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Distortion effects in electron excitation of hydrogen atoms by impact of heavy ions

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Electron excitation from the fundamental state of hydrogen atoms by impact of bare ions is studied at intermediate and high collision velocities. Total cross sections for final np states by impact of protons, alpha particles, and He^+ ions are calculated using the symmetric eikonal approximation and compared with experimental data. This comparison supports the existence of distortion effects recently predicted by Bugacov and co-workers [Phys. Rev. A **47**, 1052 (1993)]. The validity of scaling laws is analyzed.

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I. INTRODUCTION

The existence of binding and polarization effects for ionization of atomic targets by impact of lighter bare nuclei was studied by Basbas *et al.* [1,2]. Using a simple model, they have estimated that the binding effect contributes subtractively as Z_P^3 to the total cross section (TCS) for asymmetric systems that satisfy $Z_P<Z_T$, with Z_P (Z_T) the projectile (target) nuclear charge. Transition probabilities and TCS computed with the first order of the Born series ($B1$) present a Z_P^2 dependence, so that the Z_P^3 behavior has been interpreted as an interference between the first- and second-order terms of the Born series [3]. The physical picture proposed by Basbas *et al.* to support this effect is that at low impact velocities ($v<v_e$, with v the collision velocity and v_e the electron orbital velocity in the initial state), collisions with small impact parameter dominate, increasing in this way the initial binding energy and decreasing in consequence the transition probability and TCS.

The binding effect was also studied for ionization in asymmetric systems with $Z_P>Z_T$, using the continuum distorted wave–eikonal initial state model (CDW-EIS) [4]. For these systems the electron emission is produced mainly at large internuclear distances [5–7]. The intensity of the projectile field affects the dynamics of the electron even at very large distances, so that the presence of the projectile must be taken into account in the description of the initial state. The electron travels bound to the target in a continuum state of the projectile before being ionized. At large distances this continuum is well represented using an eikonal approximation. In the CDW-EIS approximation the initial bound wave function is in this way distorted by an eikonal phase associated with the projectile-electron interaction. The representation of the electron in the simultaneous presence of the projectile and target fields plays a fundamental role in the description of the experimental TCS. However, it must be noted that for systems with $Z_P>Z_T$ we lose the idea of a *perturbative* increasing of the binding energy. The projectile strongly modifies the target potential. We prefer to invoke in this case a *distortion* effect.

Bugacov *et al.* [8] have introduced the idea of the possible existence of distortion effects in reactions of electron excitation to bound states of the target. These authors and Rodríguez and Salin [9] (see also Martín and Salin [10]) proved that when $Z_P>Z_T$ the TCS, for allowed transitions, are dominated by impact parameters $\rho>r_k$, with r_k the mean initial orbital radius. Moreover, the dominant impact parameter region shifts to larger values as Z_P increases [8,9]. Using a symmetric eikonal (SE) approximation [11], they observed a decreasing of the TCS with respect to the $B1$ predictions, just like for the ionization reaction [4]. Very recently it has been shown [10] that, for electron excitation to bound states, the development of the total cross sections as a series in powers of Z_P, associated each one of them with given orders of the perturbation series, is of doubtful validity.

We show in this work that recent experimental data [12], for excitation to np final states, supports the existence of the distortion effect in electron excitation to bound states of the target. Atomic units will be used throughout except where otherwise indicated.

II. THEORY

The SE approximation is used to represent the excitation of a hydrogenic target. The initial and final bound states φ_i and φ_f are distorted by multiplicative projectile-electron eikonal phases with correct outgoing and incoming boundary conditions, respectively. Assuming that the electrons of the projectile remain frozen during the collision and following Ramírez and Rivarola [14], the transition amplitude can be written as

$$\mathscr{A}_{if}^{-}(\boldsymbol{\rho})=(-i)\int_{-\infty}^{+\infty}dt\int d\mathbf{x}\ \varphi_f^*(\mathbf{x})\varphi_i(\mathbf{x})\exp[-i(\epsilon_i-\epsilon_f)t]\times(sv-\mathbf{s}\cdot\mathbf{v})^{-i\nu}\left[-\frac{\nabla^2}{2}-\nabla\ln\varphi_i\cdot\nabla+V_{ap}(\mathbf{s})-\frac{N}{s}\right]\times(sv+\mathbf{s}\cdot\mathbf{v})^{-i\nu}\quad. \tag{1}$$

