

APPLICATION OF THE SCHWINGER PRINCIPLE FOR EXCITATION PROCESSES IN THE $H^+ + Be^{3+}$ COLLISION AT INTERMEDIATE ENERGIES

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RESUME:

Dans le formalisme du paramètre d'impact, l'approche variationnelle basée sur la forme fractionnaire du principe variationnel de Schwinger est appliquée pour l'évaluation des sections efficaces totales d'excitation directe des ions hydrogénoides béryllium (Be^{3+}) par impact de protons (H^+) (L'ion béryllium étant une des impuretés principales dans les plasmas de Tokamak). L'étude a été réalisée dans la gamme d'énergie de 40 keV à 4 MeV incluant le domaine des énergies intermédiaires (autour de 100 keV). Nos prédictions théoriques sont en bon accord avec les divers calculs théoriques disponibles comme ceux des méthodes des équations couplées.

Mots Clés : Principe variationnel de Schwinger, excitation atomique, section efficace.

ملخص:

إن الطرق النظرية المعتمد عليها في الدراسات الخاصة بالتصادمات الذرية و المرتكزة أساساً على المبدأ التغيري لشونينغر تعتبر ركيزة من الركائز الحديثة المعول عليها في حساب المقاطع الفعالة للإثارة المباشرة للذرات عن طريق الأيونات في المجال الطاقوي المتوسط و التي بإمكانها إعطاء نتائج جذ مشجعة خاصة فيما يتعلق بالايون الشبه هيدروجيني Be^{3+} في حالة تصادمه مع البروتون المرمز إليه غالباً بـ H^+ . نعرض في طيات هذا المقال طريقة جديدة مرتكزة أساساً في شكلها العام على شكل كسري للمبدأ التغيري لشونينغر. النتائج و النبوءات النظرية في توافق جيد إن لم نقل تام مع المعطيات التجريبية الخاصة بإثارة المستويات الجزئية $(1s, 2s)$, $(1s, 2p)$, فتم الكلية $(n=3, n=2)$ الخاصة بـ Be^{3+} (الذي يعتبر واحدة من الشوائب في البلازما Tokamak) في المجال الطاقوي المحدد من 40keV إلى 4MeV والذي يشمل المجال الطاقوي المتوسط.

الكلمات المفتاحية: المبدأ التغيري لشونينغر، الإثارة الذرية، المقاطع الفعالة.

I. INTRODUCTION:

During the two last decades, a considerable amount of theoretical works had been devoted to the study and the understanding of the collision between different atoms and especially the excitation occurring in the multicharged ion-atom collisions. In particular, the collisions with one active electron have been often studied with attention. These collision processes, as charge-exchange, ionization and excitation, are important essentially for the astrophysical environments, the plasma physics and the radiobiology as the cell dead induced by collision. An important difficulty arises in the description of these collisional processes as in the range of intermediate impact energies. Generally, the excitation process at intermediate impact energies is described by two theoretical methods using the perturbation methods or the close coupling calculations.

In fact, these two methods are very efficient for the high impact energies with a perturbation method and for the low impact energies with close coupling calculations. On the other hand, both methods do not describe with accuracy the intermediate impact energy range. These various fields of collision energies are defined from the capture process, especially the intermediate energy range is situated near its maximum [1]. Brendlé, Gayet and Bouamoud [2-7] have developed a new theoretical approach based on the Schwinger variational principle excluding a perturbative treatment. In fact, Luchesse et al (1980), [8], had already employed this method successfully for collisions by electron impact, then by Brendlé and Gayet [2] for the excitation process by ion impact. From 1988, the Schwinger variational procedure which was applied with great interest by Bouamoud [3-7] and then by Lasri et al [5-7] appears as a powerful tool to study the excitation processes especially for the hydrogen-like ions. One important successful of this approach has been the prediction of the saturation effect of cross sections when the projectile charge increases [4,9].

In the present work, we determine using this variational approach, the direct excitation of beryllium ions Be^{3+} by proton impact with energies from 40 keV to 4 MeV. We compare our calculations with those of Ermolaev (1994, 1996), [10,11], obtained in a Two Center Atomic Orbital (TCAO) expansion.

This manuscript is organized as follows: in section II, we present a brief theoretical recall of the transition amplitude form applicable to the excitation process. In section III, our calculations are compared with the TCAO calculations. Conclusions are drawn in section IV.

