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Abstract – We use Schwinger variational principle to evaluate excitation cross section of atomic hydrogen by proton impact at energy range between 2keV and 200keV. Contribution of the continuum near ionization threshold was introduced in a model with zero angular momentum using L^2 method developed by Yamani and Reinhardt in 1974-1975. Our results were compared with those of Bouamoud (1988-1989) using 1s, 2s and 2p state of hydrogen atom.

Keywords: Schwinger variational principle, L^2 method, J matrix method of Yamani and Reinhardt.

I. Introduction

The interaction (excitation, capture and ionization) process discussed in the light of simple systems (hydrogen and hydrogen-like) attracted a great deal of interest on behalf of theorists [1]-[8] and experimentalists [9]-[13]. Theoretical approximation methods and techniques (Already cited references) were designed and developed in this regard and calculations compared with measurements directly accessible by the experience have always been the evidence on the reliability and efficiency of advanced models. Among these techniques and methods of approximation, the variational principle of Schwinger is to him only, an extremely powerful tool in the estimation of cross sections and parameters associated. This principle has always motivated the theoretical physics group of Bouamoud [14] and it is in this same niche that we want, through this work, make our contribution in the calculation and estimation on the hydrogenic ion-Atom interaction process by including, in the later part, the continuum discretized on a set of pseudo-states of the target functions. To be, in the first part, we apply the Schwinger variational principle to estimate the excitation cross sections of atomic hydrogen by proton impact at intermediate energies. Variational transition matrix elements are developed first. It should be noted however, that the main contribution to the considered transition occurs at small angle (the forward scattering) for a collision of type $H^+ - H$ within an energy range of 50Kev [15]. In such a situation, the projectile describes a straight line trajectory and therefore we can address the problem within the eikonal approximation [16]. We wish to point out that in the majority of this part, we imitate the assumptions and developments advanced by our group [4], [5], [6], [7], [8] and that, in this work, the atomic unit was adopted except explicit mention.

II. Method and theory

In the Schwinger variational principle, the transition amplitude can be obtained in a stationary form from small changes of scattering states around their exact value.

II.1. Variational transition amplitude in the impact parameter method

In the impact parameters method where the nuclei are assumed to move in a straight line, scattering states $|\psi_\alpha^+(z)\rangle$ and $|\psi_\beta^-(z)\rangle$, eigenvectors of the total Hamiltonian of the system, each one associated to its correspondent Green's function G_T^+ and G_T^- must satisfy respectively outgoing and ingoing wave conditions in the direction $\vec{z}$. Scattering states that are solutions of the Schrödinger equation within the impact parameters approximation method are determined almost systematically by the eikonales Lippmann-Schwinger equations [17]:

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

$$|\psi_\beta^-(z)\rangle = |\beta(z)\rangle + \int_{-\infty}^{+\infty} dz'\, G_T^+(z-z')V(z')\,|\psi_\beta^-(z')\rangle \quad (2)$$

It should be noted, that initial and final states of the target are not only electronic $\vec{x}$ coordinates dependent but also

dependent on the direction $\vec{z} = \vec{\vartheta}t$ of $\vec{R} = \vec{\rho} + \vec{z}$ where $\vec{\rho}$ is the impact parameter checking the condition $\vec{\rho}.\vec{\vartheta} = 0$ with $\vec{\vartheta}$ the collision velocity reported in the frame of laboratory system. The eikonal Schwinger transition amplitude in fractional form is then written as [13]:

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

Scattering states are not known exactly. We can take as states test vectors $|\tilde{\psi}_\alpha^+\rangle$ and $|\tilde{\psi}_\beta^-\rangle$ such as:

$$|\tilde{\psi}_\alpha^+\rangle = |\psi_\alpha^+\rangle + |\delta\psi_\alpha^+\rangle \qquad (4)$$

$$|\tilde{\psi}_\beta^-\rangle = |\psi_\beta^-\rangle + |\delta\psi_\beta^-\rangle \qquad (5)$$

These states are developed later on the set of the basic elements in a vector space of dimension N with their respective coefficients $\tilde{a}_i$ and $\tilde{b}_j$. It will further be recalled that the transition amplitude $a_{\beta\alpha}(\vec{\rho})$ given by the relationship (3) is stationary with respect to small variations of the scattering states $|\psi_\alpha^+\rangle$ and $|\psi_\beta^-\rangle$ around their exact values and inserting, in this circumstances, solutions of the equation $\delta a_{\beta\alpha}(\vec{\rho}) = 0$ in the expression of the approximate transition amplitude $\tilde{a}_{\beta\alpha}(\vec{\rho})$ obtained by replacing $a_{\beta\alpha}(\vec{\rho})$, $|\psi_\alpha^+(z)\rangle$ and $|\psi_\beta^-(z)\rangle$ by test vectors $|\tilde{\psi}_\alpha^+\rangle$ and $|\tilde{\psi}_\beta^-\rangle$ respectively led us to the almost final formulation of the Schwinger variational principle:

$$\tilde{a}_{\beta\alpha}(\vec{\rho}) = \left(-\frac{i}{\vartheta}\right)\sum_{i=1}^{N}\sum_{j=1}^{N}(\beta|V|i)(D^{-1})_{ij}(j|V|i) \qquad (6)$$

where $(D^{-1})_{ij}$ represents the element (i,j) of the matrix D^{-1}, opposite of D defined by the elements:

$$D_{ij} = (j|V - VG_T^+|i) \qquad (7)$$

It should be noted however, that, during the development of approximated scattering states $|\tilde{\psi}_\alpha^+\rangle$ and $|\tilde{\psi}_\beta^-\rangle$ we took into consideration first a basis consisting only of target bound states (discrete) and we have ignored the inclusion of capture states (continuum) on the projectile. This assumes that the effect of coupling between the capture and excitation must be low for the variational principle to remains reliable and this is true when the projectile charge is lower than that of the kernel.

Subsequently, we try to estimate the continuum and its contribution in the excitation cross sections which is still not negligible in the range of energies which we are interested and more particularly between 2KeV and 40KeV.

II.2. Pseudo-continuum within L^2 method

The eigenstates of the target, the basic elements of development which we have referred in the first part are hydrogen functions or in the same way, close to a factor, Laguerre-type L^2 functions [18], [19], [20]. These polynomials or associated Laguerre-type functions, in addition to be orthogonal with some well-defined weight, they enjoy some extremely remarkable properties that offer incomparable flexibility [20], [21]. In this part, we want to take advantage of the benefits cited previously in stalking the near continuum and estimate its contribution in cross sections of excitation energy between 2KeV and 200KeV. First, we must begin an analysis of an eigenvalue equation which cries in its usual form:

$$H|\psi\rangle = E|\psi\rangle \qquad (8)$$

It should be noted that in equation (8), energy E is negative for bound states and positive for scattering states. However, in the most part of the cases, the wave function solution of (8) is generated in a space of square integrable functions with the basic elements of $\{\phi_n\}_{n=0}^{\infty}$ in the form:

$$|\psi\rangle = \sum f_n(E)|\phi_n\rangle \qquad (9)$$

The elements $|\phi_n\rangle$, which checks the eigenvalue equation $H|\phi_n\rangle = E_n|\phi_n\rangle$ and leading to a diagonal representation of H form the discrete spectrum H while the continuous spectrum is obtained by analysis of the infinite sum of the complete basic functions. To this end, we follow a strategy developed by Heller and Yamani in 1974 [22] then Yamani and Reinhardt in 1975 [23]. In doing so, we require only the hermitian matrix representing the wave operator $(H - E)$ to be tridiagonale [24], [25], [26], [27], [28]. Thus, action of the Schrödinger wave operator on the basic elements can take the form of a recurrence relation in the δ Kronecker [26]:

$$\langle\phi_n|H - E|\phi_n\rangle = (a_n - z)\delta_{n,m} + b_n\delta_{n,m-1} + b_{n-1}\delta_{n,m+1} \qquad (10)$$

A relationship in which z and the coefficients $\{a_n, b_n\}_{n=0}^{\infty}$ are real and in general functions of energy, angular momentum and parameters related to the potential. After a projection on $\langle\phi_n|$, the Schrödinger wave operator matrix obtained by development of $|\psi\rangle$ on $|\phi_m\rangle$ in equation $(H - E)|\psi\rangle = 0$ reduces to a three-term recurrence relation of the form:

$$zf_n = a_n f_n + b_{n-1}f_{n-1} + b_n f_{n+1} \qquad (11)$$

The problem is therefore reduced to solution of a recurrence relation for the expansion coefficients of the wave function ψ. It should be noted, however, that the solution to the problem stated by the above quoted recurrence is obtained for all energies E, whether discrete or continuous. Thus, the recurrence relation in δ Kronecker shows clearly that the discrete spectrum with negative energies, regular solution of the considered problem, can be obtained by Diagonalization with simply requiring that the coefficients b_n and $a_n - z$ must be zero.