In Eq. (1) an exponential factor which is irrelevant for the calculation of the impact parameter probabilities and TCS is

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neglected. In the same equation $\mathbf{x}$ ($\mathbf{s}$) represents the position of the electron with respect to the target (projectile) nucleus, ϵ_i (ϵ_f) is the initial (final) orbital energy, $\nu=(Z_P-N)/v$ with N the number of projectile electrons, and V_{ap} is the interaction potential between the electron of the target and the electrons of the projectile averaged over the spatial distribution of the latter electrons. When the projectile has one electron in a $1s$ state, as for the He^+ case, the static potential V_{ap} is

$$V_{ap}(\mathbf{s})=\frac{1}{s}[1-(1+Z_p\, s)e^{-2Z_p s}] \ , \tag{2}$$

and $N=1$.

A generating function

$$\psi(\beta,\boldsymbol{\mu},\mathbf{r})=\frac{{Z_T}^{3/2}}{\sqrt{\pi}}\ \exp[-\beta r]\ \exp[-i\boldsymbol{\mu}\cdot\mathbf{r}] \tag{3}$$

can be used to obtain the different $n,l,\pm m$ final states, so that

$$\varphi_{n,l,\pm m}(\mathbf{r})=D_{n,l,\pm m}\psi(\beta,\boldsymbol{\mu},\mathbf{r})\ |_{(\beta=Z_T/n\ ,\ \boldsymbol{\mu}=\mathbf{0})}\ . \tag{4}$$

In Eq. (4)

$$D_{n,l,\pm m}=C_{n,l}D^{(1)}_{n,l}D^{(2)}_{l,m}D^{(3)}_{\pm m}\ , \tag{5}$$

with

$$C_{n,l}=\frac{\left(\frac{iZ_T}{n}\right)^l}{n^2\ l!}\sqrt{(2l+1)\ \frac{(l+n)!}{(n-l-1)!}}\ , \tag{6}$$

$$D^{(1)}_{n,l}=\sum_{q=0}^{n-l-1}\binom{n-l-1}{q}\frac{(2Z_T/n)^q}{(2l+1+q)!}\left(\frac{\partial}{\partial\beta}\right)^q\ , \tag{7}$$

$$D^{(2)}_{l,m}=\sqrt{\frac{(l-m)!}{(l+m)!}}\sum_{k=0}^{\left[\frac{l-m}{2}\right]}\binom{l}{k}\frac{(2l-2k)!}{(l-2k-m)!}\times\left(\frac{\partial}{\partial\mu_z}\right)^{l-2k-m}\left(\frac{\partial}{\partial\beta}\right)^{2k}, \tag{8}$$

and where $[(l-m)/2]$ indicates the integer part of the fraction considered. Also in Eq. (5):

$$D^{(3)}_{\pm m}=(-1)^{\frac{1\pm1}{2}m}\left(\frac{\partial}{\partial\mu_x}\pm i\frac{\partial}{\partial\mu_y}\right)^m\ . \tag{9}$$

A generating transition amplitude is calculated with the function $\psi(\beta,\boldsymbol{\mu},\mathbf{r})$ and the corresponding transition amplitudes for the different final states are obtained applying the operator $D_{n,l,\pm m}$ on this generating amplitude.

III. RESULTS AND DISCUSSIONS

Reduced total cross section for target excitation to final np states (with n varying from 2 to 6),

