Total and state-selective electron-capture cross sections for N^{4+}-H collisions

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Electron-capture cross sections in collisions of N^{4+} ions with atomic hydrogen is studied using the close-coupling two-center atomic orbital expansion method by treating the collision system in a quasi-two-electron model. Total electron-capture cross sections to the dominant individual singlet and triplet excited states are evaluated over the energy range of 50–20 000 eV/amu. The results are compared to existing experimental data and to theoretical calculations based on the molecular orbital expansion method. It is found that while the general overall agreement is satisfactory, the large experimental uncertainty cannot be used to discriminate the different theories. For the present energy range our results are closer to the semiclassical close coupling calculations based on the molecular orbital expansion method of Shimakura *et al.* [Phys. Rev. A **45**, 267 (1993)] than the quantum calculations of Zygelman *et al.* [Phys. Rev. A **56**, 457 (1997)].
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I. INTRODUCTION

As a result of the possible important role of N^{4+}-H charge-changing collisions in plasma diagnostics and modeling [1], several experimental and theoretical studies have been undertaken in the last two decades over a broad range of collision energies for this system. Total electron-capture cross sections have been measured by Crandall *et al.* [2] in the 1–7 keV/amu region, Seim *et al.* [3] in the 1.1–3.6 keV/amu region, and Huq *et al.* [4] and Folkerts *et al.* [5] who used the merged-beam technique to obtain total charge transfer cross sections. The translational energy spectroscopy technique has been used by McCullough *et al.* [6] to obtain information on state-selective cross sections. The latter measurement, however, does not have the resolution to distinguish singlet and triplet states populated. More recently, Bliek *et al.* [7] used photon emission spectroscopy by detecting the photons emitted from the excited states of N^{3+} after the electron-capture process, and were able to differentiate the singlet and triplet excited states populated. Their measurements cover the 1–4 keV/amu energy range.

Theoretically the N^{4+}-H system was studied in the early days using a small number of molecular basis functions [8,9]. However, two elaborate calculations based on the molecular basis functions have been carried out in recent years, one by Shimakura *et al.* [10] and the other by Zygelman *et al.* [11,12]. These two calculations predict different results. As a result of the relatively large experimental errors, the existing experiments cannot be used to discriminate between these two theoretical results.

In view of the above conflicting results, we have undertaken an independent study of the present collision system within the semiclassical close coupling method by expanding the electron wave function in terms of atomic orbitals (AO's) at the two nuclear centers [13]. In this approach we have used plane-wave electron translational factors. Since the transitions for the dominant electron-capture channels occur mostly at large impact parameters, the atomic orbital expansion method is expected to be adequate down to relatively low energies. In the present calculation we treat N^{4+}-H as a two-electron collision system; this allows us to obtain state-selective electron-capture cross sections to distinct singlet and triplet final states, and to compare with the calculations of Shimakura *et al.* and Zygelman *et al.* In the semiclassical calculation straight-line trajectories were used. However, as the collision energy is decreased, the motion of the heavy particles is governed by curved trajectories. We adopt a heuristic procedure to account for the trajectory effect in order to extend the calculation to the lower energies. In Sec. II, we document the model and the parameters used in the present calculation. The results and the comparison with experiments and other theoretical calculations are presented in Sec. III. A short summary and conclusion are given in Sec. IV.

II. THEORETICAL MODEL

We first treat N^{4+}-H as consisting initially of an electron on the N^{5+} core and an electron on the proton. The time-dependent electron wave function for these two electrons is expanded in terms of the traveling two-electron atomic eigenstates, consisting of configurations where one electron is on the target and the other on the projectile to describe elastic as well as single excitation channels, and configurations where both electrons are on the projectile. The latter are final states populated by the single-electron-capture process. As the N^{5+} core potential we take the screened hydrogenic potential as proposed by Garvey *et al.* [14] with a slightly adjusted thickness parameter of $1/\xi = 0.128$ a.u. in order to fit the experimental N^{4+} $2s$ binding energy of the initial state. One-electron states of the N^{4+} ion and two-electron states of the N^{3+} ion are obtained by solving, respectively, the one-electron problem and the two-electron problem in the N^{5+} core model potential. The two-electron states of N^{3+} ions are calculated using the standard configuration-interaction approach where the two-electron eigenstates are expanded in terms of the antisymmetrized products of the wave functions of the two electrons. Since the dominant electron-capture channels are $2s3s$, $2s3p$, and $2s3d$, for both singlet and

TABLE I. Comparison of energy levels for the N^{3+} ion. Energies are given relative to the double ionization threshold.

