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A new variationnal model for the excitation of Ar^{16+} ions impinging on neutral gaseous targets at intermediate impact energies.

B. Lasri
Laboratoire de Physique Théorique, Faculté des Sciences, Université Abou-Bekr-belkaïd,
B.P 119 Tlemcen (13000), Algérie
lasribo@yahoo.fr

M. Bouamoud
Laboratoire de Physique Théorique, Faculté des Sciences, Université Abou-Bekr-belkaïd,
B.P 119 Tlemcen (13000), Algérie
m_bouamoud@yahoo.fr

J. Hanssen
Laboratoire de Physique Moléculaire et des Collisions, Université de Metz, 1 Bd Arago, 57078, Cedex 3, Metz, France
jocelyn@univ-metz.fr

Abstract

A new variational impact parameter approach, based on the fractional form of the Schwinger principle, is successfully applied to study the direct excitation of the level (1s,2p) $^1P_1$ cross section of Ar^{16+} by various atoms of nuclear charges Zp (2≤ Z_T ≤ 54) which include neutral gaseous (He, N_2 , Ne, Ar, Kr, Xe) at 13.6 MeV/u. The convergence to steady results promised by this variationnal procedure is shown to be reasonable. Our theoretical predictions of the saturation effect of the excitation cross sections stay in good agreement with experimental data of Adoui et al. [1].

1. Introduction

One-electron collision processes at intermediate velocity have been intensively investigated during these last years. In particular, it has been pointed out that excitation cross sections of He-like and H-like ions colliding with neutral atoms tend to saturate when the atom nuclear charge increases (Wohrer *et a1*. 1986 [2], Xiang-Yuan Xu *et a1*. 1988 [3], Adoui *et al*. 1995 [1]). A better under-standing of this process is of main importance both for fundamental reasons: a recent molecular approach [4-6] proposes a new interpretation of the saturation effect, and for practical reasons: inner shell excitation (ionization) has been quoted as a possible trigger phenomenon for radiation damage in inert or biological media [7,8]. Especially one still wonders whether the K cross sections remain constant (as predicted by some models [9]) or go to zero, at asymptotically high values of the exciting charge [10].This phenomenon has been related theoretically to high-order effects introduced in the frame of a Schwinger principle (Brendlé *et al.* 1985 [11]; M. Bouamoud *et al*. 1988 [12] Lasri *et al.*1998,2004,2006 [13-16]), in a distorted wave formalism (Deco *et a1* 1986 [17], Reinhold and Miraglia 1987 [18]) or in an atomic coupled-state calculation (Reading *et al.* 1981 [19], Mukoyama and Lin 1989 [20]).

The Schwinger variational approach to the process of direct electronic excitation of atoms by impact of ions at intermediate velocities was shown to be very successful in predicting the saturation of cross sections when the projectile charge is increased what means that the excitation cross section tend to a finished limit when the Z_P charge of projectile increases in total contradiction with the dependence on Z_P^2 in the first Born approximation. This characteristic is illustrated by a good agreement between the theoretical results when the wave function is enough well represented and the experimental data of the excitation.

A variational approach, based on the Schwinger variational principle, was introduced a few years ago to study electronic excitation of atoms by ion impacts. This approach that has been implemented within the impact parameter framework successfully predicted the saturation of the excitation of ions by neutral projectiles at intermediate impact velocities (Brendlé *et al.* 1985 [11], Wohrer *et al*. 1986 [2]; M. Bouamoud *et al*. (1988) [12], Lasri *et al*. (2004,2006) [13-16]).

