Single-electron capture by highly charged ions colliding with atomic and molecular hydrogen

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The ratio between the cross sections for single-electron capture by highly charged ions colliding with atomic and molecular hydrogen has been investigated within the framework of the Bohr-Lindhard theory. It is shown that $\sigma(H_2)/\sigma(H)$ can be represented as a universal function of the inherent scaling parameter over a wide range of ion energy and charge states. Generally, the ratio is different from the often-assumed value of 2.

Owing to their importance for a multitude of ion-atom and ion-solid interactions, electron-capture processes have been the subject of theoretical and experimental studies for many years. Theoretically, even the simplest case, namely, the proton–atomic-hydrogen collision system, has presented a problem of great complexity. On the other hand, early experimental efforts were concentrated on more complicated systems, owing to the technical difficulties associated with atomic-hydrogen targets. Therefore, theoretical cross sections for atomic hydrogen were often compared with experimental results for the molecular target divided by the factor of 2. This could in no sense be considered physically rigorous, and a theoretical investigation[1] on the energy dependence of the cross-section ratio $[\sigma(H_2)/\sigma(H)]$ was attempted and found to be in reasonable agreement with experiment as results on atomic hydrogen gradually became available.

During the last decade, the importance of electron-capture processes to fusion and astrophysical research has become widely realized, and this has led to a renewed interest, especially in electron capture for highly charged ions colliding with atomic hydrogen. A considerable amount of data has been obtained for both atomic- and molecular-hydrogen targets.[2] In this connection, our recent work[3] has involved the extension of experimental studies in the intermediate- and high-energy regime and has shown that the Bohr-Lindhard (BL) model[4] offers a general theoretical framework for the description of atomic collisions with highly charged ions. The present Communication reports on experimental high-energy cross sections on atomic and molecular hydrogen, which in conjunction with the previously available lower-energy results, are used to verify a universal scaling of $\sigma(H_2)/\sigma(H)$ inherent in the BL theory. This ratio for highly charged ions is not solely of interest from a practical viewpoint in so much as it has arbitrarily been assumed equal to 2 (Refs. 5–7) but also demonstrates a striking contrast to that for projectiles of low charge where a proper theoretical description must recognize the distinct features of the collisions for each individual projectile. A universal description of highly charged ion-atom collisions is of further significance for extensions to differential cross sections, describing, for example, the distribution of capture over various quantum states, a problem of great practical importance in connection with highly charged impurity atoms in thermonuclear plasmas. Thus the situation is not unlike that existing previously for experimental studies for high-energy protons in that although high-temperature ovens have facilitated the measurement of total-capture cross sections on a sufficiently dense atomic-hydrogen target, such techniques preclude study of light emission due to capture into specific quantum states. These remarks are extended and amplified below, first by a brief description of the essential features of the BL model, and second by a discussion of the scaling of the ratio $\sigma(H_2)/\sigma(H)$, which is shown to be universal with respect to all projectiles provided that the ionic charge is sufficiently high.

The theory of Bohr and Lindhard is based on a classical picture of the capture process. This is a reasonable approach if, firstly, there is a high density of final states available to the captured electron in the projectile ion. That is the case if the ion charge is high enough (say, $q \geqslant 5$); secondly, if the ion velocity V is small enough that quantal effects can be neglected in the description of the collision between the ion and the target electron. This latter condition has been shown[8] to be fulfilled when

$$2q\frac{v_0}{V} >> 1 \ , \tag{1}$$

where v_0 is the Bohr atom, electron-orbital velocity.

As a result of our calculations[3] based on the BL model, we found that the cross section for single-electron capture divided by the charge of the particle q depends only on the scaling parameter,

$$X = Eq^{-4/7} \ , \tag{2}$$

in keV/amu, where E is the ion energy. Furthermore, using a simple distribution for the target-atom electrons, we obtained an analytical expression for the cross section for single-electron capture by highly charged ions for any target atom, given by the target atomic number z, the ionization potential I, and a parameter α, which determines the smallest effective target-electron velocity for the capture process. It was shown[3] that α can be found by fitting to data for low-velocity ions.

Figure 1 presents the results of this model (solid curve) for highly charged ions in atomic hydrogen. Also shown is the majority of published experimental data with $q \geq 5$. Two sets of data known to the authors have been excluded from the figure: The iron-ion data of Gardner *et al.*[9] which have been argued to be 50% too high by Crandall *et al.*,[10] and the oscillatory data for tantalum, tungsten, and gold ions of Meyer *et al.*[11] where a special mechanism stemming from the ions not being pointlike decreases with cross sections.