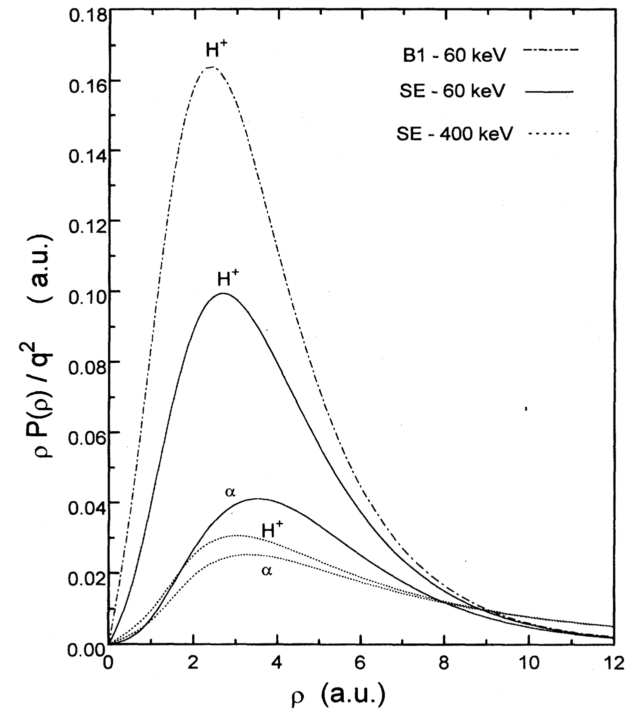

FIG. 1. SE-reduced impact parameter probability for excitation of H ($1s$) to the $2p$ final state by impact of protons and alpha particles at collision energies of 60 keV/amu (solid lines) and 400 keV/amu (dashed lines). $B1$ approximation for impact of protons at 60 keV (dashed and dotted line).

$$\sigma^*_{np}=\frac{\sigma_{np}}{q^2}=2\pi\int_0^\infty d\rho\ \ \frac{\rho\ \ |A^-_{1s,np}(\rho)|^2}{q^2}=2\pi\int_0^\infty d\rho\ \ P^*_{np}(\boldsymbol{\rho}), \tag{10}$$

are calculated for impact of H^+, He^{2+}, and He^+ ions on $H(1s)$ atoms. In Eq. (10), q is the net charge of the projectile. Results of the reduced impact parameter probability $P^*_{2p}(\boldsymbol{\rho})$ are presented in Fig. 1 for formation of a final state $H(2p)$ by impact of protons and alpha particles, illustrating the fact that for a fixed collision energy, an important decreasing of $P^*_{2p}(\boldsymbol{\rho})$ is obtained when the projectile charge increases. This indicates a remarkable deviation from the Z_P^2 predictions given by the $B1$ approximation. A similar behavior (not shown in the figure) is obtained for other np final states. The impact energies considered are 60 keV/amu and 400 keV/amu. The effect diminishes as the collision velocity increases. For forbidden transitions it has been shown that, in contrast to allowed transitions, the probabilities can increase more rapidly than Z_P^2 as Z_P increases [10]. Moreover, the maximum of $P^*_{2p}(\boldsymbol{\rho})$ shifts to larger values of ρ as Z_P increases and for all the cases studied is located at impact parameters $\rho>r_k$, as previously observed by Bugacov *et al.* [8]. For $Z_P>>1$, Rodríguez and Salin [9] have shown that the position of this maximum scales as $Z_P^{1/2}$. It also must be noted that the results for proton and alpha particle impact converge between them for large ρ, indicating thus the validity of the Z_P^2 dependence for large encounter collisions.

