

Theoretical Angular Distributions for Elastic e-H Scattering

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The differential cross section for electrons elastically scattered by hydrogen atoms are calculated for incident electron energies of 100 eV and higher. The polarization and distortion of the electronic wave function are included at second order by replacing an infinite number of virtual intermediate states by a single state with parametric energy. This parameter is evaluated by using the Schwinger variational principle. Agreement with experimental values is good.

As seções de choque diferenciais para elétrons espalhados elasticamente por átomos de hidrogênio são calculados para energias (dos elétrons incidentes) de 100 eV e mais. A polarização e a distorção da função de onda do elétron são incluídas em segunda ordem pela substituição de um número infinito de estados intermediários virtuais por um único estado com energia paramétrica. Este parâmetro é determinado pelo uso do princípio variacional de Schrödinger. O acordo com os dados experimentais é bom.

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1. INTRODUCTION

Recently experimental normalized values have been obtained for the angular distributions of the elastic $e-H$ scattering at intermediate energies¹. Being the $e-H$ scattering process one of the most schematic three body problems, it has been the objective of many theoretical calculations. The interaction between the particles is known and the accuracy of the theoretical description depends mainly on the approximation method used to solve the scattering equations. In the intermediate energy range the formalism can be based on a direct solution of the Schrödinger equation, like the close coupling method² with non-local potential correction terms³, or on the Faddeev equations⁴, or by approximate evaluation of the scattering amplitude. We will deal with the last approach mentioned.

The characteristic feature of e -atom angular distributions, at the considered energies, is a peak at small angles produced by atomic polarization effects. They have been included in the eikonal approximation by considering dynamical interactions between the incident electron and the atom. This is the base of the Glauber multiple-scattering method⁵. However the agreement between the experimental data and values obtained with the Glauber's method assuming either straightline⁶ or angle trajectories⁷ for the incident electron, are poorer than results obtained by using the first Born approximation¹. But the Born approximation consider only the contribution from the static potential of the atom. In order to include the atomic polarization and distortion it is necessary to consider second order terms. The natural way should be to introduce these terms in the perturbative expansion. However calculations in potential scattering⁸ show that two terms in that series are not enough to attain good results for the scattering amplitude, at medium energies, and other methods must be applied⁹. The eikonal-Born series allows for approximate values of the third and fourth Born term, which are obtained by expanding the Glauber amplitude¹⁰. In a precedent work¹¹ we have proposed a variational method based on the Schwinger principle. Since in this method the scattering amplitude is given by a rational expression it results equivalent to introduce some approximate value for the high perturbative orders. Only one parameter is assumed to

take account for the mass of the intermediate virtual atomic states. We applied this method to the calculation of the angular distribution for e -He elastic scattering and founded agreement with experimental data¹¹. Thereafter the variational principle was object of further studies^{10,12} but assuming a "ad hoc" non variational value for the intermediate mass. The present work reports application of the variational approach to the elastic scattering of electrons by hydrogen atoms.

2. THEORY: DIRECT AND EXCHANGE SCATTERING AMPLITUDE

We consider a particle of charge Z_1e , mass m and wave vector \vec{k} colliding with a neutral atom of nuclear charge Z_1e . We take the atomic nucleus at the origin of the coordinate system, and we denote by \vec{r} the position of the incident electron and by \vec{r}_i the coordinate of the atomic electrons. The total system is described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \nabla_r^2 + H_A + V = H_0 + V \quad (2.1)$$

where

$$V = \sum_{i=1}^{Z_1} \frac{Z_1 e^2}{|\vec{r} - \vec{r}_i|} - \frac{ZZ_1 e^2}{r} \quad (2.2)$$

is the interaction between the incident particle and the atom, and H_0 is the internal Hamiltonian of the atom. Calling $\phi_n(\vec{r}_i) \equiv |n\rangle$ the atomic wave functions

$$H_A |n\rangle = E_n |n\rangle \quad (2.3)$$

we have

$$H_0 |n, \vec{k}\rangle = E |n, \vec{k}\rangle \quad (2.4)$$

where $|n, \vec{k}\rangle = e^{i\vec{k} \cdot \vec{r}} \phi_n(\vec{r}_i)$ and $E = E_n + \frac{\hbar^2 k^2}{2m}$. Then, the direct elastic scattering amplitude is given by

$$f(E, \theta) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \langle f, \vec{k}_f | V | \Psi_i^+ \rangle = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \langle \Psi_f^- | V | i, \vec{k}_i \rangle \quad (2.5)$$

where i and f denote the initial and final state of the atom. $|\Psi_i^+\rangle$ and $\langle\Psi_f^-|$ are the outgoing and ingoing wave functions respectively, satisfying the integral equations

$$\begin{aligned} |\Psi_i^+\rangle &= |i, \vec{k}_i\rangle + G_0^+ V |\Psi_i^+\rangle \\ \langle\Psi_f^-| &= \langle f, \vec{k}_f| + \langle\Psi_f^-| V G_0^+ \end{aligned} \quad (2.6)$$