In configuration space, the wave function $\psi_E(x)$ is developed in the form of an infinite series of functions $\phi_n(x) = A_n w_n(x) P_n(x)$ with coefficients $f_n(E)$ where the factor A_n is normalization constant, $P_n(x)$ a polynomial of degree n in x and $w_n(x)$ the weight function of the polynomial $P_n(x)$. In the case of the $H^+ - H$ system, L^2 functions of the bases take a form similar to that which it has previously been suggested with P_n proportional to Laguerre polynomial with weight function $w(x) = x^\alpha e^{-\beta x}$:

$$\phi_n(r) = A_n x^\alpha e^{-\beta x} L_n^\nu(x) \qquad (12)$$

Functions ϕ_n are of Laguerre type with $A_n = \sqrt{\lambda\Gamma(n+1)/\Gamma(n+\nu+1)}$ where n can be integer 0, 1, 2...; α and β are real positives. We deliberately avoided direct resolution of the time independent radial wave equation for a particle without spin in a spherical symmetric potential V(r). In fact, running of the remarkable properties what enjoy the Laguerre polynomials and the use of differential equation and differentiation formula relating to these famous polynomials [21], [29], [30] requires the passage to a double derivation from the variable x instead of r. We followed a strategy used by Alhaidari [26] and we were able to obtain, by suggesting value $\alpha = l+1$, $\nu = 2l+1$ and $\beta = 1/2$, recurrence relation in δ Kronecker between the elements of the basis $\{\phi_n\}_{n=0}^{\infty}$ which subsequently allowed us to write, by asking $\sigma_\pm = \frac{2E}{\lambda^2} \pm \frac{1}{4}$ and $x = \frac{(2E/\lambda^2 - 1/4)}{(2E/\lambda^2 + 1/4)}$, a recurrence relationship in terms of polynomials $P_n(E) = \sqrt{\frac{\Gamma(n+2l+2)}{\Gamma(n+1)}} f_n(E)$ in the form:

$$(n+1)P_{n+1} - 2[(n+1+l)x + b]P_n + (n+1+2l)P_{n-1} = 0 \qquad (13)$$

It should be noted however, that the recurrence relationship for x values necessarily located between -1 and $+1$ for positive energies (continuum) reduces in the case which we are interested doing $l = 0$ for s states with the conditions $P_{-1} = 0$ and $P_0 = 1$ to:

$$(n+1)P_{n+1} - 2[(n+1)x + b]P_n + (n+1)P_{n-1} \qquad (14)$$

Recursive sequences obtained from (14) with the conditions $P_{-1} = 0$ and $P_0 = 1$ for integer values $m = n+1 = 1, 2, 3, \ldots$ are the pillar of our algorithm for the calculation of the target state pseudo-continuum wave functions expansion coefficients.

III. Results and discussion:

By application of the Schwinger variational principle, we reproduce in the first part, the calculation results of excitation cross sections to the state 2s (Schw55) of Bouamoud and group [14]. Cross sections are illustrated in figure 1 (HExact) where we have registered a slight shifting due probably to more meticulousness calculations than those of Bouamoud and group.

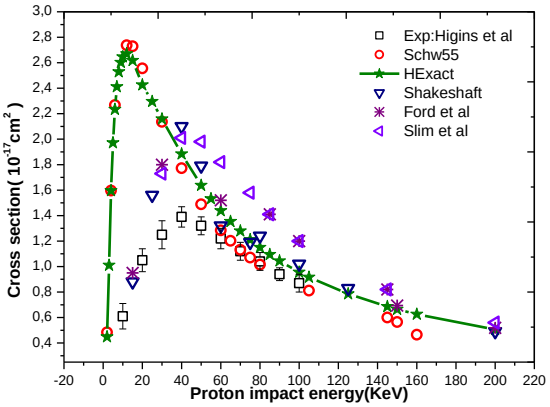

Figure 1. Excitation to the state 2s without pseudo-continuum

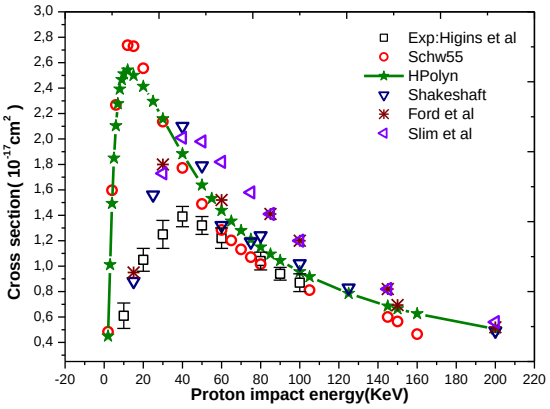

Figure 2. Excitation to 2s state within pseudo-continuum (3s)

The continuum, translated by a competition between excitation and capture in the environment near of the ionization threshold is introduced by discretization over L^2 basis function of Laguerre type generated by a set of pseudo-states functions. The results shown in figure 2 (HPolyn) mark a detachment of the maximum cross sections about 15% if there are only the contribution of the pseudo-state noted (3s) for m=3. However, a competitive convergence to literature (Schakeshaft, Ford et al and Slim et al) can be significantly improved by adding other pseudo-states $(m > 3)$ to better describe the continuum of the target state in the low energy range between 2KeV and 40KeV.

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