is noted that electron capture is dominated by transitions occurring at large impact parameters where the atomic orbital expansion method is expected to be valid.

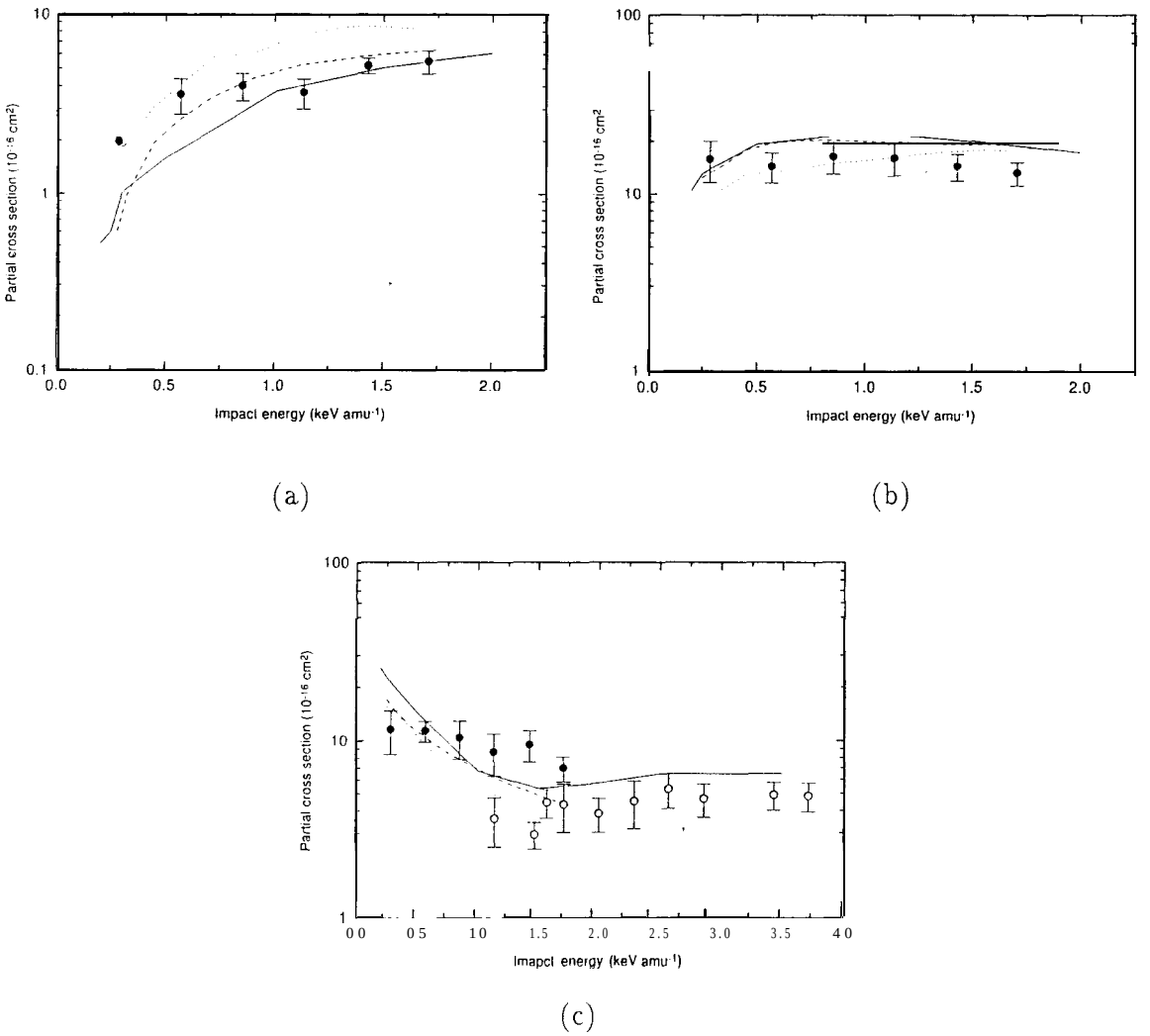

FIG. 3. Comparison of theoretical and experimental partial electron capture cross sections to (a) 3s, (b) 3p and (c) 3d states of N^{4+} ions. Present, solid line; dashed, Shimakura *et al.* [6]; dotted, Zygelman *et al.* [8]. The experimental data are from McCullough *et al.* [10] (solid circles) and Bliek *et al.* [9] (open circles).

