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Learning from Numerical Calculations of Ion-Atom Collisions

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Violent collision of two independent many-particle systems, victims, are discussed in the atomic sphere. The asymmetric region where the charge of the projectile Z_p is less than the target nuclear charge Z_n is now well understood though interesting details still need to be worked out. Negatively charged projectiles offer a new illustration of Fadeev re-arrangement collisions. Multi-electron coherence effects illustrate the richness of the field but a symmetric ($Z_p \sim Z_n$) collision treatment is needed. A new one and a half center expansion method promises a solution to this problem. Future areas of interest are discussed.

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I. Introduction

In ion-atom collisions we are concerned with the study of VICTIMS: the violent collision of two independent many-particle systems. Victims in fact are studied in all the branches of physics that use high energy nuclear accelerators. Thus progress in one particular area can be of importance elsewhere. Atomic victims play a unique role in the task of formulating a microscopic theory because the two body force is precisely known and correlations are weak. With such an advantage, is coupled the tremendous diversity of collision partners that can be used in an experiment in atomic victims. For example by using slow light ions incident on lead one can demonstrate factors of fifty in measured ionization cross sections due solely to relativistic properties of the electron wave function in the target nuclear region.¹ This provides a marvelous test of relativistic many-body theory. Alternatively using collision partners that are heavy and symmetric one can produce positrons plucked out of the Fermi sea by strong quantum electrodynamics.² Indeed there appears to be no diminishing of the rate at which new phenomena are appearing in the field even though we are well into the second decade of intense activity.

The work of our theory group has been directed towards producing accurate calculations of ion-atom collisions from first principles.³ There are always two ways of proceeding with a theoretical calculation; one can use analytic approximation schemes, or numerical approximation schemes. Because of the simple long range nature of the coulomb force tremendous progress has been made using the former approach.⁴ We have chosen the latter for three reasons. Firstly because of the analytic schemes we already know what features to include in our model and we do not need the quick felicity in that regard

that such schemes provide. Secondly we always have in mind developing methods which have wider applicability than just pure coulomb force situations. Thus from the very outset we recognize that we must eventually deal with such nasty objects as non-local potentials, configuration interaction, anti-symmetry and so on. Computers are the only way to practically handle these features. Thirdly we wanted methods that within a given model could be methodically increased in accuracy. We make no claim that our numbers are the last word for a given model, but we do have the facility to increase our accuracy if ever that is brought into question. Most analytical schemes do not. Lastly we must confess some impatience with the one electron problem that has proven to be such a barrier to theoretical research in this area. Of course the single electron atom being perturbed by a classically orbiting projectile is the first hurdle to be jumped but in of itself it is not so interesting and it denies to us the full richness of the many-particle nature of our field. We believe we are now past this barrier with a new method that we will describe here. And we look forward to exploring some of the other trees in the forest.

The rest of this talk has four parts. In part II we give a quick review of what we can do with light ions. In part III we present some interesting results for negatively charged projectiles. In part IV we discuss a new phenomena, coherent many electron effects. These are best shown in symmetric collisions. In part V we develop a new theoretical approach that helps us to calculate victims in this region of parameters.

II. Collisions of Light Ions with Light Atoms

Our work so far has been restricted to a non-relativistic treatment of the target. Thus we can only accurately treat light atoms. An extremely

interesting question in this regard is how light do the atoms have to be for a non-relativistic treatment to work; perhaps the experts here will throw some light on this.

In the independent particle model we need only calculate single electron amplitudes and use appropriately anti-symmetrized products to produce expected values of collision events. Integrating these values over the impact parameter, B , gives total cross sections. We are thus concerned with solving the single electron problem

$$\left[i\hbar \frac{\partial}{\partial t} - H \right] \psi = \left[i\hbar \frac{\partial}{\partial t} - H_e(r) - V(\vec{r}; t) \right] \psi = 0,$$

where the time dependence arises from treating the projectile as following a classical coulomb orbit $\vec{R}(t)$ with boundary conditions $\vec{R}(-\infty) = (\vec{B}, -\infty)$.

We solve this problem using a single centered expansion (SCE) method. That is we numerically determine the coefficients $c_n(t)$ in the expansion of ψ in a truncated set of Hilbert basis functions, χ_n , eigenstates to the hamiltonian projected onto the basis. Thus

$$\psi(\vec{r}, t) = \sum_{n=1}^N c_n(t) \chi_n(\vec{r}, t),$$

$$\langle \chi_n | H_e | \chi_{n'} \rangle = \delta_{nn'} \lambda_n.$$

The set χ_n are centered on the target; hence the name of the method. Charge transfer to the projectile in state ϕ_m is not included in the SCE ansatz. If it were we would be using a two centered expansion (TCE) method. However if we restrict ourselves to situations in which the charge of the projectile is much less than Z_n , the charge of the nucleus, then the transfer channel is not a dynamically important part of the process. Its amplitude

can be calculated perturbatively from

$$b_m(\infty) = -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt \langle (i\hbar \frac{\partial}{\partial t} - H) \phi_m | \psi_i \rangle_{(SCE)}, \quad (1)$$

The advantage of the SCE is that being computationally simple a large number of states χ can be included in the calculation. Thus ionization, excitation and charge transfer can be calculated simultaneously.