In the figure are also shown data for high-X values obtained in this work. We measured cross sections for 2–8-MeV N^{5+} and O^{5+} ions on atomic and molecular hydrogen. Details of the experimental technique will be discussed in a forthcoming publication.[12]

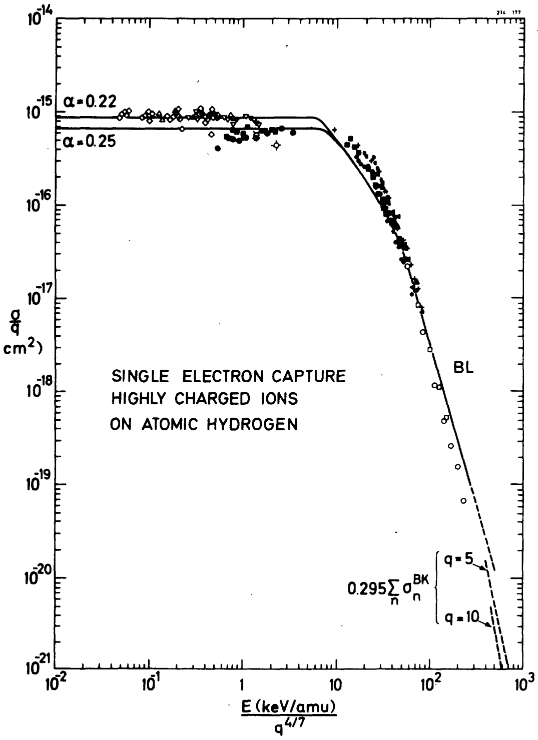

FIG. 1. Cross sections for single-electron capture for highly charged ions ($q \geq 5$) in atomic H. The data are ○: N^{5+}, □: O^{5+} (this work), ◇: Xe^{5-12+}, Δ: $Fe^{5,6+}$, ▽: Ar^{5-9+} (Ref. 13), ◀: Si^{5-7+} (Ref. 14), ▲: O^{5-7+}, ●: Fe^{5-15+}, ■: Mo^{5-18+} (Ref. 11), ◖: N^{5+}, ◗: O^{5+} (Ref. 15), +: $C^{5,6+}$, ∗: B^{5+} (Ref. 16), ⌖: B^{5+}, ⌑: C^{5+}, ⊗: N^{5+}, ⊞: $O^{5,6+}$, ⊠: F^{6+} (Ref. 10).

From the figure it can be concluded that the scaling inherent in the BL theory is obeyed for all X values. The absolute magnitude of the theoretical result is in good agreement with the data. For low X, the curve marked $\alpha = 0.25$ is that found in Ref. 3. With the advent of new accurate data (Ref. 13), a value of $\alpha = 0.22$ seems more appropriate. For high X, the data decrease more steeply with increasing X than the BL result. This is expected because here condition (1) breaks down, and quantal theories are more appropriate. In the figure it can be seen that the data tend towards the widely accepted perturbation result (dashed curves),

$$\sigma = 0.295 \sum_n \sigma_n^{BK} , \tag{3}$$

where σ_n^{BK} is the Brinkman-Kramers cross section for populating the nth energy level of the ion.

In Fig. 2, we have plotted the ratio between the electron-capture cross sections for highly charged ($q \geq 5$) ions on molecular and atomic hydrogen as a function of the scaling parameter X. To the best knowledge of the authors, the figure includes all values of the ratio $\sigma(H_2)/\sigma(H)$ that can be extracted from the published literature, using the condition that $\sigma(H_2)$ and $\sigma(H)$ must be measured in the same experimental setup.

In spite of the rather large uncertainties associated with the data, they suggest that the Bohr-Lindhard X scaling is fulfilled over the entire X range. For low X, the ratio is constant and smaller than one. For medium X, the ratio increases with increasing X, but our data for $X \gtrsim 100$ show this increase to stop and the ratio to become roughly constant close to a value of 4.

From the integrated BL cross section[3] for atomic hydrogen with $\alpha = 0.22$ (shown in Fig. 1) and the corresponding one for molecular hydrogen ($I = 15.4$ eV, $z = 2$, $\alpha = 0.30$), we obtain the solid curve in Fig. 2. The α values were found by fitting to the low-X $\sigma(H)$ and $\sigma(H_2)$ data, and hence the theoretical $\sigma(H_2)/\sigma(H)$ curve agrees with the data in this region. However, the theoretical result also agrees by and large with the medium- and high-X data, which lends support to the model used.

In Fig. 2, the dashed curve is an empirical fit to the data. It is given by

$$\frac{\sigma(H_2)}{\sigma(H)} = \begin{cases} 0.76, & X < 6 \\ 1.76 + 0.0328(X-6), & 6 < X < 100 \\ 3.84, & 100 < X \ . \end{cases} \tag{4}$$

For this fit, 80% of the data points fall within ±20%.