The G_0^+ is the Green free operator of the whole system

$$G_0^+ = (E - H_0 + i\epsilon)^{-1}$$

The scattering amplitude satisfy the Schwinger variational principle

$$f(E, \theta) = - \frac{1}{4\pi} \frac{2m}{\hbar^2} \frac{\langle f, \vec{k}_f | V | \Psi_i^+ \rangle \langle \Psi_f^- | V | i, \vec{k}_i \rangle}{\langle \Psi_f^- | V - V G_0^+ V | \Psi_i^+ \rangle} \quad (2.7)$$

being this functional stationary under variations of Ψ_i^+ and Ψ_f^- around the exact solutions of Eq. (2.6).

From (2.5) and (2.6) we can obtain the perturbative expansion of the direct scattering amplitude

$$f(E, \theta) = - \frac{1}{4\pi} \frac{2m}{\hbar^2} \left[\langle f, \vec{k}_f | V | i, \vec{k}_i \rangle + \langle f, \vec{k}_f | V G_0^+ V | i, \vec{k}_i \rangle + \dots \right] \quad (2.8)$$

When the scatterer is a hydrogen atom the matrix elements of the potential are

$$\begin{aligned} \langle \vec{k}_n, n | V | \vec{k}_m, m \rangle &= Ze^2 \int d\vec{r} d\vec{r}' \phi_n^*(\vec{r}') e^{-i\vec{k}_n \cdot \vec{r}'} \left[\frac{1}{|\vec{r} - \vec{r}'|} - \frac{1}{r} \right] \phi_m(\vec{r}) e^{i\vec{k}_m \cdot \vec{r}} \\ &= \frac{4\pi Ze^2}{|\vec{k}_n - \vec{k}_m|} \int d\vec{r} \phi_n^*(\vec{r}) \left[e^{i(\vec{k}_m - \vec{k}_n) \cdot \vec{r}} - 1 \right] \phi_m(\vec{r}) \end{aligned} \quad (2.9)$$

If we consider the elastic $e-H$ scattering with the atom in the ground state

$$\phi_{1S}(r) = \sqrt{\frac{\lambda^3}{\pi}} e^{-\lambda r}, \quad \lambda = Z/a_0, \quad Z = 1$$

we have¹³

$$\int d\vec{x} |\phi_{1s}(x)|^2 (e^{i(\vec{k}_i - \vec{k}_f) \cdot \vec{x}} - 1) = -K^2 \frac{8\lambda^2 + K^2}{(4\lambda^2 + K^2)^2} \quad (2.10)$$

where

$$K^2 = |\vec{k}_f - \vec{k}_i|^2 = 4k^2 \sin^2 \theta/2$$

The first perturbative term (in units a_0^{-2}) results¹⁴

$$f_1(E, \theta) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \langle 1, \vec{k}_f | V | 1, \vec{k}_i \rangle = \frac{1 + \frac{K^2}{2} \sin^2 \theta/2}{(1 + K^2 \sin^2 \theta/2)^2} \quad (2.11)$$

The second perturbative order

$$f_2(E, \theta) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \langle f, \vec{k}_f | V G_0^+ V | i, \vec{k}_i \rangle$$

by using the completeness condition, can be written

$$f_2(E, \theta) = \frac{1}{4\pi(2\pi)^3} \left(\frac{2m}{\hbar^2} \right)^2 \lim_{\epsilon \rightarrow 0} \sum_n \int d\vec{q} \frac{\langle f, \vec{k}_f | V | n, \vec{q} \rangle \langle n, \vec{q} | V | i, \vec{k}_i \rangle}{q^2 - k_n^2 - i\epsilon} \quad (2.12)$$

The sum is done over all the possible discrete and continuous eigenstates of the atom. The wave numbers k_n of the electron on the intermediate states are defined by

$$k_n^2 = \frac{2m}{\hbar^2} (E - E_n)$$

We shall make the usual approximation by calculating exactly the initial N terms in the sum of Eq. (2.12), and replacing in the remaining terms the k_n^2 by an average energy difference p^2 . Then

$$f_2^{(N)}(E, \theta, p^2) = \frac{1}{32\pi^4} \left[\frac{2m}{\hbar^2} \right]^2 \lim_{\epsilon \rightarrow 0} \left[\sum_{n=1}^N \int d\vec{q} \frac{\langle f, \vec{k}_f | V | n, \vec{q} \rangle \langle n, \vec{q} | V | i, \vec{k}_i \rangle}{q^2 - k_n^2 - i\epsilon} \right. \\ \left. + \int d\vec{q} \frac{1}{q^2 - p^2 - i\epsilon} \left[- \sum_{n=1}^N \langle f, \vec{k}_f | V | n, \vec{q} \rangle \langle n, \vec{q} | V | i, \vec{k}_i \rangle + \right. \right.$$

$$+ \left. \sum_{n=1}^{\infty} \langle f, \vec{k}_f | V | n, \vec{q} \rangle \langle n, \vec{q} | V | i, \vec{k}_i \rangle \right] \quad (2.13)$$