In figs. 1-2 we show examples of the efficiency of the method. Many more are extant in the literature. Generally we feel confident that in the intermediate energy region with $Z_p \ll Z_n \lesssim 30$, we can now handle most aspects of K-shell collisions. That is not to say we have nothing to learn. Now we have a good calculation we feel that if it does not fit the experiments then they are either wrong or some new physics must emerge. For example we are gradually accumulating evidence for the breakdown of the independent particle model in capture by protons of inner shell electrons due to inelastic collisions with outer shell electrons in the target. This process was suggested by us⁶ and independently by Band,⁷ some five years ago. The evidence is in two parts.⁸ Firstly as the number of electrons in the target atom is increased, measured electron capture cross sections (taken in coincidence with K-shell x-ray production) fall increasingly below the theoretical cross sections. Secondly this does not happen if we increase the charge of the projectile and bind the captured electron more tightly. More experimental and theoretical investigation of this multi-electron effect is needed.

A second piece of physics to emerge recently is the effect of target recoil as a mechanism for excitation and ionization of inner shell electrons. We first became aware of the importance of this mechanism through the work

of Kleber⁸ and a review of it will be given by Trautman in this workshop. To include it in our calculations is trivial. The set ψ_n are now chosen as eigenstates attached to the recoiling nucleus. This ensures orthogonality at all times of the basis states. It also motivates the assertion that first order perturbation theory is sensibly calculated by replacing the full wave-function not by the initial stationary target state as in the first Born approximation but by that same state attached to the recoiling nucleus. We of course do not use perturbation theory but the SCE method. In fig. 3 we show in agreement with Kleber that the small B peak is considerably reduced by inclusion of recoil. The theory is some 20% below the published experimental data⁹ and perhaps Laegsgaard will be able to tell us if it is theory or experiment that is at fault.

There are other experiments in this "well understood" region that do not agree with our calculations such as illustrated in fig. 4. But we have no explanation other than the obvious one that the normalization of the experiment is wrong.

Thus though there may be some surprises it would appear that the theory in this region is well in hand.

III. Negative Projectiles

Brandt¹⁰ was the first author to realize that a parameter available to an atomic experimentalist studying victims is the coupling constant which can be varied by using projectiles of different nuclear charge. He explored the Born series by this device and gave us a very useful and insightful way to view the interference between the first and second Born terms. This theory called the perturbed stationary state (PSS) method introduced the concepts

of increased binding and polarization. Later work added terms to include the effect of coulomb deflection and the relativistic effects, which topics will be covered by Kocbach and Paul in this workshop.

An interesting extension of this idea is to use negatively charged projectiles such as muons. It was proposed at the first Linz workshop (FLW) to perform such an experiment so we have calculated the type of effect that might be obtained in Table 1. Naturally all of the terms change sign for negative projectiles and there is "decreased binding" and so on. It would be very useful if the experiment could be performed to check this prediction but we do not regard the result as particularly exciting. It just illustrates the expected symmetry about the Born result.

A result of much greater importance is obtained by repeating the calculation in a symmetric situation where we would use for example anti-protons and protons on hydrogen, figs. 5-6. Here the expected symmetry about the Born result has largely disappeared. There is little difference between using positive and negative projectiles! The explanation lies in the role that charge transfer plays in the collision. We can turn this channel off in a theoretical calculation. If we do this the symmetry about the Born result for ionization, mainly dominated by the "polarization" returns. The reason that the true calculation for positive projectiles gives the result below the Born is that the "polarization" in this symmetric collision turns into "capture". Electrons which would have been first pulled towards the proton before ionization are now actually captured into bound states on the projectile. They therefore disappear from the ionization channel which destroys the expected symmetry about the Born result. This is a beautiful illustration

of the Brandt picture of the collision and is a logical development that we should have anticipated. Nevertheless we were surprised. The result also dramatically illustrates the "failure" of the Born series to explain what is happening and the importance of "rearranging" the series to allow for capture explicitly. This of course was first pointed out by Fadeev but we do not believe such a clear example has been demonstrated before because usually one does not have the facility to change the coupling constant from positive to negative.

The result was so surprising that we decided to check our code by comparing to the only negative projectile that is easily available as an experimental collision partner with hydrogen, i.e. an electron. Now an electron is very light and using a straight line path is a much poorer approximation than for an anti-proton. Also antisymmetry is being neglected. Another effect is the disparity between the Born cross section calculated in the wave picture and the SCA approach used in our code. To offset this we included a "fudge" factor of this ratio before comparing to experiment. The predicted electron results are in reasonable agreement with experiment, fig. 7. In fact the agreement is so good that it points to another unexpected bonus to wit the possibility of using our codes to explain high energy electron atom scattering. An investigation of this is underway but as it is outside the scope of this workshop it is properly described elsewhere. This does however illustrate directly our opening remarks and the theme of this talk that we do learn a lot about how to calculate many different things when we study victims in atomic processes.

IV. Coherent Multi-electron effects and the Symmetric Region

So far the processes we have talked about are mainly concerned with producing single electron events. But the full richness of our field lies in its many body aspects. Now we must be careful in our understanding here. As we have already pointed out, the great advantage of atomic victims is that two electron correlation effects caused by the two body force in the target are very weak. i.e. the independent particle model is good. Thus atomic victims is not the place to study these two body correlation effects. In fact atomic physics is not the place to study two body force correlations period. It hardly plays any role at all, compared say to nuclear physics. But there is a two body correlation that is important in atomic physics i.e. that due to the exclusion principle. The great advantage atomic physics has is that this is the dominant two body correlation and may therefore be studied separately before embarking on the full problem which we are forced immediately into in nuclear physics.

Because two body force correlations are weak the rearrangement energy is small. Thus when a projectile causes multiple vacancies in the target we may initially at least neglect changes in the average potential that the electrons move in. Experimentalists in atomic physics have instinctively recognized this for a long time, because they often measure inclusive cross sections. This is because the signal that is used to identify a K-shell vacancy is an x-ray. This is emitted whether simultaneously with the K-shell vacancy production there were say two holes produced in the L-shell, and three produced in the M-shell of the target, or not. Inclusive cross sections are now used extensively in other areas of physics but they were first measured in atomic victims.