Two-electron state	Energy level from model (a.u.)	Experimental value (a.u.)
$2s^2\ ^1S^e$	−6.45	−6.46
$2p^2\ ^1S^e$	−5.38	−5.31
$2s3s\ ^{1(3)}S^e$	−4.68(−4.73)	−4.67(−4.73)
$2p3p\ ^{1(3)}S^e$	− (−4.20)	−4.09(−4.19)
$2s2p\ ^{1(3)}P^o$	−5.85(−6.14)	−5.76(−6.10)
$2s3p\ ^{1(3)}P^o$	−4.60(−4.60)	−4.59(−4.60)
$2p3s\ ^{1(3)}P^o$	−4.29(−4.33)	−4.23(−4.32)
$2p3d\ ^{1(3)}P^o$	−4.08(−4.12)	−4.07(−4.11)
$2s3d\ ^{1(3)}D^e$	−4.49(−4.53)	−4.48(−4.52)
$2p3p\ ^{1(3)}D^e$	−4.17(−4.24)	−4.19(−4.22)

triplet states, and to a lesser extent, the $2p3s$ singlet and triplet states, we compare in Table I the calculated energies of these states using the model potential approach and the experimental values.

In the calculation, the two-electron basis functions included are the two-electron states listed above, as well as some two-electron pseudostates to improve convergence. Since no spin interaction is considered, the total spin is conserved and thus the calculations are carried out separately for the spin singlet and spin triplet symmetries. In total, including the two-electron capture states and the one-electron elastic and excitation states, the singlet and triplet cases are 35-state and 33-state calculations, respectively. With the basis set chosen, the standard close-coupling equations are solved for each impact parameter. We only considered straight-line trajectories in the calculation.

The merged-beam experiments of Huq *et al.* and of Folkert *et al.* covered mostly the energy region below 1000 eV/amu. Within the atomic orbital expansion method, it is straightforward to perform calculations based on the straight-line trajectories. For energies below 100 eV/amu we found that the Coulomb repulsion between N^{3+} and H^+ is no longer negligible. Thus the use of straight-line trajectories in the AO calculations becomes questionable. In the semiclassical approach, it is possible to perform AO calculations using curved trajectories [15]. However, there is not a well-defined procedure to decide the effective interaction between the two heavy particles from which the trajectory can be calculated.

To account for the trajectory effect at low collision energy where the straight-line trajectory approximation is not valid, we use the same ansatz as in the calculation of the electron-capture cross section of $C^{4+}+H$ collisions [16]. In the ansatz, we assume that the incoming part is a straight-line trajectory and the outgoing part is a curved trajectory determined by the Coulomb force between N^{3+} and H^+. Instead of performing calculations with such a trajectory, we assume that the distance of closest approach is approximated by the mean of the impact parameter b and the distance of closest approach r_c for the Coulomb trajectory on the outgoing path. We then interpret the probability for electron capture at impact parameter b for a curved trajectory as the electron-capture probability for a straight-line trajectory which has an impact parameter of $(b+r_c)/2$. The above assumption implies that the electron-capture cross section will be suppressed by the repulsive Coulomb interaction at the lower-energy range. We have also used a variation of this model by taking the effective distance of closest approach as resulting from half of the Coulomb repulsion, in the outgoing capture channel, but acting along the whole projectile trajectory. The two models differ little but each model does reduce the calculated electron-capture cross sections from those calculated with straight-line trajectories. In Table II we tabulate the total electron-capture cross sections calculated. We tabulate results from both the straight-line and ''corrected'' trajectories.

