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Application of the Schwinger variational principle to the excitation of Kr^{34+} by impacts of bare atoms at intermediate energies

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Abstract

In the impact parameter formalism, variational approach based on the fractional form of Schwinger's variational principle is applied to evaluate the total direct excitation cross sections to n=2, n=3 and 2p+3 of the helium like ion Kr^{34+} by impact of various atoms Z_p charges including those of rare gases (C, Si, Ar, Cu, Zr) at an energy equal to 33.9 $MeV.u^{-1}$. Our theoretical predictions of the saturation for total excitation cross sections, obtained by this new variational approach are compared with the experimental results of Chabot et al.

Key words: *Atomic collision; Schwinger variational principle; Atomic excitation; Excitation cross sections.*

Introduction

The excitation process at intermediate speeds has been extensively examined in recent years. Specifically, it was reported that the excitation cross sections of helium like ion by impact of neutral atoms, tend to saturate when the atomic nucleus number increases. This phenomenon was predicted theoretically in the Schwinger's variational principle formalism [1] [2]. We present here the development of this new approach based on the Schwinger variational principle.

The scattering amplitude variational, established in the impact parameter formalism, is used to study the electronic excitation of highly charged ions by impact of ions at intermediate speeds [3].

We applied this method to determine, In addition, the excitation total cross sections of the helium like ion Kr^{34+} ($1s^2$) colliding with neutral atoms of various charges ranging from 1 to 56 including those of rare gases (C, Si, Ar, Cu, Zr) at intermediate speeds (35a.u) This corresponds at 33.9$Mev.u^{-1}$ energy. We subsequently compared the various theoretical predictions obtained by this new variational approach with the experimental results of Chabot et al [4].

In recent decades, variational methods can be a tool for investigating that takes relays perturbative treatment in the study of atomic collisions. These variational methods can be grouped into two categories: those based on the Schrödinger equation {method Hulthén Khon-[5-7], variational method called matrix-R (R-matrix) [8-10].} and those based on the Lippmann-Schwinger equations {variational method, Schwinger in person that presented in his lectures at Harvard University and was published in 1947 [11].}.

The greatest importance in the collision problem is the determination of the wave function which represents the wave scattering because it contains all information on system state. To resolve this problem, some approximations have been widely used in recent decades: The Born approximation [12], the method of VPS (Vaishtein, Presnyakov and Sobelman) [13], the eikonal approximation « Impact Parameter Method » and the Glauber approximation [14] [15].

Several approaches have been formulated to give adequate models for studying the collisions processes: model of Cheshire and Sullivan established in 1967 [16], the potential model of second order proposed by Coleman in 1972 and Brensden [17], the pseudo-states model used for the first time by Reading and his collaborators in 1976 [18], then taken by Fitchard and his collaborators in 1977[19].

Owing to the insufficiency of these methods and difficulties of implementation methods based on the perturbation theory, we are interested in this new approach excluding a perturbative treatment [20], and based on a variational theory. This approach is called the Schwinger variational principle.

Theoretical treatment:

We are interested in an approach called Schwinger variational principle based on the Lippmann-Schwinger equations:

$$\left|\Psi_\alpha^+\right\rangle = |\alpha\rangle + G_c^+ V_c \left|\Psi_\alpha^+\right\rangle \quad (1a)$$

$$\left\langle\Psi_\beta^-\right| = \langle\beta| + \left\langle\Psi_\beta^-\right| G_c^- V_c \quad (1b)$$

where: $\left|\Psi_\alpha^+\right\rangle$, $\left\langle\Psi_\beta^-\right|$, Eigen-states of total Hamiltonian of the system H respectively satisfying to the input and output waves conditions knowing that the Hamiltonian system is decomposed as follows:

$$H = H_c + V_c \quad (2)$$

where: H is the Hamiltonian of no-interacting particles and V_c interaction potential between particles in this way and G_c^+ the Green operator defined by [21]:

$$G_c^+ = \lim_{\varepsilon \to 0^+} \left(E - H_c + i\varepsilon\right)^{-1} \quad (3)$$

