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VARIATIONAL SCHWINGER APROACH TO DIRECT EXCITATON OF HYDROGEN-LIKE (Li^{2+} (1s)) TARGET TO THE STATE n=2 BY PROTON IMPACT ENERGIES FROM 9 keV to 3 MeV

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ABSTRACT: The *1s → 2s, 2p, 3s, 3p* and *3d* excitation cross sections for hydrogen-like (Li^{2+}) by proton impact have been calculated in a wide energy range from 9 keV to 3 MeV, using Schwinger's variational principle within the impact parameter formalism. These cross sections are relevant to controlled nuclear fusion studies. They are also important in fusion plasma research [1]. The behavior of the computed cross sections are in excellent agreement with available theoretical results, obtained by the close-coupling method which is that of TCAO (Two-centre Atomic Orbital expansion) of Ermolaev and co-workers [1] and SCE (Single Centre Expansion) of Hall and co-workers [2].

KEYWORDS: fusion plasma, excitation cross section, Schwinger variational principle, atomic collision

Introduction:

Inner-shell processes in ion-atom collisions have been extensively studied in the past, both experimentally and theoretically, covering a wide range of impact velocities. In this paper, we have performed an application of the fractional form of the Schwinger principle to study the direct excitations of the hydrogen-like by proton impact. This approach was applied to study the direct excitation of hydrogen atom by proton impact at energies, from 10 keV to 200 keV [3]. We extend our variational Schwinger approach to direct excitation of Lithium ion (Li2+) target by proton impact at energies from 9 keV to 3 MeV.

The total cross sections for target excitation Li2+(1s) to the states Li^{2+}(2s ,2p, n=2) are presented in this energy range by the Schwinger's variational principle which is performed by expanding the wave functions $|\psi_\alpha^+\rangle$ and $\langle\psi_\beta^-|$ on five-states basis set as {1s, 2s, $2p_0$, $2p_{+1}$, $2p_{-1}$}.

We also present several results obtained from others theoretical models as single and two-centre close-coupling approaches [1] [2].

Currently there are no experimental results for any of the above stated transitions. While an experimental preparation of the Li^{2+}(1s) with a merged proton beam may be feasible, it appears unrealistic that an excited Li^{2+} ion target could be prepared [2] .

These cross sections are important in fusion plasma research [4]. Lithium pellets are used to condition the plasma confinement walls, i.e. to reduce edge influx from H and C impurities which reduce confinement times. Lithium pellets are also used in diagnostic procedures, e.g. the measurement of hydrogen ion temperatures in the plasma core after neutral beam injection. Also, electron removal from Li ions and charge transfer to D^+ constitutes increased radiative power losses and decreased deuteron fuel densities [2].

Schwinger's variational principle and close-coupling method applied to direct excitation:
Several theoretical approaches have been made to the problem of excitation of Lithium ion (Li^{2+}) target by proton impact. A M Ermolaev and M R C McDowell (1987) used the close-coupled atomic orbital model within the impact parameter formalism [1] in the energy region 17.5 keV to 3.0 MeV to calculate the cross section of the direct excitation:

$$H^+ + Li^{2+}(1s) \rightarrow H^+ + Li^{2+}(nl)^*. \qquad n=2 \qquad (1)$$

Two different TCAO bases have been used in the calculations:

1- A 32-state basis AO32 which have been applied to the problem of 1s → 2s, 2p excitations of (Li^{2+}) by proton impact varying the incident energy from 17.5 keV to 3.0 MeV

2- A 59-state basis AO59 which have been applied to the problem of 1s→ 2s, 2p and 1s → 3s, 3p, 3d excitations of (Li^{2+}) by proton impact varying the incident energy from 17.5 keV to 3.0 MeV.