The ratio $\sigma(H_2)/\sigma(H)$ has been investigated theoretically by Olson and Salop[17] and by Bottcher[18] for highly charged ions. Using their absorbing-sphere model, Olson and Salop calculated for $V = 7 \times 10^7$

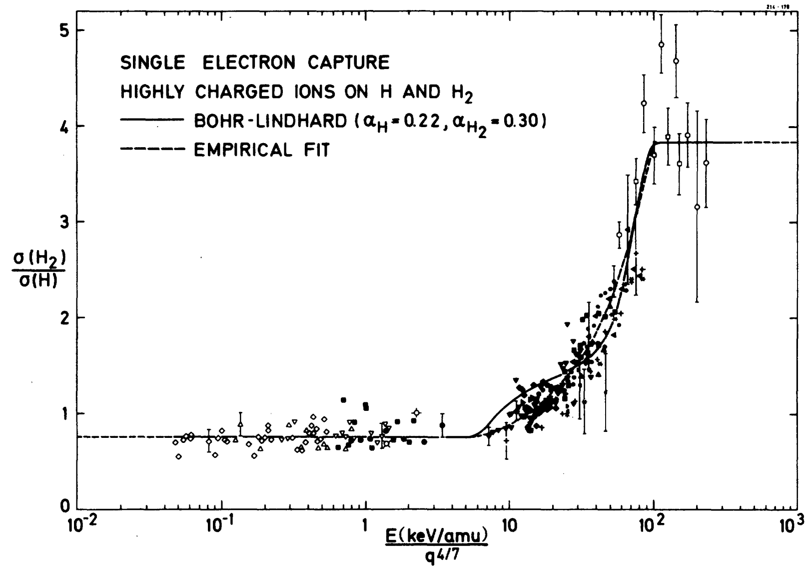

FIG. 2. Ratio $\sigma(H_2)/\sigma(H)$. The data symbols are the same as in Fig. 1. In this figure are also included the heavy-ion data of Ref. 11: ▼: Ta^{5-19+}, ◆: W^{5-15+}, ▶: Au^{5-16+}.

cm/sec the ratio to be 0.44 for $q=5$ and 0.30 for $q=20$. These results should be compared to the present value of 0.76. Although there is a numerical difference, this theory does predict a value smaller than 1. Olson and Salop explained the smallness of the ratio as being due to two factors: (1) The larger ionization potential of H_2 (more tightly bound electrons), which results in electron capture not being possible at as large an internuclear separation for H_2 as for H. (2) The presence of Frank-Condon factors in the molecular matrix elements. At medium-X values, Bottcher[18] applied a two-center, coherent-scattering model to calculate $\sigma(H_2)/\sigma(H)$. Using two adjustable parameters, he was able to obtain a rather good fit to the data of Refs. 11 and 19. His theoretical results decrease with decreasing velocity from close to 4 to slightly above 1 in the same region as does our result, but at lower velocities, Bottcher's $\sigma(H_2)/\sigma(H)$ increases again, contrary to the experimental findings. The theory of Bottcher does not predict a scaling like that found in this work.

As can be concluded from Fig. 2, the scaling of $\sigma(H_2)/\sigma(H)$ with X is fulfilled for highly charged ions. This is not the case when the same ratio measured with ions of low charge is considered. For example, for $X=1$, $\sigma(H_2)/\sigma(H) \approx 0.4$ for both H^+ (Ref. 20) and He^{2+} (Ref. 21) ions. Furthermore, for decreasing X, the ratio decreases steeply for H^+ ions,[20] whereas it increases and reaches values above 3 for He^{2+} ions.[21] For $X>1$, the ratio $\sigma(H_2)/\sigma(H)$ measured using H^+ (Ref. 20) and He^{2+} ions (Refs. 20, 22, and 23) shows the same general dependence on X as does the ratio for highly charged ions. It increases for X going from 1 to 100, and for higher X values, it reaches a constant value, which for H^+ ions is 2.3–2.4 (Refs. 24 and 25) and for He^{2+} ions is ~3.3 (Ref. 24).

Tuan and Gerjuoy[1] have discussed $\sigma(H_2)/\sigma(H)$ in the case of medium-to-high X and ions of low charge on the basis of the Oppenheimer-Brinkmann-Kramers theory. They mention a number of mechanisms that make the H_2 molecule act differently from two separate hydrogen atoms in the electron-capture process. For high energies, for example, they find that the capture amplitude is approximately proportional to the probability that the electron being captured has the velocity of the incoming ion, and that probability is higher in the more tightly bound H_2 molecle than in the hydrogen atom. For high-energy protons, they calculate that $\sigma(H_2)/\sigma(H) \sim 2.4$–2.8, depending on which molecular wave function is employed.

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