In order to obtain a stationary form of the transition amplitude $T_{\beta\alpha}$ relative to small variations arbitrary around their exact values:

$$T_{\beta\alpha} = \left\langle\beta\right| V_c \left|\Psi_\alpha^+\right\rangle \quad (4a)$$

$$T_{\beta\alpha} = \left\langle\Psi_\beta^-\right| V_c \left|\alpha\right\rangle \quad (4b)$$

$$T_{\beta\alpha} = \left\langle\Psi_\beta^-\right| V_c - V_c G_c^+ V_c \left|\Psi_\alpha^+\right\rangle \quad (4c)$$

Since the scattering states $\left|\Psi_\alpha^+\right\rangle$ and $\left\langle\Psi_\beta^-\right|$ cannot be exactly known, we will take as test states the approached vectors $\left|\tilde{\Psi}_\alpha^+\right\rangle$ and $\left\langle\tilde{\Psi}_\beta^-\right|$ such as:

$$\begin{cases} \left|\tilde{\Psi}_\alpha^+\right\rangle = \left|\Psi_\alpha^+\right\rangle + \left|\delta\Psi_\alpha^+\right\rangle & (a) \\ \left\langle\tilde{\Psi}_\beta^-\right| = \left\langle\Psi_\beta^-\right| + \left\langle\delta\Psi_\beta^-\right| & (b) \end{cases} \quad (5)$$

that we develop in a finite dimensional vector subspace (N), whether:

$$\begin{cases} \left|\tilde{\Psi}_\alpha^+\right\rangle = \sum_{i=1}^{N} \tilde{a}_i \left|i\right\rangle & (a) \\ \left\langle\tilde{\Psi}_\beta^-\right| = \sum_{i=1}^{N} \tilde{b}_j^* \left\langle j\right| & (b) \end{cases} \quad (6)$$

By expressing the fractional transition amplitude based on these test vectors, we thus obtain the approached transition amplitude $\tilde{T}_{\beta\alpha}$:

$$\tilde{T}_{\beta\alpha} = \sum_{i=1}^{N}\sum_{j=1}^{N} \langle\beta| V_c |i\rangle \left(D^{-1}\right)_{ij} \langle j| V_c |\alpha\rangle \quad (7)$$

where $\left(D^{-1}\right)_{ij}$ is the inverse of the matrix $D_{ji} = \langle j|V_c - V_c G_c^+ V_c|i\rangle$.

As the principal contribution to the transition considered occurs at small angles (<10^{-3}radian for the collision $H^+ \rightarrow H$), considering that the projectile describes a rectilinear trajectory and therefore treat this problem in the eikonal approximation [14] [15].

We consider a collision between a projectile of mass M_p, of charge Z_p and a target of mass M_T, of charge Z_T. the inter-nuclear separation is given by:

$$\begin{cases} \vec{R} = \vec{\rho} + \vec{Z} & (a) \\ \vec{Z} = \vec{v}.t & (b) \\ \vec{\rho}.\vec{v} = 0 & (c) \end{cases} \quad (8)$$

where $\vec{\rho}$ is the impact parameter, $\vec{v}$ relative velocity of projectile, $\vec{R}$ defines inter-nuclear distance.

t: is the time taken arbitrarily equal to zero when $\vec{R} = \vec{\rho}$, $\vec{Z}$ is the projection of $\vec{R}$ on the path of the projectile.

The Schrödinger's time-dependent equation $i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle$ [22], is written in another form said eikonal scattering equation deduced by differentiation with respect to Z rather than t and using expression (8b) $\vec{Z} = \vec{v}t$. We will then have:

$$\left(-iv\frac{\partial}{\partial Z} + H_T + V_c\right)\left|\Psi(Z)\right\rangle = 0 \quad (9)$$

The resolution of this last equation implicates us to solve the following Schrödinger's eikonal equation of the target:

$$\left(-iv\frac{\partial}{\partial Z} + H_T\right)\left|k(Z)\right\rangle = 0 \quad (10)$$

The long range projectile-target coulomb interaction between the projectile and the target $V_{int} = \left(Z_P(Z_T - 1)\right)/R$ must be added to the Hamiltonian H_T equation (10), to obtain the eikonale Eigen-states of the target, multiplied by a phase factor nominated «of Coulomb»: $i\left(Z_P(Z_T - 1)/v\right)\ln(vR - vZ)$ with $R - Z = \rho$.