K A Hall, J F Reading and A L Ford (1996) used also the close-coupled atomic orbital model, based on a development at a single center within the impact parameter formalism [2] but their theoretical cross sections of the reaction (1) have been obtained by performing a large single Finite Hilbert Basis Set (FHBS) calculation including states with angular momentum up to l =6, in the energy region from 30 keV to 600 keV The results of this approach are in very good agreement with the experiment results for the P + H collision[5] .
In the present work, the calculations, based on the fractional form of the Schwinger variational principle, are performed. The variational approach reported here uses methods that have been described previously and so will be recalled [6] [7].
Let $|\psi_\alpha^+\rangle$ and $\langle\psi_\beta^-|$ be the scattering Eigen-states of the Hamiltonian satisfying outgoing and incoming wave boundary conditions defined, in a collision without rearrangement, by the eikonal Lippmann-Schwinger equations:

$$\left|\psi_\alpha^+(z)\right\rangle = \left|\alpha(z)\right\rangle + \int_{-\infty}^{+\infty} dz'\, G_T^+(z-z')\, V(z')\, \left|\psi_\alpha^+(z')\right\rangle \qquad (2a)$$

$$\left\langle\psi_\beta^-(z)\right| = \left\langle\beta(z)\right| + \int_{-\infty}^{+\infty} dz'\, \left\langle\psi_\beta^-(z')\right| G_T^-(z-z')\, V(z') \qquad (2b)$$

where V is the potential responsible for the excitation and obtained by omission of the long-range projectile-target coulomb interaction [8], i.e., $V = Z_P\left(R^{-1} - |\vec{R}-\vec{x}|^{-1}\right)$, $|\alpha(z)\rangle$ and $\langle\beta(z)|$ are the initial and final states of the target respectively. Where z is the coordinate along the straight trajectory of the projectile and $G_T^{\pm}$ are target Green's operators.
The transition amplitude, for the impact parameter $\vec{\rho}$, may be written for $\alpha \neq \beta$, as:

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

where the notation $(\ |\ |\ )$ indicates the integration over the electronic coordinates as well as over z only when G_T^+ does not appear, and over z' when G_T^+ is present, and v is the impact velocity. It can be easily shown that the expression (3), for the transition amplitude $a_{\beta\alpha}(\vec{\rho})$ is stationary under arbitrary variations on $|\psi_\alpha^+\rangle$ and on $\langle\psi_\beta^-|$. Indeed, it is easy to show that:

$$\delta a_{\beta\alpha}(\vec{\rho}) = 0 \qquad (4)$$

Until first order for $|\delta\psi_\alpha^+\rangle$ and $\langle\delta\psi_\beta^-|$. By expanding $|\psi_\alpha^+\rangle$ and $\langle\psi_\beta^-|$ on two truncated basis sets $\{|i\rangle\}$ and $\{\langle j|\}$ respectively, one calculates approximate transition amplitude $\tilde{a}_{\beta\alpha}(\vec{\rho})$. The two basis sets are not necessarily identical but they must have the same finite dimension N. Then, using the variational condition $\delta\tilde{a}_{\beta\alpha}(\vec{\rho}) = 0$, one gets two separate finite sets of linear equations for the coefficients of the expansions: one for $|\psi_\alpha^+\rangle$ and one for $\langle\psi_\beta^-|$. Solving these sets of linear equations provide approximate solutions $\left|\tilde{\psi}_\alpha^+\right\rangle$ and $\left\langle\tilde{\psi}_\beta^-\right|$ for $\left|\psi_\alpha^+\right\rangle$ and $\left\langle\psi_\beta^-\right|$, respectively. Finally, the insertion of their solutions in eq. (3) leads to the following practical form of the approximate transition amplitude:

$$\tilde{a}_{\beta\alpha}(\vec{\rho}) = \left(-\frac{i}{\mathrm{v}}\right)\sum_{i=1}^{N}\sum_{j=1}^{N} (\beta|V|i)\left(D^{-1}\right)_{ij}(j|V|\alpha) \qquad (5)$$