Like in our previous Fe^{24+}, Kr^{34+} , Xe^{52+} excitation studies, the process under consideration in these former references is the excitation of 13.6 MeV/u $Ar^{16+}(1s^2)$ helium-like ions colliding with various rare gases (He, N_2 , Ne, Ar, Kr, Xe) whose neutral atoms play the role of projectiles. At a given impact velocity, the saturation of excitation appears when one increases the projectile nuclear charge to a value comparable to (or greater than) the target nuclear charge. With a neutral projectile, the electron capture process is strongly inhibited because it is a second order process that can occur only if at least one electron is removed from the projectile. Therefore, the coupling between excitation and capture channels may be neglected, thus making the approach easy to implement to study excitation. An experimental study of the levels excitation cross sections 1s→2p of 13.6 MeV/u Ar^{16+} ions colliding with various target atoms ($2 \leq Z \leq 54$) have been measured by looking at the projectile emission with a high-resolution X-ray spectrometer were shown the saturation of the total excitation cross sections of each transition when the nuclear charge of targets is increased [1]. Our theoretical calculations have been performed using the first and the second Born approximation, the Schwinger-Born approximation and principally the Schwinger variational principle which are directly compared with experimental data of Adoui *et al*. [1].

2. Theoretical treatment

2.1. Excitation cross section

We feature briefly the treatment and computational details are given elsewhere [13-16].

In the impact parameter method and in collisions without rearrangement, the scattering wave functions $|\psi_\alpha^+(z)\rangle$ and $|\psi_\beta^-(z)\rangle$ are defined by the eikonal Lippmann-Schwinger equations:

$$|\psi_\alpha^+(z)\rangle = |\alpha(z)\rangle + \int_{-\infty}^{+\infty} dz'\, G_T^+(z-z')\, V(z')\, |\psi_\alpha^+(z)\rangle \tag{1a}$$

$$|\psi_\beta^-(z)\rangle = |\beta(z)\rangle + \int_{-\infty}^{+\infty} dz'\, G_T^-(z-z')\, V(z')\, |\psi_\beta^-(z)\rangle \tag{1b}$$

Where z is given by $\vec{R} = \vec{\rho} + \vec{z}$; $\vec{z} = \vec{\mathrm{v}}.t$ and $\vec{\rho}.\vec{\mathrm{v}} = 0$.

$|\alpha(z)\rangle$ and $|\beta(z)\rangle$ are the initial and final states of the target respectively and V is the projectile-target interaction and $G_T^{\pm}(z-z')$ are target Green's operators.

If we denote by $|\phi_\nu\rangle$ a target eigenstate associated with the eigenenergy ε_ν and by $|\nu(z)\rangle$ the corresponding solution of the eikonal Schrödinger equation for the unperturbed target. In the configuration space, with the origin of coordinates taken on the target nucleus, $\nu(z)$ may be written as:

$$\nu(z) = \phi_\nu(\vec{x}) \, \exp\left(-i\frac{\varepsilon_\nu}{\mathrm{v}} z\right) \tag{2}$$

$\vec{x}$ denote the nucleus-electron separation.

The well-known Schwinger amplitude for a genuine transition, i.e., for $\alpha \neq \beta$:

$$a_{\beta\alpha}(\vec{\rho}) = -\frac{i}{\mathrm{v}} \frac{(\beta|V|\psi_\alpha^+)\ (\psi_\beta^-|V|\alpha)}{(\psi_\beta^-|V - VG_T^+V|\psi_\alpha^+)} \tag{3}$$

where v is the collisions velocity and the notation $(\,|\,|\,)$ indicates integrations over electronic coordinates and over the coordinate z or (z, z') for matrix element V or VG_T^+V respectively.

The expression (3), that is nothing but an eikonal form of the Schwinger variational principle, is stationary for small errors on $|\psi_\alpha^+(z)\rangle$ and on $|\psi_\beta^-(z)\rangle$. Indeed, it is easy to show that $\delta a_{\beta\alpha}(\vec{\rho})$ is zero to first order in $|\delta\psi_\alpha^+(z)\rangle$ and $|\delta\psi_\beta^-(z)\rangle$. To calculate $a_{\beta\alpha}(\vec{\rho})$, one expands $|\psi_\alpha^+\rangle$ and $|\psi_\beta^-\rangle$ on truncated basis sets $\{|i\rangle\}$ and $\{|j\rangle\}$ respectively. The two basis sets are not necessarily identical but they must have the same finite dimension *N*. As in previous developments made [12-16], the two sets are simply made up of the ground state and of some excited states of the target with time-independent coefficients for the two expansions. Then, using the variational condition $\delta a_{\beta\alpha}(\vec{\rho}) = 0$, one gets two separate finite sets of linear equations for the coefficients of the expansions: one for $|\psi_\alpha^+(z)\rangle$ and one for $|\psi_\beta^-(z)\rangle$. Solving these sets of linear equations provide approximate solutions for $|\psi_\alpha^+(z)\rangle$ and $|\psi_\beta^-(z)\rangle$. Finally, replacing in eq.(3) $\left|\psi_\alpha^+(z)\right\rangle$ and $\left|\psi_\beta^-(z)\right\rangle$ by their approximate expressions leads to the following practical form of the transition amplitude:

$$a_{\beta\alpha}(\vec{\rho})=\left(-\frac{i}{\mathrm{v}}\right)\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\beta\,|V|\,i\right)\left(D^{-1}\right)_{ij}\left(j|V|\alpha\right) \quad (4)$$

$\left(D^{-1}\right)_{ij}$ is the element of the matrix D^{-1} between states $|i\rangle$ and $|j\rangle$ of the basis set. D^{-1} is the inverse of a matrix D whose elements between states $|i'\rangle$ and $|j'\rangle$ are:

$$D_{j'i'}=\left(j'\left|V-VG_T^+V\right|i'\right) \quad (5)$$

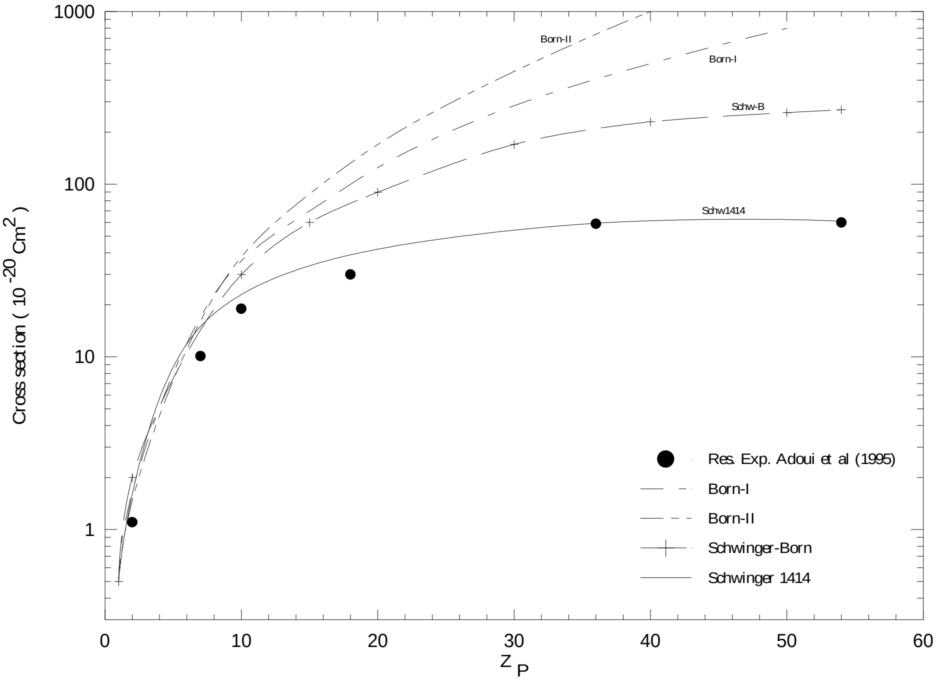
In what follows, we are dealing with the excitation of the target from its ground state to the first excited state. Hence, the basis set, which is made up of eigenstates of the target is restricted to the lowest target states, including the initial state $|\alpha\rangle$ and the final state $|\beta\rangle$. Then, tow matrix elements have to be calculated; one first Born-type matrix elements $\left(j|V|i\right)$ and one Second Born-type matrix elements $\left(j\left|VG_T^+V\right|i\right)$.In the evaluation of $\left(j\left|VG_T^+V\right|i\right)$, one has to perform a sum over an infinite set of intermediate states $|\nu\rangle$. A first step toward the exact evaluation of $\left(j\left|VG_T^+V\right|i\right)$ has been accomplished by taking into account the contribution of the whole discrete spectrum of the set $\{|\nu\rangle\}$ [11,12]. The contribution of the continuum has been taken into account using an analytical continuation which consists to evaluate the part close to ionisation threshold [13-16].