Having made this approximation the completeness property of the atomic wave functions can be used to evaluate the infinite sum. Comparing with Eq. (2.9), we can write this last term in the following way

$$\int d\vec{q} \frac{1}{q^2 - p^2 - i\epsilon} \frac{1}{|\vec{k}_f - \vec{q}|^2 |\vec{k}_i - \vec{q}|^2} \langle \phi_f | (e^{-i(\vec{k}_f - \vec{q}) \cdot \vec{r}} - 1) (e^{i(\vec{k}_i - \vec{q}) \cdot \vec{r}} - 1) | \phi_i$$

We can give a simple interpretation for the approximation performed. If we consider the formal expression of the Green function

$$G_0^+(E) = - \frac{1}{(2\pi)^3} \frac{2m}{\hbar^2} \sum_{n=1}^{\infty} \int d\vec{q} \frac{|n, \vec{q}\rangle \langle n, \vec{q}|}{q^2 - k_n^2 - i\epsilon} \quad (2.14)$$

we have replaced it by

$$G_0^{(N)}(E, p^2) = - \frac{1}{(2\pi)^3} \frac{2m}{\hbar^2} \left[\sum_{n=1}^N \int d\vec{q} \frac{|n, \vec{q}\rangle \langle n, \vec{q}|}{q^2 - k_n^2 - i\epsilon} + \int d\vec{q} \frac{1}{q^2 - p^2 - i\epsilon} (|\vec{q}\rangle \langle \vec{q}| - \sum_{n=1}^N |n, \vec{q}\rangle \langle n, \vec{q}|) \right] \quad (2.15)$$

At the real axis of the complex E plane the function G_0 has an infinite set of poles in the range $-|E_1| \leq E < 0$ corresponding to the bound states and a cut from 0 to $+\infty$. By using $G_0^{(N)}(E)$ we are considering exactly a set of N poles and we replace all the other singularities by a pole with parametrized position. Since the ground state lies quite apart from the other bound states and from the continuum we will assume $N=1$ in our calculations. Then Eq. (2.13) can be written

$$f_2^{(1)}(E, \theta, p^2) = f_{1s}(E, \theta, k_1^2) + f_c(E, \theta, p^2) \quad (2.16)$$

where $f_{1s}(E, \theta)$ is the exact contribution of the state $1s$. The integrals in the Eq. (2.13) contain only $1s$ hydrogen orbitals, and can be written

$$f_{1s}(E, \theta, k_1^2) = \frac{2Z^2}{\pi^2 \alpha_0^2} \int d\vec{q} \frac{\langle \phi_{1s} | e^{i(\vec{q}-\vec{k}_f) \cdot \vec{r}} - 1 | \phi_{1s} \rangle \langle \phi_{1s} | e^{i(\vec{k}_i - \vec{q}) \cdot \vec{r}} - 1 | \phi_{1s} \rangle}{(q^2 - k_1^2 - i\epsilon) |\vec{q} - \vec{k}_f|^2 |\vec{k}_i - \vec{q}|^2}$$

$$f_c(E, \theta, p^2) = \frac{2Z^2}{\pi^2 \alpha_0^2} \int d\vec{q} \frac{\langle \phi_{1s} | e^{i(\vec{k}_i - \vec{k}_f) \cdot \vec{r}} - 1 - (e^{i(\vec{q} - \vec{k}_f) \cdot \vec{r}} - 1) - (e^{i(\vec{k}_i - \vec{q}) \cdot \vec{r}} - 1) | \phi_{1s} \rangle}{(q^2 - p^2 - i\epsilon) |\vec{q} - \vec{k}_f|^2 |\vec{k}_i - \vec{q}|^2} - f_{1s}(E, \theta, p^2)$$

The matrix elements between atomic states can be evaluated to obtain

$$f_{1s}(E, \theta, k_1^2) = \frac{2Z^2}{\pi^2 \alpha_0^2} \left[16 \lambda^2 J(2, 2, 2\lambda, 2\lambda; k_1) + 8 \lambda^2 J(2, 1, 2\lambda, 2\lambda; k_1) + J(1, 1, 2\lambda, 2\lambda; k_1) \right]$$

$$f_c(E, \theta, p^2) = \frac{2Z^2}{\pi^2 \alpha_0^2} \left[8 \lambda^2 J(2, 1, 2\lambda, 0; p) + 2 J(1, 1, 0, 2\lambda; p) - \frac{K^2(8\lambda^2 + K^2)}{(4\lambda^2 + K^2)^2} J(1, 1, 0, 0; p) \right] - f_{1s}(E, \theta, p^2) \quad (2.17)$$

where

$$J(n, m, a, b; p) = \int \frac{d\vec{q}}{(q^2 - p^2 - i\epsilon) [|\vec{k}_f - \vec{q}|^2 + a^2]^n [|\vec{q} - \vec{k}_i|^2 + b^2]^m}$$

By using the Dalitz's transform¹⁵ this integral can be reduced to an one-dimensional integral. Analytical expressions are given in Appendix I.