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

$$D_{ij} = \left(i\left| V - VG_T^+V \right| j\right) \qquad (6)$$

Quantum transition amplitude between initial and final states of the system (projectile-Target): $|\alpha\rangle\otimes|\vec{k}_\alpha\rangle \rightarrow |\beta\rangle\otimes|\vec{k}_\beta\rangle$ is:

$$\begin{aligned} T_{\beta\alpha} &= \left\langle\vec{k}_\beta\right|\otimes\left\langle\beta\right|V\left|\psi_\alpha^+\right\rangle && (a)\\ &= \left[\left\langle\vec{k}_\beta\right|\otimes\left\langle\beta\right|\right]V\left[\left|\psi_\alpha^{+E}\right\rangle\otimes\left|\vec{k}_\alpha\right\rangle\right] && (b)\\ &= \left\langle\vec{k}_\beta,\beta\right|V\left|\vec{k}_\alpha,\psi_\alpha^{+E}\right\rangle && (c)\end{aligned} \qquad (7)$$

Where $|\alpha\rangle\otimes|\vec{k}_\alpha\rangle, |\beta\rangle\otimes|\vec{k}_\beta\rangle$ the initial and final are states of the system target-projectile respectively and $\left|\psi_\alpha^{+E}\right\rangle$ is eikonal scattering state of the target.
Equations (7 b, c) result by taking the first order of the expansion in power of $(1/\mu)$ (μ is reduced mass of collisional system) for the scattering wave because our study is based on the impact parameter formalism.
Using the energy conservation, quantum transition amplitude can be written:

$$T_{\beta\alpha}(\vec{\eta}) = i\mathrm{v}\int d^2\vec{\rho}\; e^{i\vec{\eta}.\vec{\rho}}\; \rho^{2i\frac{Z_P(Z_T-1)}{\mathrm{v}}}\; a_{\beta\alpha}(\vec{\rho}) \qquad (8)$$

Where Z_P and Z_T are the charge of projectile and the target nucleus respectively and $\vec{\eta}$ is the transverse impulsion transfer ($\vec{\eta}.\vec{\mathrm{v}}=0$). From this relation we can see that the phase factor $\rho^{\frac{2iZ_P(Z_T-1)}{v}}$ is reintroduced, it represents the potential contribution between the projectile and the whole target inter-aggregate contribution [6].
For an excitation process, the differential cross section is given by the relation:

$$\frac{d\sigma_{\beta\alpha}}{d\Omega} = \frac{\mu^2}{4\pi^2}\frac{k_\alpha}{k_\beta}\left|T_{\beta\alpha}(\vec{\eta})\right|^2 \qquad (9)$$

where Ω indicates the solid angle. Using the case of little longitudinal impulsion transfer $\frac{k_\alpha}{k_\beta}\approx 1$, the total cross section will be:

$$\sigma_{\beta\alpha} = 2\pi\int_0^{+\infty} d\rho\;\rho\;\left|a_{\beta\alpha}(\vec{\rho})\right|^2 \qquad (10)$$

In the present calculations, the total cross section has been evaluated by substituting the expression of the approximate transition amplitude (5) in (10) and omission of the integration over the range of impact parameters $[\rho_0, +\infty[$ in our case $\rho_0 = 11.2au$. Therefore, the total cross section may be approximated as:

$$\sigma_{\beta\alpha} = 2\pi\int_0^{\rho_0} d\rho\;\rho\;\left|\tilde{a}_{\beta\alpha}(\vec{\rho})\right|^2 \qquad (11)$$

In the code, a piecewise Simpson integration is made. An automatic procedure manages to ensure a given accuracy of the outcome. The target operator G_T^+ has been expanded on the whole discrete spectrum. The contribution of the continuum has been taken into account using an analytical continuation which consists to evaluate the art close to ionization threshold.

In our study, we are dealing with target excitation from the ground state. Hence, the states $|i\rangle$ and $|j\rangle$, in the expression (5), are chosen to be in the set $\{|\upsilon\rangle\}$ of Eigen-states of the target, which are solutions of the eikonal Schrodinger equation of the target:

$$\left(-i\mathrm{v}\frac{\partial}{\partial z}+H_T\right)|\upsilon(z)\rangle=0 \tag{12}$$

Further, they are restricted to a subset which contains the lowest target states, including $|\alpha\rangle$ and $\langle\beta|$ .Using the steps of our calculations, we find the results of the following approximations:

1- The first Born approximation (Born-I): $\tilde{a}_{\beta\alpha}(\vec{\rho})$ is replaced by $-\frac{i}{\mathrm{v}}(\beta|V|\alpha)$ in (11).