II. THEORETICAL TREATMENT:

In Lasri et al. [7], more details on the theoretical treatment and the calculations are given. In the impact parameter method and in collisions without rearrangement, the scattering initial and final wave functions $\psi_a^+(z)$ and $\psi_b^-(z)$, respectively, are defined by the eikonal Lippmann-Schwinger equations:

$$\psi_a^+(z) = \alpha(z) + \int_{-\infty}^{+\infty} dz' G_r^+(z-z') V(z') \psi_a^+(z) \quad (1a)$$

$$\psi_b^-(z) = \beta(z) + \int_{-\infty}^{+\infty} dz' G_r^-(z-z') V(z') \psi_b^-(z) \quad (1b)$$

With the inter-nuclear distance $\vec{R} = \vec{\rho} + \vec{z}$; $\vec{z} = \vec{v} \cdot \vec{t}$ the azimuthally axis; $\vec{\rho} \cdot \vec{v} = 0$, $\vec{\rho}$ being the impact parameter; $\vec{v}$ the collision velocity; $\alpha(z)$ and $\beta(z)$ are the initial and final states of the target, respectively; V is the projectile-target interaction and $G_T^\pm(z-z')$ are target Green's operators. If we denote by $\phi_v(\vec{x})$ a target eigenstate associated with the eigenenergy ε_v , where $\vec{x}$ is the electron-nucleus separation, the corresponding eikonal Schrödinger solution for the unperturbed target $v(z)$ may be written as (in the configuration space, with the origin of coordinates taken on the target nucleus):

$$v(z) = \phi_v(\vec{x}) \exp\left(-i \frac{\varepsilon_v}{v} z\right) \quad (2)$$

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

$$a_{\beta\alpha}(\vec{\rho}) = -\frac{i}{v} \frac{\langle \beta | V | \psi_\alpha \rangle \langle \psi_\beta | V | \alpha \rangle}{\langle \psi_\beta | V - V G_T^+ V | \psi_\alpha \rangle} \quad (3)$$

We note that the integrations (scalar products) are over z and $\vec{x}$.

As showed in [4], the expression (3) is stationary for small errors on the initial and final wave functions and it is easy to show that $\delta a_{\beta\alpha}(\vec{\rho})$ is zero to first order in $\delta \psi_\alpha^+(z)$ and $\delta \psi_\beta^-(z)$. The wave functions $\psi_\alpha^+(z)$ and $\psi_\beta^-(z)$ are developed 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 [3-7], the two sets are simply built from ground state and excited states of the target with time-independent coefficients for the two expansions. Finally, using $\delta a_{\beta\alpha}(\vec{\rho}) = 0$ with the development of $\psi_\alpha^+(z)$ and $\psi_\beta^-(z)$ on $\{|i\rangle\}$ and $\{|j\rangle\}$ respectively, the Eq. (3) can be written as:

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

Where $(D^{-1})_{ij}$ is the element (i, j) of the matrix D^{-1} inverse of the matrix D defined by the elements:

$$D_{ji} = \langle j | V - V G_T^+ V | i \rangle \quad (5)$$

Let remember that the i which appear in the term $\left(-\frac{i}{v}\right)$ at the beginning of the relation (3) and (4) represent the complex number i .

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 $|\beta\rangle$.

In the Eq. 4, we have two matrix elements, one of first Born-type $\langle j | V | i \rangle$ and the other of second Born-type $\langle j | V G_T^+ V | i \rangle$. In the evaluation of $\langle j | V G_T^+ V | i \rangle$, one has to perform a sum over an infinite set of intermediate states $|\nu\rangle$. A first step toward the exact evaluation of $\langle j | V G_T^+ V | i \rangle$ has been accomplished by taking into account the contribution of the discrete spectrum of the set $\{|\nu\rangle\}$ [3-5].

The contribution of the continuum has been taken into account using an analytical continuation that consists to evaluate the part close to ionisation threshold [7].

Finally, the direct excitation cross section $\sigma_{exc}(nl)$ from $\alpha=1s$ to $\beta=nl$ states is given by:

$$\sigma_{exc}(nl) = \int |a_{\beta\alpha}(\vec{\rho})|^2 d\vec{\rho} \quad (6)$$

In consequence, the direct excitation production for n level $\sigma_{exc}(n)$ is:

$$\sigma_{exc}(n) = \sum_{l=0}^{n-1} \sigma_{exc}(nl). \quad (7)$$

III. RESULTS AND DISCUSSIONS

We present in this paper the $\text{Be}^{3+}(1s)$ direct excitation cross sections to $n=2$ and $n=3$ states according to two expansions. For an nl excitation, the first is calculated with a basis of two states $\{1s, nl\}$ (called Schwinger-Born [4] and denoted Schw-B). The second is calculated with a basis of 14 states (denoted Schw1414) $\{1s, 2l_m, 3l_m\}$ for the $2l$ excitation and of 10 states (denoted Schw1010) $\{1s, 3l_m\}$ for $3l$ excitation where $0 \leq l \leq n-1$ and $-l \leq m \leq l$. Our cross-sections are compared with the TCAO calculations of Ermolaev [10, 11] obtained with a 55 two centre AO expansion.