In addition to the total cross section, partial cross sections or the fractions of electron capture to the $N^{3+}(2s3\ell), \ell = s$, p, d states have been determined at energies above 250 eV/u in a number of experiments [2,9,10]. In Figs. 3(a), (b) and (c) we compare the present partial cross sections with the recent result of Bliek *et al.* [9] in the 1- 4 keV/u region and the result of McCullough *et al.* [10] in the region of 250 eV/u -1.6 keV/u. The present results are in general good agreement with experimental data for all the channels considered.

In Figs. 3(a)-3(c) we also include the theoretical cross sections from Zygelman *et al.* [8] and Shimakura et al. [6]. These cross sections show good agreement with experiments at higher energies. It is interesting to note that electron capture to the 3d state increases with decreasing collision velocity below 250 eV/u. This result is similar to the C^{4+} on H system [13]. In terms of diabatic molecular potential curves this increase results from the crossing between the entrance channel and the 3d exit channel at R=7 a.u. for triplet states and R=8 a.u. for singlet states. At higher energies this crossing is diabatic but it becomes effective in populating 3d states at lower energies: as expected from a typical Laudau-Zener model.

IV. Summary and conclusions

We have performed careful calculations for single electron capture cross sections for the N^{4+} on H system based on the two-center atomic orbital close-coupling expansion method. In view that two electron processes such as double capture and simultaneous projectile-core excitations are small, we adopted a one-electron model in the calculation. The results show that the present quasi-one electron AO calculation can describe successfully the electron capture processes in N^{4+} on H collisions quantitatively. While the present total cross sections are in general agreement with the other MO calculations and with existing experimental data [2,6,8,9,10], there are still significant discrepancies among the theoretical results. The existing experimental data also have large discrepancies which are not useful for discriminating the different theoretical results. Until more precise experimental data become available the limitation of the theoretical models cannot be exposed.

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References

[1] P. C. Stancil *et al.*, J. Phys. B30, 1013 (1997).
[2] M. S. Huq, C. C. Havener, and R. A. Phaneuf, Phys. Rev. A40, 1811 (1989).
[3] L. Folkerts *et al.*, Phys. Rev. A51, 3685 (1995).
[4] S. E. Bulter and A. Dalgarno, Astrophys. J. 241, 838 (1980).
[5] C. A. Feikert *et al.*, Astrophys. J. 286, 371 (1984).
[6] Shimakura, M. Itoh, and M. Kimura, Phys. Rev. A45, 267 (1993).
[7] B. Zygelman *et al.*, Phys. Rev. A46, 3846 (1992).
[8] B. Zygelman *et al.*, Phys. Rev. A56, 457 (1997).
[9] F. W. Bliek *et al.*, Phys. Rev. A57, 221 (1998).
[10] R. W. McCullough et *al.*, Nucl. Instrum. Methods Phys. Res. B98, 199 (1995).
[11] W. E. Seim *et al.*, J. Phys. B14, 3475 (1981).
[12] D. H. Crandall, R. A. Phaneuf, and F. W. Meyer, Phys. Rev. **A19**, 504 (1979).
[13] H. C. Tsengand C. D. Lin, Phys. Rev. A58, 1966 (1998).
[14] Jiyun Kuang and C. D. Lin, J. Phys. B29, L889 (1996).

[15] R. W. Brankin, I. Gladwell, and L. F. Shampine, 1992 RKSUITE: a suite of Runge-Kutta codes for the initial value problem for ODEs, Softreport 92-S1, Department of Mathematics, Southern Methodist University, Dallas, Texas, USA.

[16] W. Fritsch and C. D. Lin, Phys. Rep. 202, 1 (1991).