2- The second Born approximation (Born-II): $\tilde{a}_{\beta\alpha}(\vec{\rho})$ is replaced by $-\frac{i}{\mathrm{v}}(\beta|V-VG_T^+V|\alpha)$ in (11).

3- Schwinger-Born-approximation: $\tilde{a}_{\beta\alpha}(\vec{\rho})$ is replaced by $-\frac{i}{\mathrm{v}}\frac{(\beta|V|\alpha)(\beta|V|\alpha)}{(\beta|V-VG_T^+V|\alpha)}$ in (11).

4- Schwinger55 approximation (Schw55): $|\psi_\alpha^+\rangle$ and $|\psi_\beta^-\rangle$ are expanded on the above-mentioned five-state basis set as {1s, 2s, $2p_0$, $2p_{+1}$, $2p_{-1}$}. This approximation is used to study the excitation of Li^{2+}(1s) to the states 2s, 2p.

Results and discussions:

The present 1s→2s excitation total cross sections, represented by Figure 1, show that the Schw55 results, which refer to the approach of Schwinger with 5 states, have a peak located around 75 keV. But above 800 keV this procedure, even in the Figure 2 and Figure 3, represented the total cross sections for excitation to the state 2p and to the level n=2 respectively, join with an almost similar results obtained using different theoretical approaches: TCAO-32, TCAO-59 of Ermolaev et al [1] and FHBS of Hall et al [2].

The approach FHBS (Finite Hilbert Basis Set) gives results slightly higher than those of Ermolaev et al [1]. Although the cross sections arising from TCAO-32, TCAO-59 and FHBS are generally above our Schw55 results, their behavior is similar to the behavior of cross sections obtained by our theoretical procedure. The two theories provide also up to proton energy around 75 keV.

the behavior of our results, for the excitation 1s → 2p of the approximation Schw-B, presented in Figure 2 proved in very good agreement with the behavior of the results of both approaches TCAO-32 and TCAO-59. While those arising from Schw55 are slightly lower in the energy range 30-300 keV.

In Figure 3, one reports total cross sections for excitation to the level n = 2 which are obtained by summing excitation cross sections to 2s and 2p states. It is essential to note that the theoretical results provided by the first and second Born approximations greatly overestimate the total cross sections for the excitation to the level n = 2 in the field of low energy. But they give the same pace as other theoretical results for high energies.

In the TCAO-32, TCAO-59, Schw-B, Schw55 results presented here, we have small values of the excitation total cross sections at high impact velocities where we have the requisite energy to remove the electron. Then the ionization process is the most dominant in this energy range. At low and intermediate energies the results differ due to the existence of multiple scattering, but they have the same behavior. The lack of experimental results cannot rule on the validity of each theoretical calculation presented here.

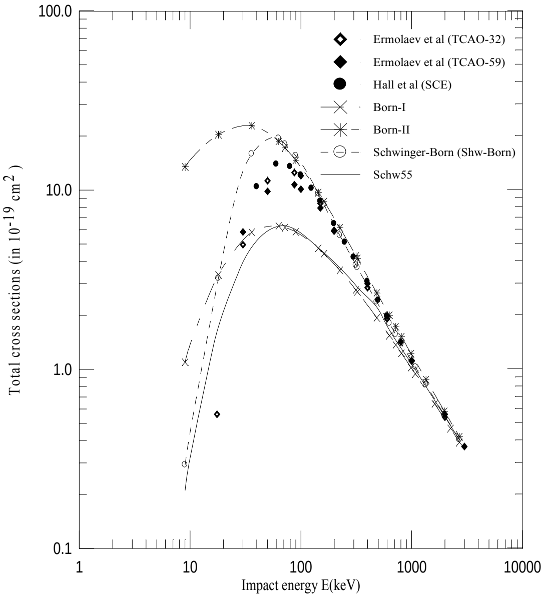

Figure 1 : cross sections for the excitation to the state 2s of Li^{2+} by proton impacts