In the e - H scattering process allowance must be made for the possible electron's exchange. The exchange amplitude $g(E, \theta)$ for the e - H elastic scattering, in the first Born approximation, is obtained by using the explicitly symmetrized or antisymmetrized incident waves in the Eq. (2.5)

$$\Psi_i^\pm(\vec{r}_1, \vec{r}_2) = e^{i\vec{k}_i \cdot \vec{r}_1} \phi_{1s}(\vec{r}_2) \pm e^{i\vec{k}_i \cdot \vec{r}_2} \phi_{1s}(\vec{r}_1) \quad (2.19)$$

This gives the Born-Oppenheimer exchange amplitude¹⁶

$$g_1(E, \theta) = -\frac{1}{4\pi} \frac{2me^2}{\hbar^2} \int d\vec{r}_1 d\vec{r}_2 e^{-i\vec{k}_f \cdot \vec{r}_1} \phi_{1s}(\vec{r}_2) \left(\frac{1}{|\vec{r}_1 - \vec{r}_2|} - \frac{1}{r_1} \right) e^{i\vec{k}_i \cdot \vec{r}_2} \phi_{1s}(\vec{r}_1) \quad (2.20)$$

It can also be obtained from the Kohn-Hülden variational principle. At intermediate energies $g_1(E, \theta)$ is much smaller than the direct amplitude, and it is unnecessary to consider higher perturbative orders. However when the energy decreases the Oppenheimer approximation rises steply. This is originated by the high terms of the expansion of $g_1(E, \theta)$ in a power series of $1/k$. Ochkur and Bonham propose to keep only the leading term in that expansion¹⁶

$$\begin{aligned} g_1^{OB}(E, \theta) &\xrightarrow{k \rightarrow \infty} -\frac{2me^2}{\hbar^2 k^2} \int d\vec{r} e^{i(\vec{k}_f - \vec{k}_i) \cdot \vec{r}} |\phi_{1s}(\vec{r})|^2 \\ &= \frac{|\vec{k}_f - \vec{k}_i|^2}{k^2} \left[f_1(E, \theta) - \frac{2me^2}{\hbar^2 |\vec{k}_f - \vec{k}_i|^2} \right] \\ &= -\frac{2}{k^2 (1 + k^2 \sin^2 \theta/2)^2} \end{aligned} \quad (2.21)$$

This approximation can not be obtained from a variational principle, to achieve that Rudge introduces a slightly modified form¹⁶. In our calculation we will use the Eq. (2.21).

3. DIFFERENTIAL CROSS SECTION FOR e-H SCATTERING

We can apply the second perturbative term, as obtained in the precedent section, to the calculation of the cross section. The standard way is to assume that perturbative theory is applied to solve the wave

equation and that the approximate value for the scattering amplitude, obtained by keeping the first two terms in the expansion (2.8), should be assumed as the true value of $f(E, \theta)$. Then

$$\sigma_2(E, \theta) = |f_1(E, \theta) + f_2(E, \theta)|^2 \quad (3.1)$$

or, by including the exchange contribution,

$$\sigma_2(E, \theta) = \frac{1}{4} |f_1 + f_2 + g_1|^2 + \frac{3}{4} |f_1 + f_2 - g_1|^2 \quad (3.2)$$

It is also possible to assume that a fix perturbative order must be retained in the cross section: then Eq. (3.1) contains a term of order V^4 , but another term of order V^4 would enter from the cross product $f_1 \cdot f_3$. Only terms to order V^3 are consistently included¹⁷; then

$$\sigma_3(E, \theta) = |f_1(E, \theta)|^2 + 2f_1(E, \theta) \operatorname{Re} f_2(E, \theta) \quad (3.3)$$

or

$$\sigma_3(E, \theta) = |f_1|^2 + |g_1|^2 - f_1 g_1 + (2f_1 - g_1) \operatorname{Re} f_2$$

All these cross sections depend on the parameter p^2 introduced in Eq. (2.13). When using Eq. (3.3) it was usually set $p_N^2 = k_{N+1}^2$ ¹⁷. This choice is justified by observing the stability of the value of $\operatorname{Re} f_2^{(N)}(E, 0, k_{N+1}^2)$ when N is increased¹⁸. For $N=1$ that means that in the Green function the first pole is exactly evaluated, and the contribution from the order should be well approximated by the modified residue of the second pole. This is not a reliable approximation because the cross section given by Eq. (3.3) is not a positive definite quantity¹¹.