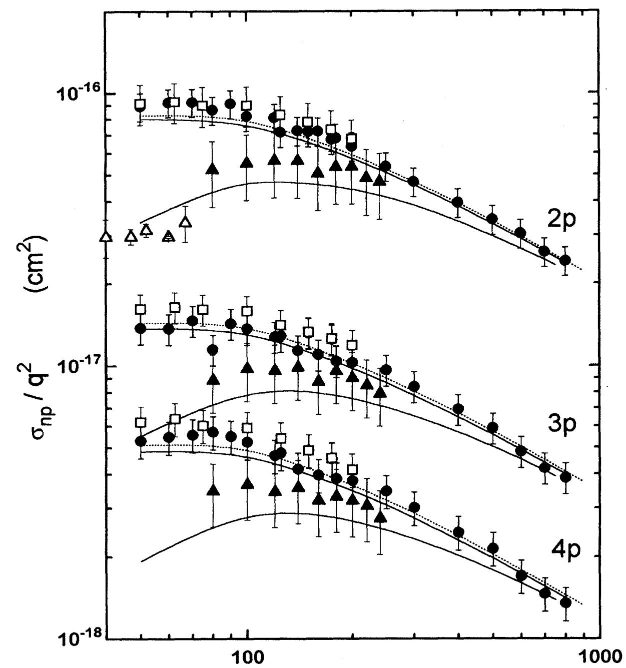

FIG. 2. SE-reduced cross section for excitation of H $(1s)$ to the $2p$, $3p$, and $4p$ final states by impact of: (solid lines) H^+ and He^{2+}; (dotted lines) He^+. Experimental data: (solid circles) H^+; (solid triangles) He^{2+}; (open squares) He^+, from Ref. [12]. Experimental data: (open triangles) He^{2+}, from Ref. [13].

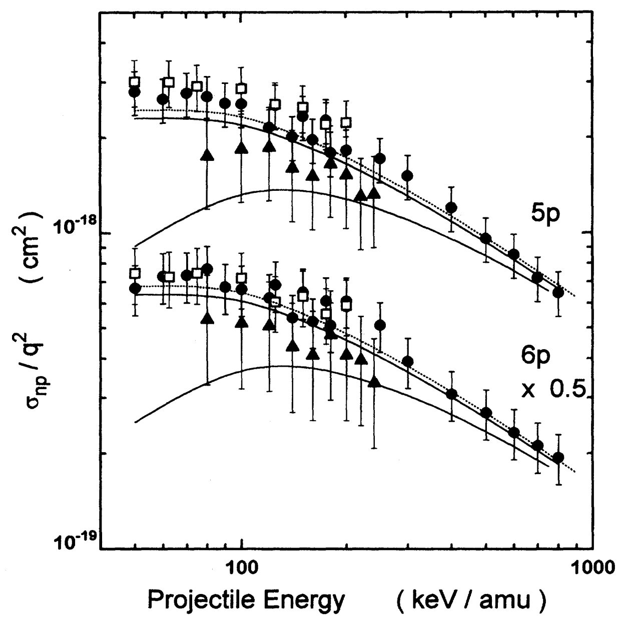

FIG. 3. SE-reduced cross section for excitation of H $(1s)$ to the $5p$ and $6p$ final states by impact of: (solid lines) H^+ and He^{2+}; (dotted lines) He^+. Experimental data: (solid circles) H^+; (solid triangles) He^{2+}; and (open squares) He^+, from Ref. [12].

The probability $P^*_{2p}(\boldsymbol{\rho})$ calculated within the $B1$ approximation at 60 keV/amu laboratory energy is also included in the figure to show the validity of $B1$ at large impact parameters.

The decreasing of $P^*_{np}(\boldsymbol{\rho})$ as Z_P increases provokes a similar behavior in the reduced cross sections σ^*_{np}, as can be seen in Figs. 2 and 3. In these figures, SE calculations are compared with recent experimental data. Distortion effects are observed at intermediate $(v \sim v_e)$ energies. The reduced cross sections converge at high collision velocities $(v >> v_e)$. At high impact energies the $B1$ approximation is expected to be valid. Cross sections σ^*_{np} for He^+ ions are close to the corresponding ones for protons over all the energy region considered.

Theoretical and experimental σ^*_{np} are in good agreement for all np final states analyzed. As the principal quantum number increases, the theoretical results tend to underestimate the experimental data at intermediate impact energies. It must be noted that the measurements have been normalized to the $B1$ approximation at high velocities, but cascade contributions were not explicitly taken into account at lower energies. The qualitative agreement between SE and experiments supports thus the existence of a distortion effect for np final states.

We also must note that, from a numerical analysis of our theoretical total cross sections, a scaling law is obtained:

$$\sigma_{np}^{scaled} = \frac{\sigma_{2p}}{(n-1)^k}, \quad k = 2.58 \ . \tag{11}$$

This law does not depend on the collision energy considered and is valid for impact of both protons and alpha particles. The value of k is determined with an uncertainty of less than 1%.