TABLE II. Comparison of total capture cross section computed with straight-line trajectories versus the heuristic correction for curved trajectories. The correction due to the trajectory effect was only computed for projectile energies less than 301 eV/amu.

Projectile energy (eV/amu)	Raw $\sigma_{capt}(10^{-16}\ cm^2)$	Corrected $\sigma_{capt}\ (10^{-16}\ cm^2)$
50	31.86	28.23
70	33.64	30.55
85	35.52	32.98
100	35.65	33.60
125	35.83	34.18
151	36.10	34.52
175	35.34	34.01
201	34.52	33.52
225	34.26	33.26
250	34.09	33.24
275	34.39	33.60
301	34.75	33.97
500	34.37	
1000	33.50	
1500	31.58	
2000	30.26	
3000	28.29	
4000	26.68	
5000	24.96	
7000	22.62	
10000	20.45	
20000	17.67	

III. RESULTS AND DISCUSSION

In Fig. 1 we compare the total electron-capture cross sections from the different experiments and from the other molecular orbital (MO) theoretical calculations over the energy range of 10 eV/amu to 20 keV/amu. We stopped our calculations at 50 eV/amu since below that the trajectory ''correction'' becomes quite significant in our heuristic approach. Within the error bars of the experiments there is an overall general agreement. However, the degrees of disparities in the finer details are not satisfactory. For example, Folkerts *et al.* emphasized the apparent dip in their measured total cross section near 100 eV/amu, while the calculation of Zygelman *et al.* shows a minor dip near 80 eV/amu and the calculation of Shimakura *et al.* shows a dip near 40 eV/amu. Does the total electron-capture cross section indeed have a small dip

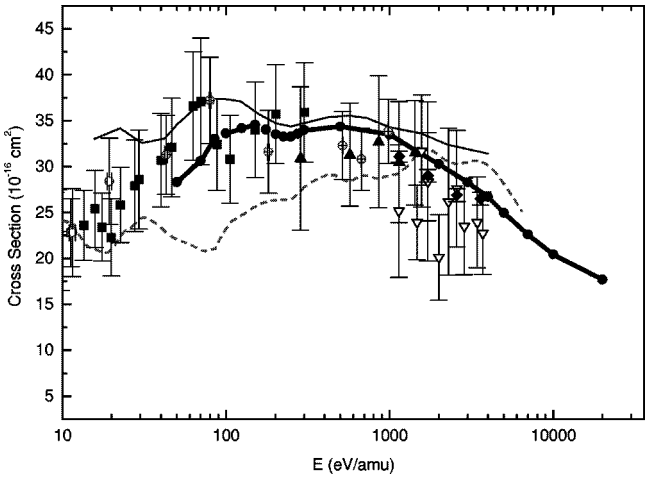

FIG. 1. Present total capture cross section results for $N^{4+}+H$ compared with other theories and experimental data. Theoretical results: thick solid line with solid circles, this work; thin solid line, Shimakura *et al.* [10]; dotted line, Zygelman *et al.* [12]. Experimental results: solid squares, Folkerts *et al.* [5]; open circles, Huq *et al.* [4]; solid up triangle, McCullough *et al.* [6]; open down triangle, Bliek *et al.* [7]; solid diamond, Seim *et al.* [3].