The advantage that an inclusive measurement has is that in spite of correlations produced by the exclusion principle a very useful theorem can be proven i.e. the single electron theorem. This states that the probability, P_1 , for inclusively producing a hole in state $|1\rangle$ of the original system is given by calculating the probability of a single electron being scattered into any state on the target or projectile that was not occupied before the collision. Mathematically stated this reads as

$$P_1 = \sum_{\text{un-occupied}} |a_{j1}|^2 = 1 - \sum_{\text{occupied}} |a_{k1}|^2$$

Thus strangely enough the many electron richness of an atomic victim is completely suppressed by the lack of two body force correlations. In fact K-shell hole production is a single particle event or more strictly a single anti-particle (or hole) phenomena.

However the many electron aspect of the problem immediately reasserts itself if we ask for the probability P_{12} for producing two holes in states $|1\rangle$ and $|2\rangle$.

$$P_{12} = \begin{vmatrix} 1 - \sum_k |a_{k1}|^2 & - \sum_k a_{k1}^* a_{k2} \\ - \sum_k a_{k1}^* a_{k2} & 1 - \sum_k |a_{k2}|^2 \end{vmatrix} \leq P_1 P_2$$

Here the off diagonal terms in the matrix elements represent a new and dramatic phenomena. i.e. a coherent effect of all the electrons in the system suppressing the single event probabilities. This phenomena is unique to atomic

physics because two body force correlations are unimportant. If they were not, the simplicity of the result would be swamped in the details of two body dynamics.

To evaluate f_{12} we need to be able to calculate the amplitudes with phases of everything that occurs to every electron in the system that possibly connects to the states $|1\rangle$ and $|2\rangle$. Fortunately this information is available from the U matrix method which we use to solve the SCE.

Unfortunately the off-diagonal terms are of lower order in the perturbing coupling constant than the direct terms. Thus in fig. 8, a first attempt to demonstrate these terms, we see that the effect is not large enough to be determined experimentally at least in the region $Z_p \ll Z_n$ unless one proceeds to rather lower velocities.

A simple way out of this experimentally is to raise Z_p to values comparable with Z_n . But how are we to follow theoretically? We need a new method. This is described in the next section.

V. Symmetric collisions: A one and a half centered expansion

As the coupling constant is increased charge transfer plays an important role in electron flux loss from the target. In this region the SCE breaks down. This is illustrated in fig. 9 for protons on hydrogen where the SCE calculation is the solid curve.

A way out of this is to use a TCE method i.e. write

$$\psi_1(\text{TCE}) = \sum_{n=1}^N a_n(t) \chi_n(\vec{r}, t) + \sum_{m=1}^M b_m(t) \phi_m(\vec{r}, t).$$

Unfortunately this method is expensive to use in practice. Also as χ_n and ϕ_m in principle are linearly dependent at convergence the equations to determine a_n and b_m become ill conditioned. If the number of states to included in the calculation is small neither of these problems is too severe but to study these coherent effects we need to include in the calculation all of the occupied states on the target and the projectile, as well as enough positive energy states to span the continuum.

Mathematically speaking there is nothing wrong with an SCE method, it is just difficult to account for the two centered feature of the collision without using a prohibitively large number of states.

We may improve the convergence of the method and solve the linear dependence problem by using a one and a half centered expansion (OHCE) method.

$$\psi_i(\text{OHCE}) = \sum_{n=1}^N a_n(t) \chi_n(\vec{r}_j t) + \sum_{m=1}^{M-1} b_m(\omega) \beta_m(t) \phi_m(\vec{r}_j t).$$

Here the coefficients $a_n(t)$ and $b_m(\omega)$ are unknown. But $\beta_m(t)$ is specified as some given function satisfying boundary conditions

$\beta_m(-\infty) = 0$, $\beta_m(\infty) = 1$. This device allows the two centered aspect to be handled while leaving the set $\{\chi_n\}$ to handle the variation of ψ_i in the interaction region.

The coefficients $b_m(\omega)$ can be found by applying one of two sets of constraints. A constraint

$$\int_{-\infty}^{\infty} dt \langle \phi_m | i\hbar \frac{\partial}{\partial t} - H | \psi_i(\text{OHCE}) \rangle = 0,$$

is identical to that of eq (1) and is therefore called a perturbative approach.

An alternative method is to use the ansatz

$$\int_{-\infty}^{\infty} dt \beta_m(t) \langle \phi_m | i\hbar \frac{\partial}{\partial t} - H | \psi_1(OHCE) \rangle = 0.$$

This guarantees that $|\psi_1|^2$ is unity at large positive or negative times. It is therefore called the unitary approach. In fig. 9 application of this method is seen to remove the problem that the SCE method developed at low energies in proton-hydrogen ionization. In figs. 10-13 we compare the perturbation method with experiment and other theories for the proton, alpha particle and single electron system. It works very well. Thus the symmetric region no longer presents a theoretical problem.

VI. Future Problems

At FLW we outlined several aspects of ion-atom collisions which we intended to investigate. We feel that negatively charged particles can be handled and the theoretical difficulties of symmetric collisions has now been largely removed. At last we are penetrating into the really interesting many electron properties of our field. But many things remain to be done.

1) The single electron problem has not been solved when the charge of the projectile is much greater than that of the target.

2) High Rydberg states offer a fascinating area of study in the future. The classical treatments of these states assume that just because the initial state of the target is classical that it follows that it will remain classical throughout the collision. That assumption must be tested.

3) Recoil effects are present when neutrons collide with atoms. It would be interesting to see impact parameter measurements of ionization due to this mechanism. Potentially accurate measurements of the long range nuclear force are possible by this method.