We will use the Schwinger variational principle, given by Eq. (2.7), to obtain a stationary value for p^2 . Let us use the simplest trial function

$$\Psi(\vec{x}_1, \vec{x}_2) = A e^{i\vec{k} \cdot \vec{x}_1} \phi_1(\vec{x}_2) \quad (3.4)$$

in the Eq. (2.7), to obtain

$$f(E, \theta) = \frac{f_1^2(E, \theta)}{f_1(E, \theta) - f_2(E, \theta)} \quad (3.5)$$

However, the exact Green function is unknown and we are using the approximate expression $G_0^{(1)}(E)$. That means that the exact wave function for the $e-H$ system is approximated by the solution of the integral equation

$$|\Psi_1\rangle = |1s, \vec{k}\rangle + G_0^{(1)}(E, p^2)V|\Psi_1\rangle$$

In the corresponding functional

$$f^{(1)}(E, \theta) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \frac{\langle f, \vec{k}_f | V | \Psi_1^+ \rangle \langle \Psi_1^- | V | i, \vec{k}_i \rangle}{\langle \Psi_1^- | V - V G_0^{(1)}(E, p^2) V | \Psi_1^+ \rangle}$$

we can use Eq.(3.4) to obtain the following approximate scattering amplitude

$$f_P(E, \theta, p^2) = \frac{f_1^2(E, \theta)}{f_1(E, \theta) - f_2^{(1)}(E, \theta, p^2)} \quad (3.6)$$

This is identical to the $[1, 1]$ Padé approximant to the expansion $f_1 + f_2^{(1)}$. To consider exchange scattering we must use the trial function given in the Eq.(2.19). According to the relative sign of the two terms in Eq. (2.19) we obtain the variational singlet f_{Ps} and triplet f_{Pt} amplitudes. Neglecting higher orders in the exchange terms, we get

$$\sigma_P(E, \theta, p^2) = \frac{1}{4} \left| \frac{(f_1 + g_1)^2}{f_1 + g_1 - f_2^{(1)}} \right|^2 + \frac{3}{4} \left| \frac{(f_1 - g_1)^2}{f_1 - g_1 - f_2^{(1)}} \right|^2 \quad (3.7)$$

According to the variational principle we should determinate p^2 by requiring the stationarity of the approximate scattering amplitude, for each energy and angle. In general, it is not possible to make the real and imaginary parts of f_{Ps} and f_{Pt} stationary, with a single parameter. Following ideas developed in Ref.11 we will choose p^2 such that the forward scattering cross section $\sigma_P(E, 0, p^2)$ is stationary. A single value of p^2 exist for each energy bigger than 100 eV. Writing $p^2 = k^2 - W$, it results $W = 5.5, 6.4, 7.1$ and 7.6 (units α_0^{-2}) for $E = 100, 200, 400$ and 680 eV, respectively. We observe that these values are larger than

the values employed by other authors^{10,12,17}. These smaller p^2 are necessary to have a good approximation for f_2 , but in our case the p^2 is taking account of high perturbative orders and gives a good description of the forward peak. That do not seems possible when using "ad hoc" values of p^2 (12,20).

In Figs.1 to 4 we present our results for the differential cross section of $e-H$ scattering, as given by Eq. (3.7). They are compared with the experimental values obtained by Williams¹. We see that, for all the energies considered, the agreement is between the experimental errors for angles smaller than 60° . For large angles the variational approaches produces values too small for the cross sections. We can give an interpretation for this fact. For large momentum transfers the static field of the atom is the dominating force in electron atom scattering. The term f_{1s} in Eq.(2.16) is the second perturbative order for the scattering amplitude $f^{(s)}$ by the static field. Hence for large angles f_{1s} will be much bigger than f_c . Calling

$$f_P^{(s)} = \frac{f_1^2}{f_1 - f_{1s}}$$

the variational approximation to $f^{(s)}$, we can expand the Eq. (3.6):

$$f_P = f_P^{(s)} \left(1 + \frac{f_c}{f_1^2} f_P^{(s)} + \left(\frac{f_c}{f_1^2}\right)^2 (f_P^{(s)})^2 + \dots \right)$$

Since $f_c \ll f_1$ and $f_1 \sim f_P^{(s)}$ we see that, for large angles, the value provided by Eq. (3.6) will be, essentially, $f_P^{(s)}$. From Ref.11 we know that for potential scattering f_P is smaller than the exact amplitude at large angles. That indicates that corrections for f_{1s} are necessary.