The Fig. 1a, 1b and 1c show the $2s$, $2p$ and $n=2$ excitation cross sections, respectively, for energies between 40 keV and 4 MeV. For $\sigma(2s)$ (Fig. 1a), we observe an important dispersion between the three calculations (Schw-B, Schw1414 and TCAO) at intermediate energies, says between 40 and 400 keV. On the other hand, above 400 keV the three calculations converge. Whereas for $\sigma(2p)$ (Fig. 1b), the cross sections are very similar over all the energy range. As the $\sigma(n=2)$ (Fig. 1c) is the sum of $\sigma(2s)$ and $\sigma(2p)$ And furthermore the $\sigma(2p)$ is dominant, the three calculations are globally in agreement. The situation is appreciably different for the excitation of $n=3$ (Fig. 2), because the cross sections given by Schw-B and TCAO are similar over all the energy range, on the other hand the Schw1010 results overestimate the cross sections at low energies unlike at the excitation of the level $n=2$. The difference in the calculations between the levels $n=2$ and $n=3$ comes from the choice of basis set. Indeed, the basis with 14 states for the excitation of $n=2$ contains the all degenerates states of the level $n=3$ $\{3l_m \text{ with } l=0 \text{ to } 2 \text{ and } -l \leq m \leq l\}$ which lie just above.

As a consequence, this level absorb an important part of the excitation towards the $n=2$ level and this is contrary to the calculation of the excitation of $n=3$ level for which the basis set do not includes the upper level. Careful examination of results shows that, this explanation may be seem contradictory with the Schw-B results, which contains only two basis set (initial and final states), that is the excited intermediate states are excluded. Indeed, this shows that, in the intermediate energy range dominated by the charge exchange, the excitation channels are strongly coupled with the capture channels. In high collision energies ($E > 500$ keV) and in all cases, the calculations give same results because in this energy range the three processes capture, excitation and ionisation become decoupled.

IV. CONCLUSION

This calculation shows the powerful of the Schwinger method, in particular at intermediate collision energy range, to describe the excitation processes and furthermore it illustrates the important role of capture channels in the excitation processes for the low energies. It appears that in further research, the best improvement for the Schwinger method will consist to include the capture channels in the calculations.

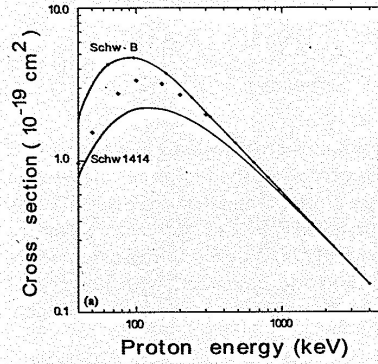


Fig. 1a: 2s excitation cross sections of Be^{3+} (1s) by proton impact with Schw1414 (full curve), Schw-B (dashed curve) and TCAO (open diamond) [10,11]

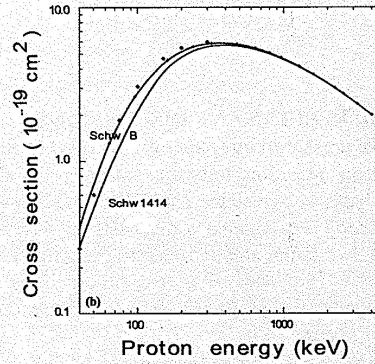


Fig. 1b: Same as Fig.1a, but for the excitation of 2p state.

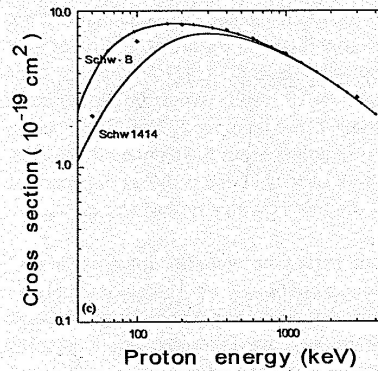


Fig. 1c: Same as Fig.1a, but for the excitation of $n=2$ level

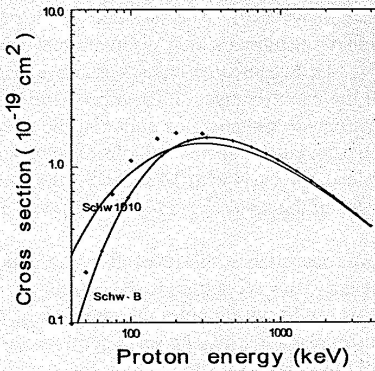


Fig. 2: Same as Fig.1a, but with Schw1010 for the excitation of $n=3$ level.

V. REFERENCES BIBLIOGRAPHIQUES

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