4) L-shell ionization is still an area that is largely untouched theoretically by modern techniques.

5) Interference between nuclear and atomic processes is only just getting started but promises many interesting problems.

In summary, though much has been learned we need still to learn much more about how to perform numerical calculations of ion-atom collisions.

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Table 1. K Shell Ionization Cross Sections (Barns)
Effect of Deflection and Increased (Decreased) Binding
Illustrated with Positive and Negative Muons
Bombarding a Copper Target

Energy (MeV/amu)	1	1.7	2.2
<u>Positive Muons</u>			
Deflection & Binding	7	41	89
Binding, no Deflection	16	62	109
<u>Straight Line Born</u>	22	74	128
<u>Negative Muon</u>			
Binding, no Deflection	32	95	151
Deflection & Binding	56	117	178

Figure Captions

Fig. 1. Expected value as a function of impact parameter for ionization of a K-shell electron by protons at 700 keV in collision with Neon. Experimental results from Pedersen.⁵

Fig. 2. Expected value as a function of impact parameter for K-shell electron capture by protons at 1 MeV in collision with Neon. Experimental results from Pedersen.⁵

Fig. 3. The expected value of K-shell vacancy production by 0.5 MeV protons in collision with a copper atom. The dashed curve is a calculation including Coulomb deflection but not recoil, the solid curve includes the recoil of the copper nucleus. Experiments are from Anderson et al.⁹

Fig. 4. Expected value for K-shell ionization by protons at 200 keV in collision with a carbon target atom. Experiments from Pedersen.⁵

Fig. 5. Total excitation and ionization cross sections divided by the first born cross section for protons and anti-protons on the hydrogen atom. The results are plotted as a function of the projectile laboratory energy in keV.

Fig. 6. Total excitation cross sections divided by the first born cross sections as in fig. ⁵/₆.

Fig. 7. Cross sections in units of πa_0^2 multiplied by incident laboratory energy in electron volts plotted against that energy for electrons incident on hydrogen. For $1s \rightarrow 2s$ the experimental points are from Kauppila et al.,¹¹ with the $0.23 \cdot (1s \rightarrow 3p)$ cascade contribution subtracted (using our calculated $1s \rightarrow 3p$ cross section). The absolute normalization of the Kauppila et al. results is fixed by that of the $1s \rightarrow 2p$ cross section. For $1s \rightarrow 2p$ the experimental points are constructed from the measurements of Long et al.¹¹ using

the Lyman- α polarization fractions of Ott et al.¹¹ In their paper Long et al. placed their measurements on an absolute scale by normalizing at 200 ev to the PWBA. We have normalized their experiment to our coupled state cross section at 200 ev; this increases their cross section by about 5%.

Fig. 8. Charge-transfer-K-shell hole coincidence cross sections $\sigma_{C,VK}^{IPM}$ and $\sigma_{C,VK}^{SP}$ for protons, alpha-particles and lithium ions in collision with Neon. The experimental points are from Rydberg et al, except the solid squares which are from Cocke et al.¹³ The cross section $\sigma_{C,VK}^{IPM}$, calculated in the independent particle model (IPM), includes multi-electron contributions. It rises as the perturbation increases to lie above the calculation performed as if there were only a single electron present, σ_{CK}^{SP} . More experiments with more highly charged projectiles are needed to verify this theoretical prediction. The cross section σ_{CK}^{SP} can be measured by adding and subtracting electrons on the projectile.

Fig. 9. Cross section (in units of 10^{-15} cm^2) for ionization in proton-hydrogen collisions. The solid curve, crosses, and open circles are the results of our single centered expansion, perturbative OHCE, and unitary OHCE calculations, respectively. The experimental points (with error bars) are from the following sources: triangles, Park et al¹⁴; squares, Fite et al¹⁵; circles, Gilbody and Ireland.¹⁶

Fig. 10. A comparison of theoretical cross sections for protons on singly charged helium ions initially in the 1s, 2s, and 2p states. The triangles are an eleven state TCE calculation by Rapp,¹⁷ and the solid curves are by the same author with an eight state calculation. The solid squares connected by a smooth curve are the results of the perturbative OHCE calculation.

Fig. 11. Comparison of cross sections for ionization of singly charged helium by protons. The solid curve through solid squares is the OHCE calculation. The experimental data by Angel et al.¹⁸ is indicated by closed triangles. The open squares are the results of a classical calculation by Olsen.¹⁹