Therefore the transition amplitude is also multiplied by a phase factor which depends on impact parameter $\vec{\rho}$ that goes be overlooked in the calculation of the cross section and reintroduced thereafter in the calculation of the differential cross section.

The scattering states $\left|\Psi_\alpha^+(Z)\right\rangle$ and $\left\langle\Psi_\beta^-(Z)\right|$, solutions of the Schrödinger equation in the formalism of the impact parameter, are then determined within the eikonal approximation by the Lippmann-Schwinger equations [23]:

$$\left|\Psi_\alpha^+(Z)\right\rangle = \left|\alpha(Z)\right\rangle + \int_{-\infty}^{+\infty} dZ' G_T^+(Z - Z') V(Z') \left|\Psi_\alpha^+(Z')\right\rangle \quad (11a)$$

$$\left\langle\Psi_\beta^-(Z)\right| = \left\langle\beta(Z)\right| + \int_{-\infty}^{+\infty} dZ' G_T^-(Z - Z') V(Z') \left\langle\Psi_\beta^-(Z')\right| \quad (11b)$$

Adopting the notation (| |) indicating the integration over the electronic coordinates as well as over Z the expression of the transition amplitude for the impact parameter $\vec{\rho}$ may be written for $\alpha \neq \beta$, as:

$$a_{\beta\alpha}(\vec{\rho}) = -\frac{i}{v} \frac{\left(\beta|V|\Psi_\alpha^+\right)\left(\Psi_\beta^-|V|\alpha\right)}{\left(\Psi_\beta^-\left|V - VG_T^+V\right|\Psi_\alpha^+\right)} \quad (12)$$

In a manner similar to quantum treatment, the expression (12) for the transition amplitude $a_{\beta\alpha}(\vec{\rho})$ is one hand stationary relative to small variations of the scattering states $\left|\Psi_\alpha^+\right\rangle$ and $\left\langle\Psi_\beta^-\right|$ round their exact values and leads in other hand, to the following approximate form:

$$\tilde{a}_{\beta\alpha}(\vec{\rho}) = \left(-\frac{i}{v}\right)\sum_{i=1}^{N}\sum_{j=1}^{N} (\beta|V|i)\left(D^{-1}\right)_{ij} (j|V|\alpha) \quad (13)$$

The eikonal quantum transition amplitude can be expressed as:

$$T_{\beta\alpha}(\vec{\eta}) = i\,\mathrm{v}\int \mathrm{d}\vec{\rho}\; e^{i\vec{\eta}.\vec{\rho}}\,\rho^{2i\frac{Z_p(Z_T-1)}{\mathrm{v}}}\; a_{\beta\alpha}(\vec{\rho}) \qquad (14)$$

In this last expression the potential inter-aggregate contribution $\rho^{2i\frac{Z_p(Z_T-1)}{\mathrm{v}}}$ depending on the impact parameter, has finally been reintroduced in the total excitation cross section:

$$\sigma_{\beta\alpha} = 2\pi\int_0^{+\infty} d\rho \quad \rho \quad \left| a_{\beta\alpha}(\vec{\rho}) \right|^2 \qquad (15)$$

In the evaluation of the approached variational transition amplitude $\tilde{a}_{\beta\alpha}(\vec{\rho})$, mainly two kinds of matrix elements are calculated:

• The $\left(i\left|V\right|j\right)$ Matrix element (Born- I):

$$(i|V|j) = \int_{-\infty}^{+\infty} dz\; e^{i\frac{\varepsilon_i-\varepsilon_j}{\mathrm{v}}z}\, W_{ij}(\vec{\rho},z) \qquad (16)$$

where [24]:

$$W_{ij}(\vec{\rho},z) = \int d\vec{x}\;\; \varphi_i^*(\vec{x})\, V\left(\vec{R},\vec{x}\right)\; \varphi_j(\vec{x}) \qquad (17)$$

•The $\left(i\left|VG_T^+V\right|j\right)$ Matrix element (Born-II):

$$\left(i\left|VG_T^+V\right|j\right) = \left(-\frac{i}{\mathrm{v}}\right)\left[\sum + \int\right]\int_{-\infty}^{+\infty} dz\; e^{i\frac{\varepsilon_i-\varepsilon_v}{\mathrm{v}}z}\, W_{iv}(\rho,z)\int_{-\infty}^{z} dz'\; e^{i\frac{\varepsilon_v-\varepsilon_j}{\mathrm{v}}z'}\, W_{vj}(\rho,z') \qquad (18)$$

The contribution of the continuum states near the ionization threshold could be evaluated by an extension of analytical calculation of first term of this expression:

$$\left(i\left|V\,G_T^+V\right|j\right) = \left(-\frac{i}{\mathrm{v}}\right)\sum_{l=0}^{+\infty}\left[\sum_{v=l+1}^{+\infty}\mathscr{H}_{ij}^{(v,l)} + \int_0^{+\infty} dk\;\mathscr{H}_{ij}^{(k,l)}\right] \qquad (19)$$

by substituting υ by Z_T/ik.

Now, the contribution of continuum states to the elements of Born-II $\left(i\left|VG_T^+V\right|j\right)$ can be evaluated in an interval $[0,k_0]$, thus, the sum along the domain of the continuum, where the analytic continuation is still valid, can be approximated by:

$$\int_0^{k_0} dk\;\mathscr{H}_{ij}^{(k,l,m)} \approx \frac{A}{{Z_T}^2}\frac{{k_0}^2}{2} \qquad (20)$$

In our study, the adapted model to examine the excitation process of the ion Kr^{34+} by impingement of neutral atoms is based on the fractional form of the Schwinger variational principle illustrated previously [25]. Moreover, the base on which the wave functions $\left|\Psi_\alpha^+\right\rangle$ and $\left\langle\Psi_\beta^-\right|$ have been developed, is enlarged from 5 states (1s, ns, np_0, np_{+1}, np_{-1}) denoted Schw 55 to 10 states (1s, 3s, $3p_0$, $3p_{+1}$, $3p_{-1}$, $3d_0$, $3d_{+1}$, $3d_{-1}$, $3d_{+2}$, $3d_2$) denoted Schw 1010 order to arrive at a better representation of the propagator G_T^+ that surely leads us to a more precise description and fairly complete of that process. All the results obtained (the total cross sections calculated from these approximations) were compared with experimental data Chabot et al [4].

To describe the excitation of helium-like Kr^{34+} we assume that the passive electron behaves like a screen with respect to each other, reducing load on of the kernel at Z_T = 35 . Taking account of simplifications introduced by the scaling laws, all calculations concerning the total cross sections of excitation has been made for a collision proton-hydrogen atom but at a reduced velocity u=v/Z_T and for a reduced impact parameter $\gamma = Z_T\rho$.

Convergence test and discussion:

In our treatment, five theoretical approaches were compared:

• The first Born approximation (Born-I).
• The second Born approximation (Born-II).
• Schwinger-Born-approximation (Schw-B).
• Schwinger55 approximation (Schw55).
• Schwinger1010 approximation (Schw1010).