2. Results and discussions

In fact, the process under consideration in these former references is the excitation of 13.6 MeV/u $Ar^{16+}(1s^2)$ helium-like ions colliding with various rare gases whose neutral atoms play the role of projectiles. At a given impact velocity, the saturation of excitation appears when one increases the projectile nuclear charge to a value comparable to (or greater than) the target nuclear charge. With a neutral projectile, the electron capture process is strongly inhibited because it is a second order process that can occur only if at least one electron is removed from the projectile. Therefore, the coupling between excitation and capture channels may be neglected, thus making the approach easy to implement to study excitation. Further, neglecting this coupling presents a noticeable advantage: it enables us to make predictions for any projectile nuclear charge once calculations have been carried out for one projectile charge (Brendlé *et al.* 1985 [11]). However, when the excitation is due to a genuine ion, the capture process cannot be neglected for impact velocities lower than the electron velocity on the initial orbital (Gayet 1983 [17]). Therefore, one expects the application of the variational approach to be limited to a domain of impact energies where the capture process is less important than all other processes. Experimental study of this excitation process have been measured by looking at the projectile emission with a high-resolution X-ray spectrometer were shown the saturation of the total excitation cross sections of each transition when the nuclear charge of targets is increased [11]. The target propagator G_T^+ has been expanded on the whole discrete spectrum of the target [11,12]. In a new implementation of the formalism the contribution of the continuum has been taken into account using an analytical continuation which consists to evaluate the part close to ionisation threshold [13-16].

Initially, the excitation of $Ar^{16+}(1s^2)$ to the levels (1s,*nl*) was made with a set of 5 orbitals: $B_1 = B_2 =\{1s, ns, np_0, np_{+1}, np_{-1}\}$ where n = 2, 3. The procedure was called the Schwinger5-5 approximation. In the present study, and in order to refine this varaiational procedure, the calculations are performed and the wave functions $\left|\psi_\alpha^+\right\rangle$ and $\left|\psi_\beta^-\right\rangle$ are expended on fourteen-states basis set as $B_1 = B_2 =\{1s , 2s , 2p_0 , 2p_1 , 2p_{-1} ,3s , 3p_0, 3p_1, 3p_{-1}, 3d_0, 3d_1, 3d_{-1}, 3d_2, 3d_{-2}\}$ which is called Schwinger14-14.

The total excitation cross section of the level (1s,2p) of $Ar^{16+}(1s^2)$ by various atoms of nuclear charges Zp, are plotted as function of Zp. The present results are nearly close to the previous Schw55 results up to a nuclear charge of 17. Beyond this charge, the saturation effect is more pronounced owing to the coupling between the ionisation and excitation channels which becomes important when the projectile and the target charges are comparable. All obtained results stay in good agreement with experimental data of Adoui *et al*. [1].



Excitation Cross sections of the level (1s , 2p) of Ar^{16+} ($1s^2$) impinging at an energy 13,6 MeV/u on various target of nuclear charge Z_P indicated in the abscise. The experimental errors do not reach 1%.

Conclusion

Our new theoretical approach show a reasonable convergence of the variational procedure when one increases the number of target states on which the scattering wave functions are expended. As expected, good results are obtained when the basis set is restricted to the initial state, to the final state and to other states, whose energy is degenerated with the final state energy (14 states). Although it is an improvement, the inclusion of the whole discrete and continuum spectrum in the expansion of the propagator of the second Born-like matrix elements results in slight changes in the total cross section. Good results are obtained when the wave functions $\left|\psi^{+}(z)\right\rangle$ and $\left|\psi^{-}(z)\right\rangle$ are expanded on the 14 states basis set.

Finally, the present-day variational procedure appears to be a powerful tool to investigate the excitation process in atomic collisions at intermediate impact velocities.

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