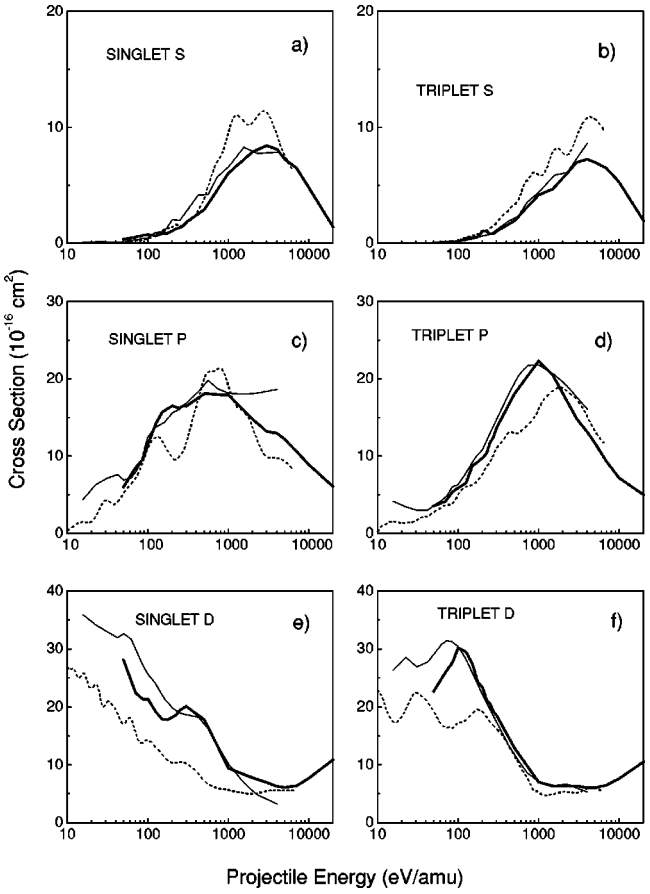

FIG. 2. Comparison of various theoretical results for partial capture cross sections. The statistical weight has been divided out; so singlet capture results have been multiplied by 4 and triplet by 4/3. Thick solid line, this work; thin solid line, Shimakura *et al.* [10]; dotted line, Zygelman *et al.* [12].

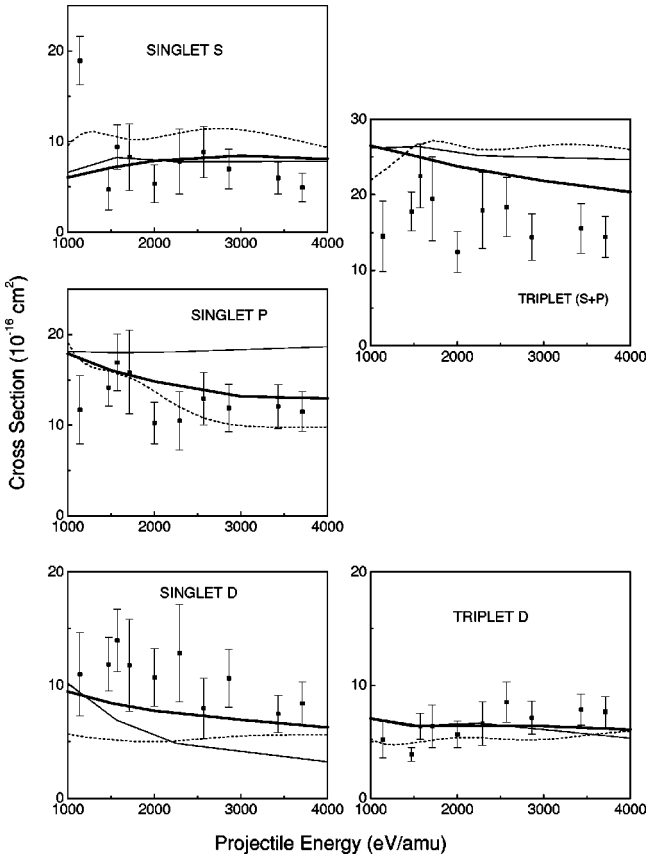

FIG. 3. Comparison of various theoretical results for singlet and triplet partial capture cross sections with experimental results of Bliek *et al.* The statistical weight has been divided out; so singlet capture results have been multiplied by 4 and triplet by 4/3. Thick solid lines, this work; thin solid lines, Shimakura *et al.* [10]; dotted lines, Zygelman *et al.* [12].

in this energy region? Our calculation does not show much structure there. Since the trajectory effect is not insignificant in this energy region, we cannot make this claim with assurance. A similar dip from the merged-beam experiment was reported for the C^{4+} on H [17] system at the higher energy around 1 keV/amu where the trajectory effect does not play a role but the dip was never reproduced in the calculation [16] using the AO expansion method.