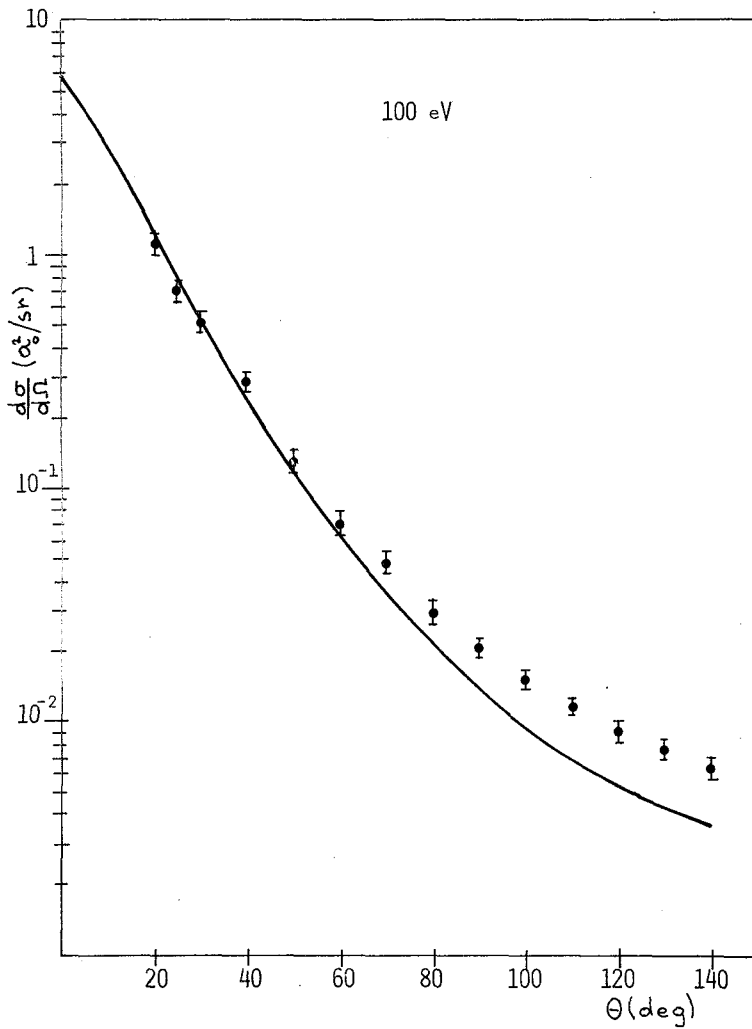


Fig.1 - Elastic differential cross section of 100 eV electrons scattered from atomic hydrogen. \bullet absolute experimental data measured by Williams¹.

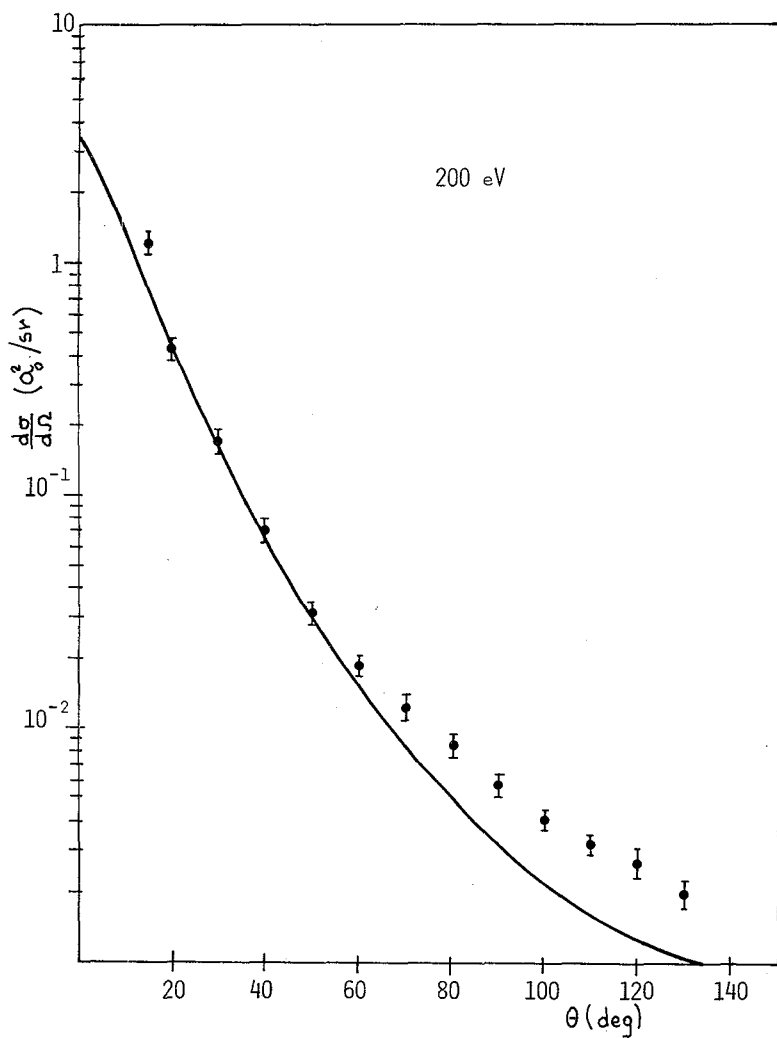


Fig.2 - Elastic differential cross section of 200 eV electrons scattered from atomic hydrogen. \blacksquare absolute experimental data measured by Williams¹.