For the excitation to the level n=2 (Figure 3), the base series used will include five following states {1s, 2s, $2p_0$, $2p_{+1}$, $2p_{-1}$}. All intermediate states need to be included In order to adequately describe the excitation to the level n=3.This has been pushing us to expand the basis on which the propagator is developed in order to reach a better representation of the wave function thus, the base series $\{|i\rangle\}$ and $\{|j\rangle\}$ is expanded from 5 to 10 states {1s, 3s, $3p_0$, $3p_{+1}$, $3p_{-1}$, $3d_0$, $3d_{+1}$, $3d_{-1}$, $3d_{+2}$, $3d_{-2}$}. Concerning excitation to the states 2p+3, we have added the total excitation cross sections to the 2p state of the level n=2 to those of the level n=3.

Our theoretical treatment has been successfully applied to the excitation of $Kr^{34+}(1s^2)$ interacting with various atoms at the energy 33.9MeV.u^{-1}.Since targets are neutral atoms; no capture process can intervene during the collision. The total experimental excitation cross sections to the final states 2s, n=2 and 2p+3 [4] of 33.9MeV.u^{-1} Kr^{34+} ions are shown only for C, Si, Ar, Cu and Zr atoms in Figs (1, 3, 8). The corresponding theoretical cross sections of the first Born approximation, the second Born approximation, Schwinger-Born-approximation, Schwinger 55 and Schwinger1010 are also shown in these figures.

The present results thus show that the Schwinger variational principle predicts that the total excitation cross section is characterized by a low variation from Z_p = 7 when Z_p increases. This is called a saturation effect. On the other hand, the results of Schwinger-Born approximation (Schw-B) do not represent well the saturation, particularly for excitation to the 2p state; unlike to the 3p state where they tend to get saturate for large values of Z_p. This inability to reproduce the phenomenon of saturation for excitation to the 2p state is due to a strong coupling with the 2s state.

The good agreement between our results (Schw55, Schw1010) with experimental measurements for large values of Z_p (Z_p =40) result from the fact that for Z_p >7 the total excitation cross sections are not very sensitive to variations of the target atomic number.

• By observing the various results in Figures 1, 3 and 8, the following comments also need to be made:

For the Kr^{34+}→ C System, all calculations give similar values that remain in good agreement with the

experimental results. The high asymmetry of the Born approximation show us that the treatment is valid solely for relatively low speeds of collision of the system ($Z_T / Z_p = 0.17$).

• By considering of systems with heavier targets, divergences more and more pronounced of the Born theory appear. By against, our predictions given by a new variational procedure remain in perfect agreement with experiment.

The most remarkable result is the experimental proof of the saturation excitation cross sections obtained by the theoretical predictions of the variational method. It can be seen that even in these cases the experimental cross sections deviate and remain much below the first Born-approximation and same for the various theoretical predictions: Schwinger 55 (Schw55) and Schwinger1010 (Schw1010). The values provided by Born-II are even further above Z_p=7 where perturbation conditions are checked.

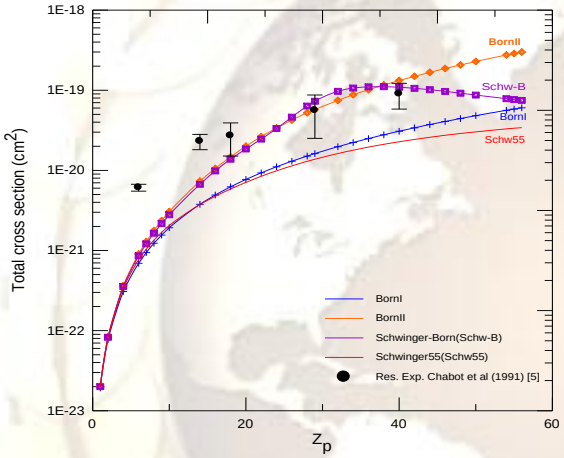

Figure 1: Excitation total cross section to the 2s state of the ion Kr $^{34+}$ ($1s^2$) at the energy 33.9 MeV.u^{-1} as function of the target atomic number.