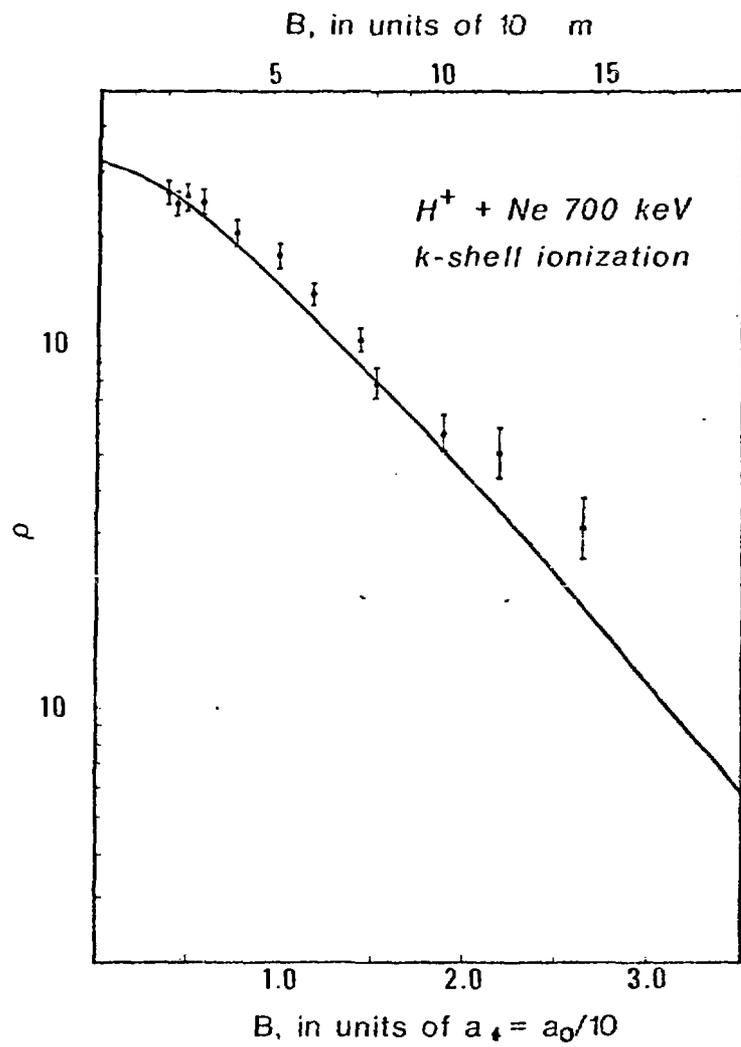
Fig. 12. Comparison of OHCE experimental and classical cross sections for total electron loss caused by protons incident on singly charged helium. Notation as in fig. 11. The circles are from experiments by Peart et al.²⁰

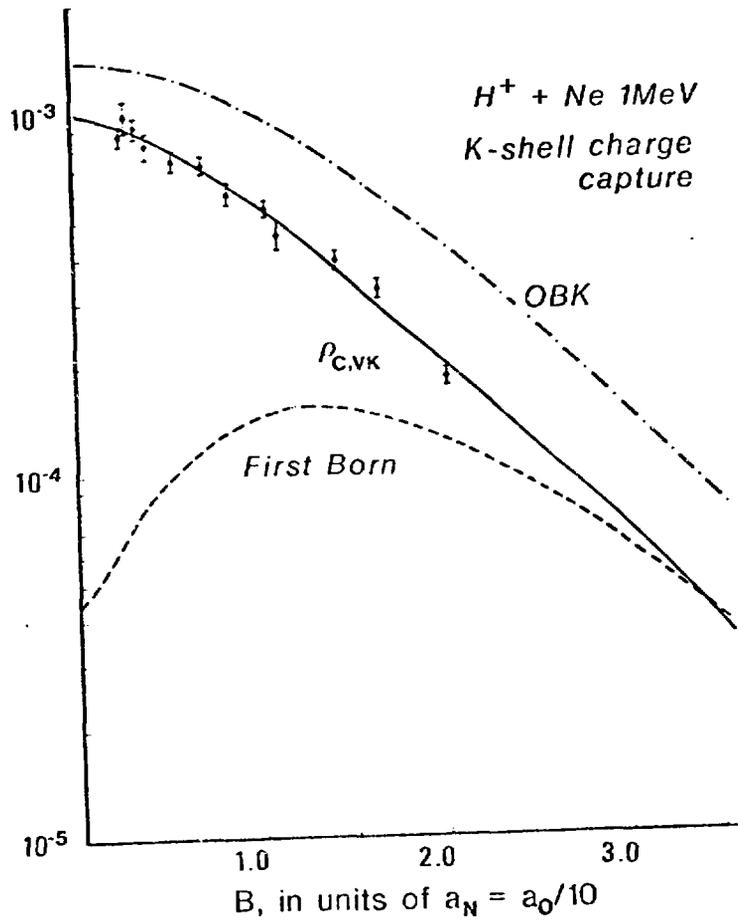
Fig. 13. Comparison of OHCE and experimental cross sections for alpha particles incident on hydrogen. The diamonds are the results of our OHCE calculation. The solid line with dots is the experimental result due to Olsen et al.²¹