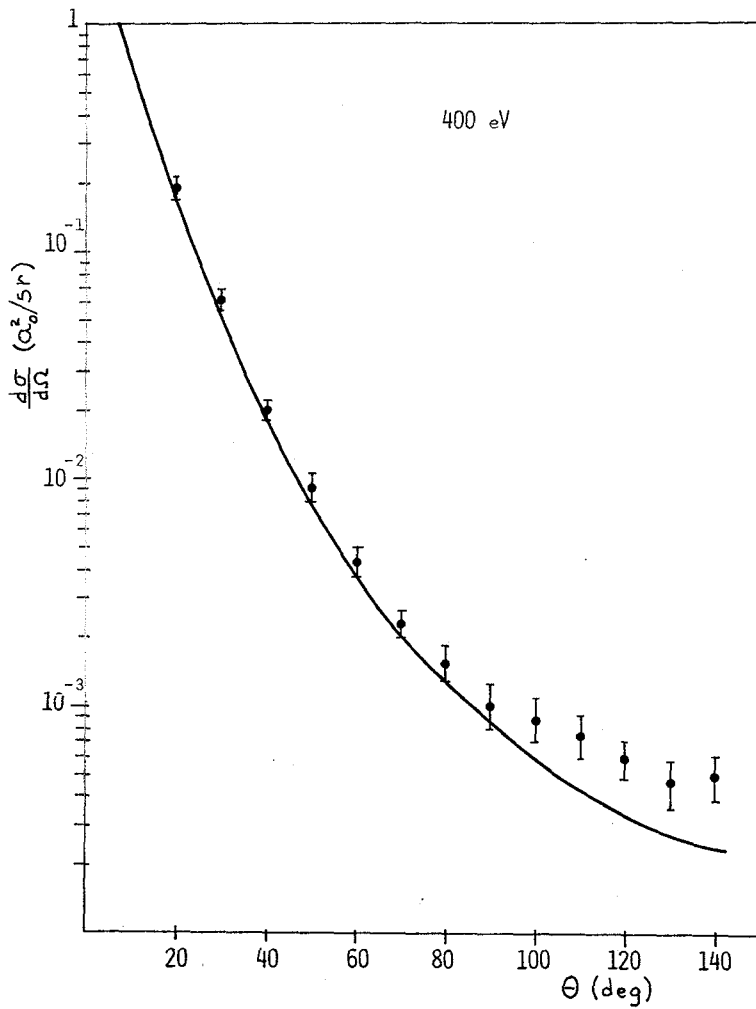


Fig.3 - Elastic differential cross section of 400 eV electrons scattered from atomic hydrogen, \times absolute experimental data measured by Williams¹.