The scaling law (11) is in close numerical agreement with the corresponding one introduced by Detleffsen *et al.* [12]

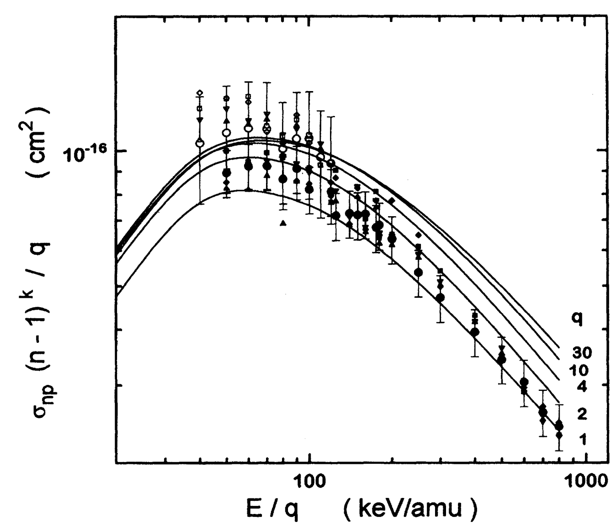

FIG. 4. Theoretical and experimental cross sections scaled by ordinate formula, for excitation of H $(1s)$ by impact of particles with $q = 1$, 2, 4, 10, and 30. Experimental data [10]: (solid circles) $2p$; (solid triangles up) $3p$; (solid triangles down) $4p$; (solid squares) $5p$, and (solid diamonds) $6p$ for protons. Corresponding open symbols are for alpha particles. The error bars are for measured points with $q = 1$ and 2 to the $2p$ final state.

for the case of protons, and supported by their experimental data. This law is given by

$$\sigma_{np}^{scaled}=\frac{\sigma_{np}\sigma_{2p}}{\sigma_{np}(800\ \text{keV})\sigma_{2p}^{max}}, \qquad (12)$$

where σ_{2p}^{max} denotes the maximum of the $2p$ cross section.

Janev and Presnyakov [15] derived a scaling law using a base set of three atomic states in a close coupling calculation. A dipole approximation was used to represent the interaction potential for the case of excitation of H atoms by impact of ions with net charge q, so that

$$\frac{\sigma_{np}^{scaled}}{q}=f\left(\frac{v^2}{q}\right), \qquad (13)$$

where f is a universal function. The validity of the dipole approximation has been tested for $Z_P \gg 1$ by Rodríguez and Salin ([9], and references therein) except for small impact parameters, at collision energies large enough to neglect electron capture.

In order to verify the validity of the scaling laws (11) and (13) for the energy range here considered, we represent in Fig. 4 a combination of both: $\sigma_{np}(n-1)^k/q$ versus E/q, with E the laboratory collision energy per nucleon. Theoretical and experimental scaled cross sections are compared. The theoretical predictions for alpha particles differ from the proton ones by approximately a constant multiplicative factor equal to 1.18. This difference remains at high impact velocities where the $B1$ approximation is expected to be valid. The experimental data supports the validity of the theoretical law given by Eq. (11) even when SE underestimates the measurements at intermediate energies. On the contrary, as pointed out by Detleffsen *et al.* [12], the comparison of the experimental data for protons and alpha particles shows that the function $f(v^2/q)$ differs slightly for both projectiles. This assertion is confirmed by our calculations, which present a similar profile of $f(v^2/q)$ for both projectiles but differ in absolute value by the multiplicative factor mentioned above. Calculations for bare projectiles with nuclear charges up to $Z_P=30$ for excitation to $2p$ final states are also included in the figure, showing that the scaled cross sections tend to converge quickly to the same curve as q increases. This behavior confirms previous predictions for $Z_P \gg 1$ [9].

IV. CONCLUSIONS

The excitation of hydrogen atoms from the fundamental state to final np states by impact of protons and helium ions is theoretically studied using the symmetric eikonal approximation. Special attention has been paid to distortion effects. Recent experimental data support the existence of these effects, predicted by the theory.

The validity of the scaling law given by Eq. (11) is confirmed by experiments for impact of protons and alpha particles. Theoretical calculations present the same qualitative behavior as the experimental data when the validity of the Janev and Presnyakov scaling law is analyzed.

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