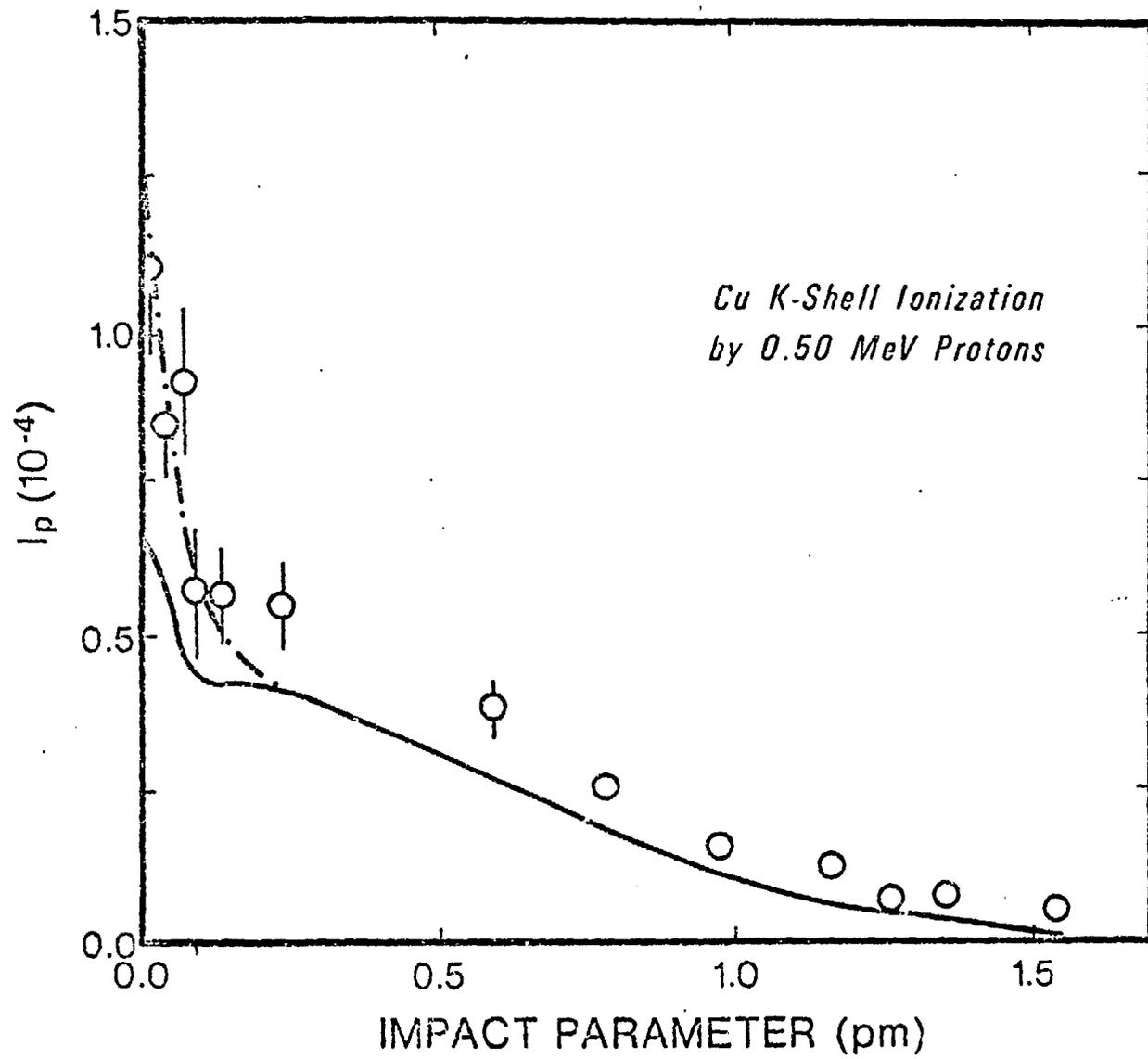
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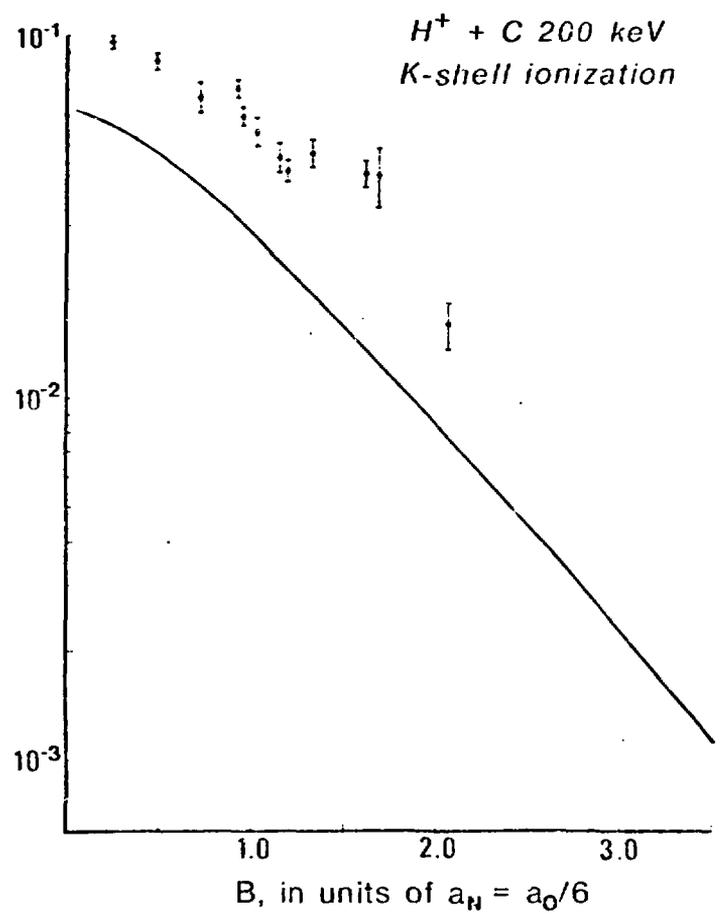
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