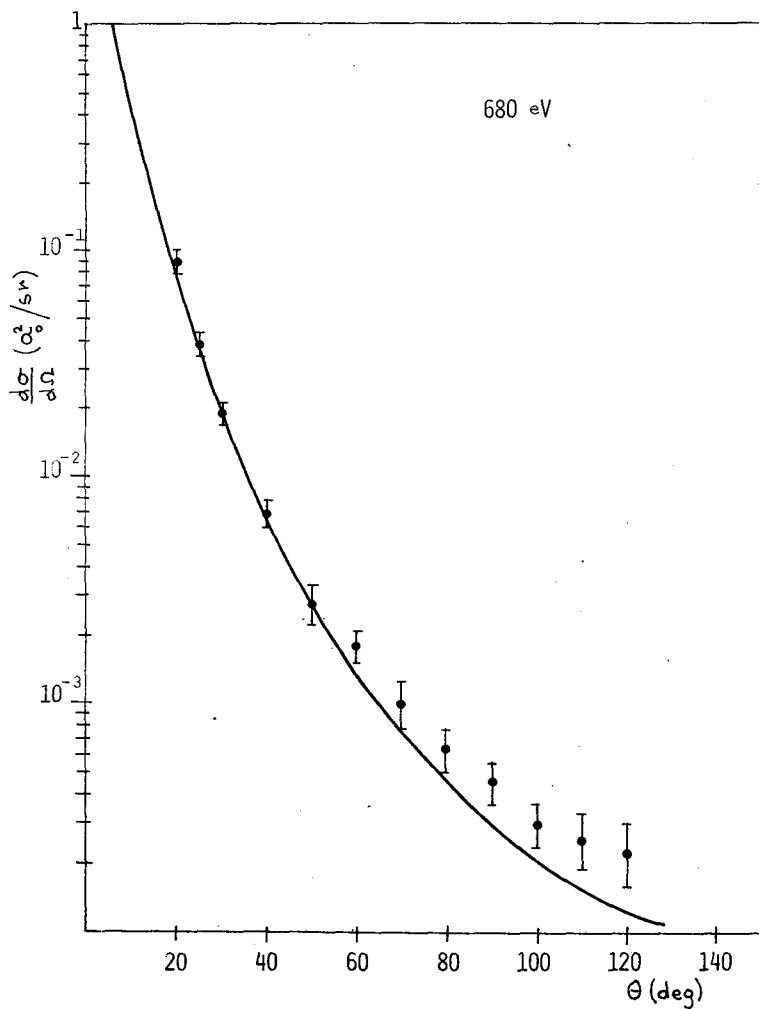


Fig.4 - Elastic differential cross section of 680 eV electrons scattered from atomic hydrogen. \blacksquare absolute experimental data measured by Williams¹.

APPENDIX I

The integrals

$$J(n, m, a, b; p^2) = \frac{d\vec{q}}{(q^2 - p^2 - i\varepsilon) [|\vec{k}_f - \vec{q}|^2 + a^2]^n [|\vec{q} - \vec{k}_i|^2 + b^2]^m} \quad (1.1)$$

can be obtained from the simpler integral

$$J(1, 1, a, b; p^2) = \frac{d\vec{q}}{(q^2 - p^2 - i\varepsilon) [|\vec{k}_f - \vec{q}|^2 + a^2] [|\vec{q} - \vec{k}_i|^2 + b^2]} \quad (1.2)$$

by derivation on a and b . This can be reduced to an one-dimensional integral by using the Dalitz transformation¹⁵. The calculation can be carried out to obtain the following analytical expression for his real and imaginary parts

$$\begin{aligned} \text{Re } J(1, 1, a, b; p^2) &= \frac{\pi^2}{8kpu^{1/2}} [(a^2 + b^2 + 2k^2 - 2p^2) (I(x_1) - I(x_2)) + \\ &\quad + (a^2 - b^2) (x_1 I(x_1) - x_2 I(x_2))] \\ \text{Im } J(1, 1, a, b; p^2) &= \frac{\pi^2}{ku^{1/2}} \ln \left| \frac{(P + a^2)(P + b^2) - 4k^2 p^2 \cos \theta + 2kpu^{1/2}}{(P + a^2)(P + b^2) - 4k^2 p^2 \cos \theta - 2kpu^{1/2}} \right| \end{aligned} \quad (1.3)$$

where

$$I(x) = \text{Re} \left\{ v^{-1/2} \ln \left[\frac{(x+1) [(3a^2 + b^2 + k^2) + (a^2 - b^2 - k^2)x + 4av^{1/2}(x)]}{(x-1) [(a^2 + 3b^2 + k^2) + (a^2 - b^2 + k^2)x + 4bv^{1/2}(x)]} \right] \right\} \quad (1.4)$$

and

$$P = k^2 + p^2$$

$$u = (P + a^2)^2 + (P + b^2)^2 - 2(P + a^2)(P + b^2) \cos \theta - 4k^2 p^2 \sin^2 \theta$$

$$k^2 = 4k^2 \sin^2 \theta / 2$$

$$x_1 = \left[-\frac{1}{2} (a^2 - b^2) \left[P + \frac{1}{2} (a^2 + b^2) \right] + kpu^{1/2} \right] \left[\frac{1}{2} (a^2 - b^2) - p^2 K^2 \right]^{-1}$$

$$x_2 = \left[-\frac{1}{2} (a^2 - b^2) \left[P + \frac{1}{2} (a^2 + b^2) \right] - kpu^{1/2} \right] \left[\frac{1}{2} (a^2 - b^2) - p^2 K^2 \right]^{-1}$$

$$v(x) = \frac{1}{2} (a^2 + b^2 + K^2/2) + \frac{a^2 - b^2}{2} x - \frac{K^2}{4} x^2$$

Let us note that x and x are real quantities, u is always positive, but $v(x)$ can be negative being necessary some are when dealing with the logarithm in Eq. (1.4). With these formulas we can evaluate the integrals appearing in Eqs. (2.17):

$$J(2, 1, a, a; p^2) = -\frac{1}{2a} \frac{\partial}{\partial a} J(1, 1, a, b; p^2) \Big|_{a=b} \quad (1.5)$$

$$J(2, 2, a, a; p^2) = -\frac{1}{2a} \frac{\partial^2}{\partial a \partial b} J(1, 1, a, b; p^2) \Big|_{a=b}$$

Some care should be taken when evaluating the limits $a=b$, $a=b \rightarrow 0$ and $\theta=0$ (Ref.19).

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