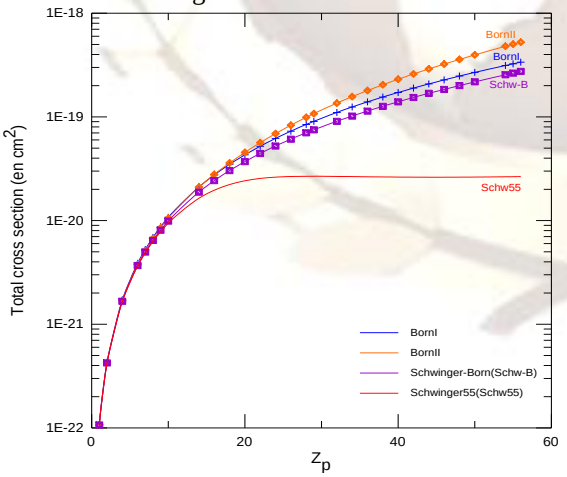

Figure 2: Excitation total cross section to the 2p state of the ion Kr $^{34+}$ ($1s^2$) at the energy 33.9 MeV.u^{-1} as function of the target atomic number.

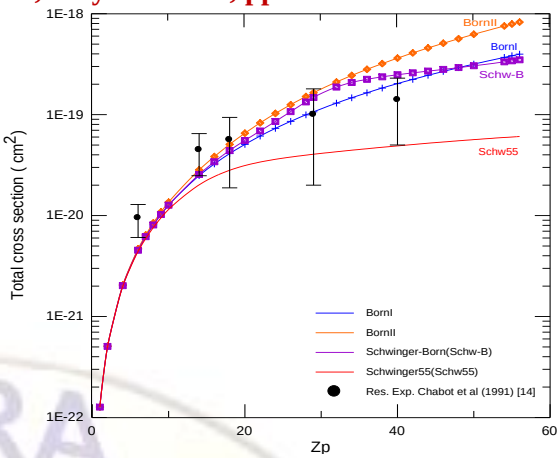

Figure 3: Excitation total cross section to the level n=2 of the ion Kr $^{34+}$ ($1s^2$) at the energy 33.9 MeV.u^{-1} as function of the target atomic number.

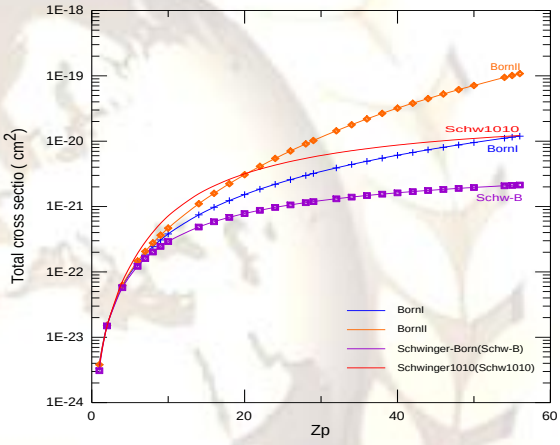

Figure 4: Excitation total cross section to the 3s state of the ion Kr $^{34+}$ ($1s^2$) at the energy 33.9 MeV.u^{-1} as function of the target atomic number.

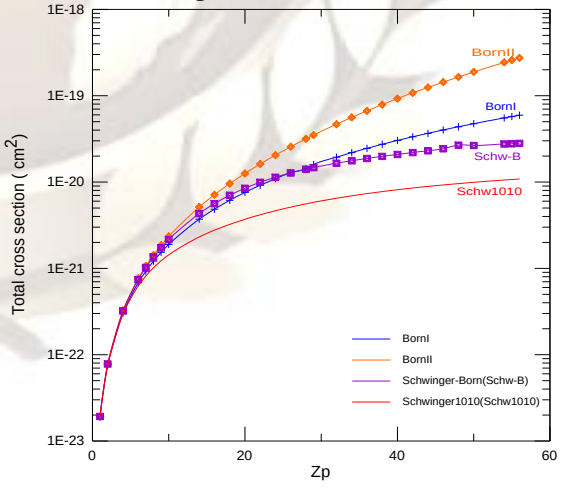

Figure 5: Excitation total cross section to the 3p state of the ion Kr $^{34+}$ ($1s^2$) at the energy 33.9 MeV.u^{-1} as function of the target atomic number.