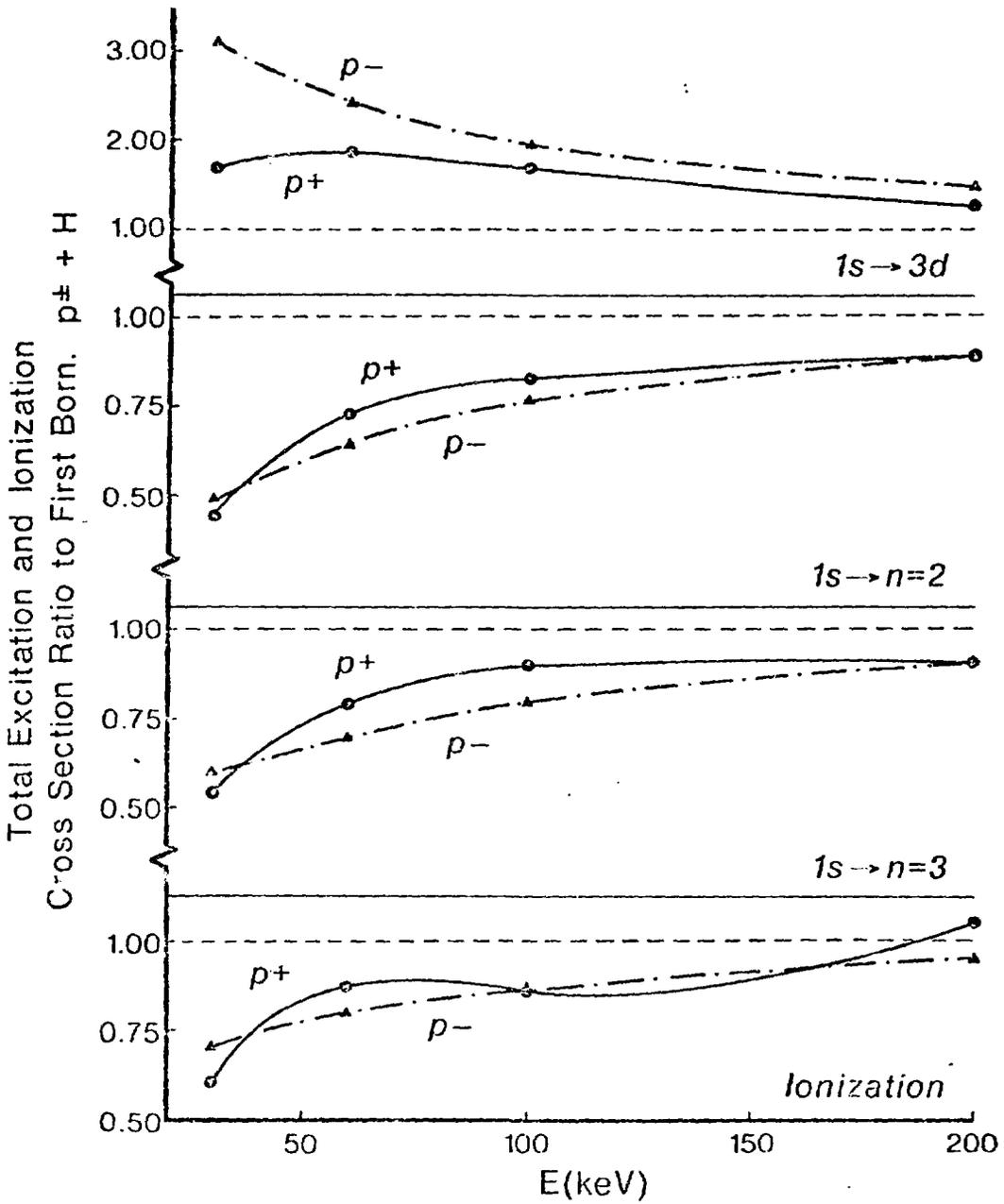
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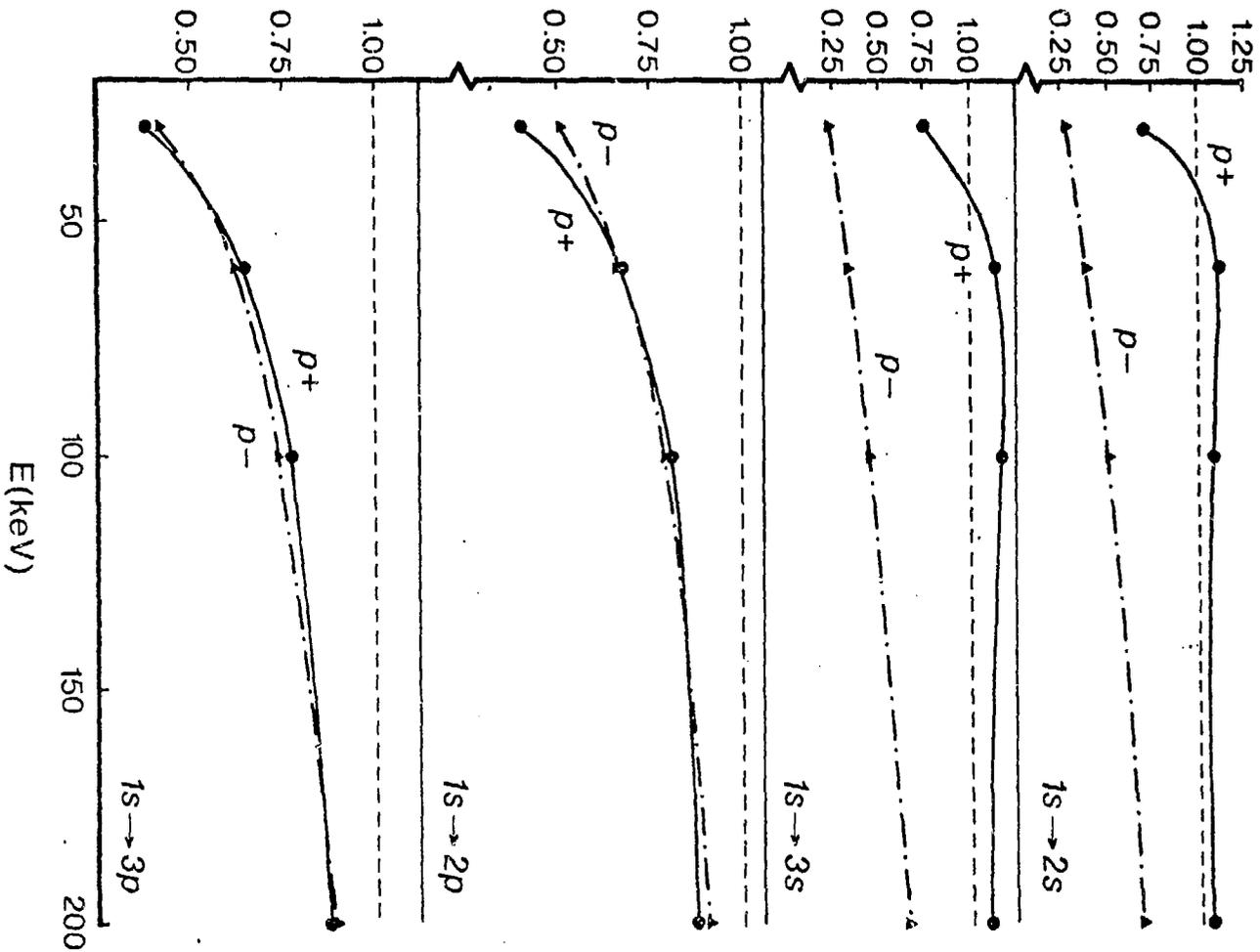