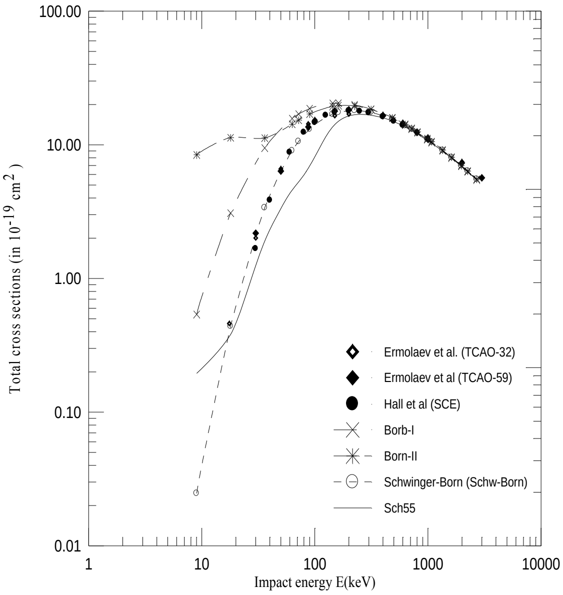

Figure 2 : cross sections for the excitation the state 2p of Li^{2+} by proton impacts.

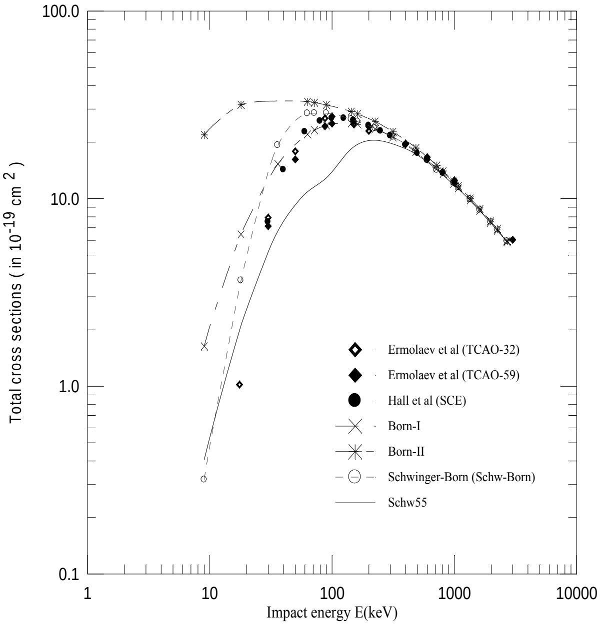

Figure 3 : cross sections for the excitation to the level n=2 of Li^{2+} by proton impacts.

Conclusion:

We have successfully applied the Schwinger variational method to study the excitation of the ion Li^{2+} (1s) to the Li^{2+} (n=2) state by impact of protons with energies ranging from 9 keV to 3 Mev. The direct excitation cross sections, deduced from this new approach, show very good convergence of the variational approach when one increases the number of the target states on which the scattering states are expanded. Good results are obtained when the scattering states $|\psi_\alpha^+\rangle$ and $\langle\psi_\beta^-|$ are developed on the basis of 5 states, compared with those of Ermolaev et al [1] and those of Hall et al [2].

At higher energies, the various total cross sections prove to be comparable. This deduction should be supported, of course, by the new close-coupling calculations which are constantly used bases of atomic orbitals increasingly large.

In this case, for the excitation the ion Li^{2+} (1s) by a bare ion, it should be possible to improve the present variational approach by introducing at least the capture ground state 1s in the expansion of both $|\psi_\alpha^+\rangle$ and $|\psi_\beta^-\rangle$.

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

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