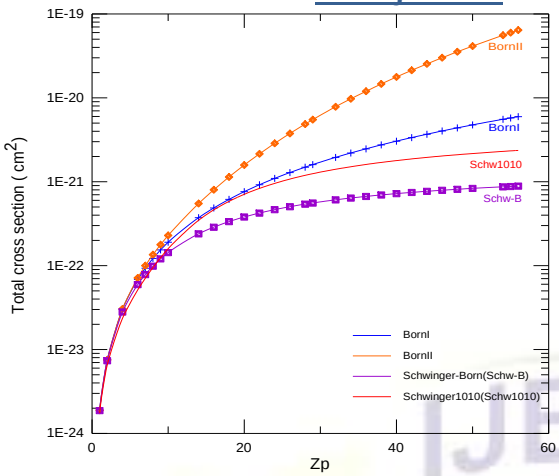

Figure6: Excitation total cross section to the 3d state of the ion Kr $^{34+}$ ($1s^2$) at the energy 33.9 MeV.u^{-1} as function of the target atomic number.

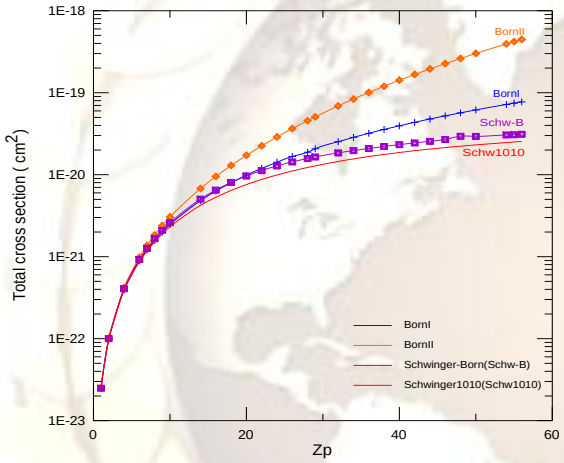

Figure 7: Excitation total cross section to the level n=3 of the ion Kr $^{34+}$ ($1s^2$) at the energy 33.9 MeV.u^{-1} as function of the target atomic number.

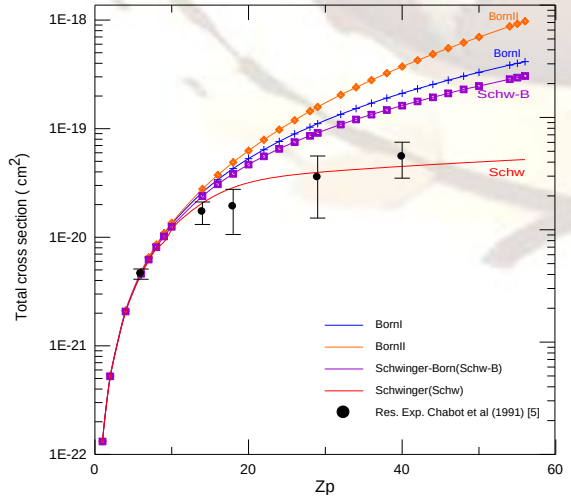

Figure 8: Excitation total cross section to the states 2p+3 of the ion Kr^{34+} ($1s^2$) at the energy 33.9 MeV.u^{-1} as function of the target atomic number.

Conclusion:

In conclusion, our objective was to give a performance calculation tool to determine the total excitation cross sections in multi-charged ion-atom interactions at intermediate speeds and to see the discrete spectrum contribution well as that of continuum in the total excitation cross sections.

The method based on the fractional form of Schwinger's variational principle allows a systematic study of total excitation cross section as a function of the projectile atomic number Z_p=7 well as the prediction with success of this phenomenon When the projectile atomic number increases.

Finally, the variational methods based on Schwinger's variational principle thus can be a powerful tool for investigating and takes the relays of perturbative treatments in the study of atomic collisions at intermediate speeds.

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