Figure 1 shows that our present results are in better agreement with the calculation of Shimakura *et al.* than with the calculation of Zygelman *et al.* In fact the present calculation appears to go through all the experimental data, noting that the data all have large error bars. The present results agree well with Shimakura *et al.* in the 200–1500 eV/amu range. The discrepancy between the two at energies below 200 eV/amu is largely due to the ''correction'' we have made on the curved trajectories. The calculation of Shimakura *et al.* in this energy region used straight-line trajectories with MO's. Our straight-line results would agree with the results of Shimakura *et al.* below 200 eV/amu. The discrepancy at energies above 2000 eV/amu may be due to the limited form of the ETF's used in the calculation of Shimakura *et al.* or the lack of convergence in the MO calculation.

The experimental total electron-capture cross sections do not allow a clear discrimination of the theoretical results. In Fig. 2 we show the comparison among the three theoretical

calculations for the dominant state-selective total electron-capture cross sections. In Fig. 2(a) the electron-capture cross sections to the $2s3s\,^1S^e$ state are shown. The results of Zygelman *et al.* are further off from the present result than that of Shimakura *et al.* This is also true for capture to the $2s3s\,^3S^e$ state [see Fig. 2(b)]. Figure 2(c) shows the cross sections for capture to the $2s3p\,^1P^o$ state. Results from Zygelman *et al.* display much more oscillatory structures which are not as pronounced in the present calculation nor in the calculation of Shimakura *et al.* For the $2s3p\,^3P^o$ state, the results from Zygelman *et al.* are lower while the other two theories agree rather well. The calculation by Zygelman *et al.* was intended primarily for lower energy where rotational coupling was not included. In the higher-energy region studied here rotational coupling is known to be more important. For $2s3d\,^1D^e$ and $2s3d\,^3D^e$, the electron-capture cross sections rise rapidly below 1000 eV/amu. We have good agreement with Shimakura *et al.* except at energies below about 100 eV/amu where we have included the trajectory effect while Shimakura *et al.* did not. At the lower energies our straight-line results compare well with those from Shimakura *et al.*

The recent data of Bliek *et al.* reported the singlet and triplet state-selective electron-capture cross sections in the narrow energy range of 1–3.5 keV/amu. In Fig. 3 we compare their measured cross sections with the three theoretical results. While the agreement is satisfactory for all three calculations, it appears that the present calculation provides the best overall agreement with the experimental data. We comment that in this energy region the trajectory effect is negligible and thus the present calculation is a genuine AO calculation without any corrections.

IV. SUMMARY AND CONCLUSION

In this paper we reported the total and the state-selective single-electron-capture cross sections for N^{4+} on H collisions over the energy range of 50–20 000 eV/amu using the close-coupling expansion using two-electron atomic basis functions. In terms of the total electron-capture cross section, there is a general agreement among the experiments and theoretical calculations. However, the experimental uncertainties are still too large and the results from two calculations based on the molecular basis function expansion method do not agree with each other. Our calculations for energies above 200 eV/amu agree better with the MO calculations based on the semiclassical approximation [10]. At lower energies we found that accounting for the trajectory effect in an approximate manner allows us to obtain total cross sections in much better agreement with the experimental data. The MO calculations where the motion of the heavy particles is described quantum mechanically gave results which are at variance with our results and with the MO results of Shimakura *et al.* The difference may be attributable to the lack of rotational coupling in the quantum calculation. At the level of the state-selective electron-capture cross sections again the AO results from the present calculation agree better with those of Shimakura *et al.* The MO calculations of Zygelman *et al.* tend to show more oscillatory structure not found in our calculation. The state-selective total capture cross sections have been measured over a narrow energy range only and it appears that the present AO results have the better overall agreement with the data. Despite the much better agreement between our results and those of Shimakura *et al.*, it is still desirable to have more accurate experimental data which can confirm these two calculations with smaller errors.

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