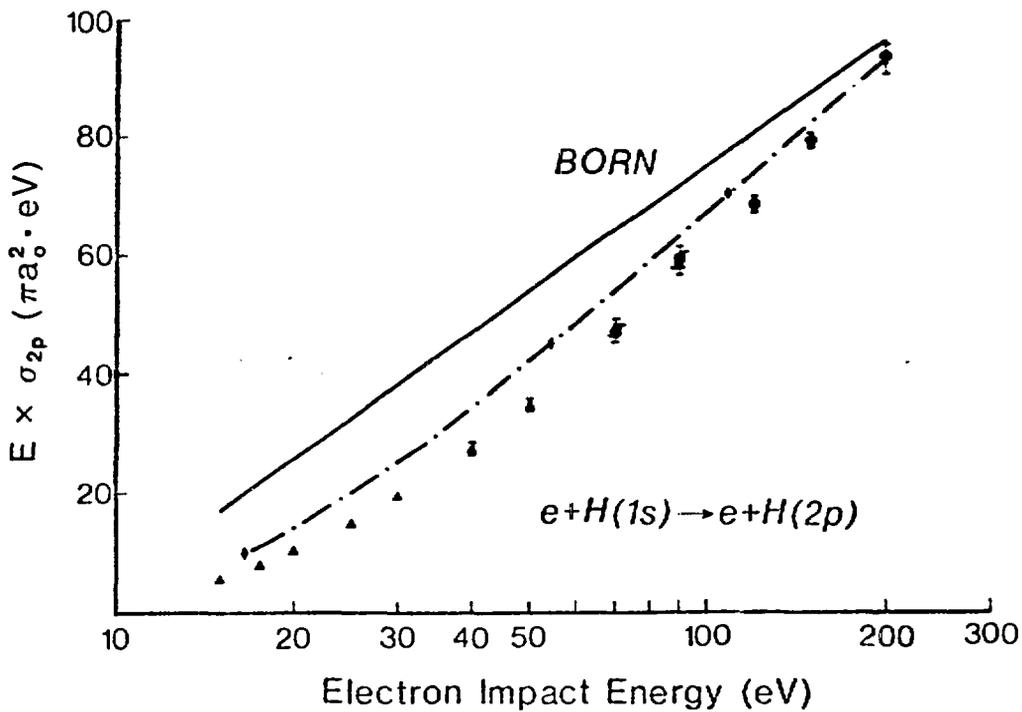
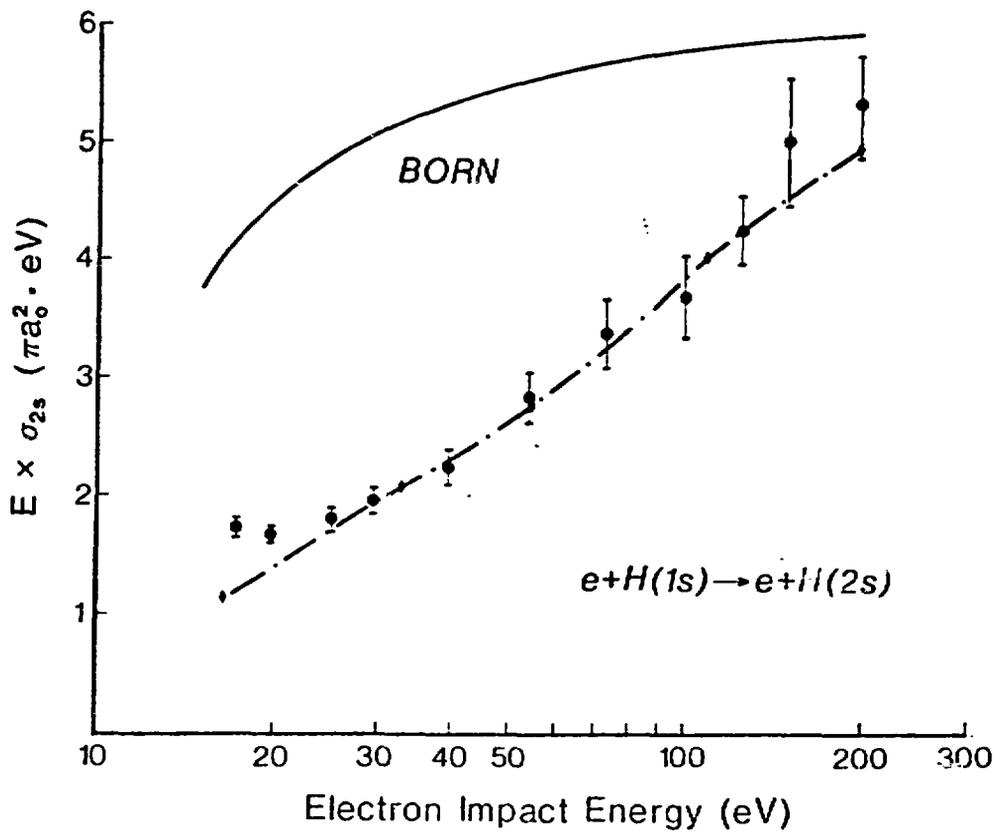






$n = 2,3$ Ratio of Cross Section to First Born. $p^\pm + H$





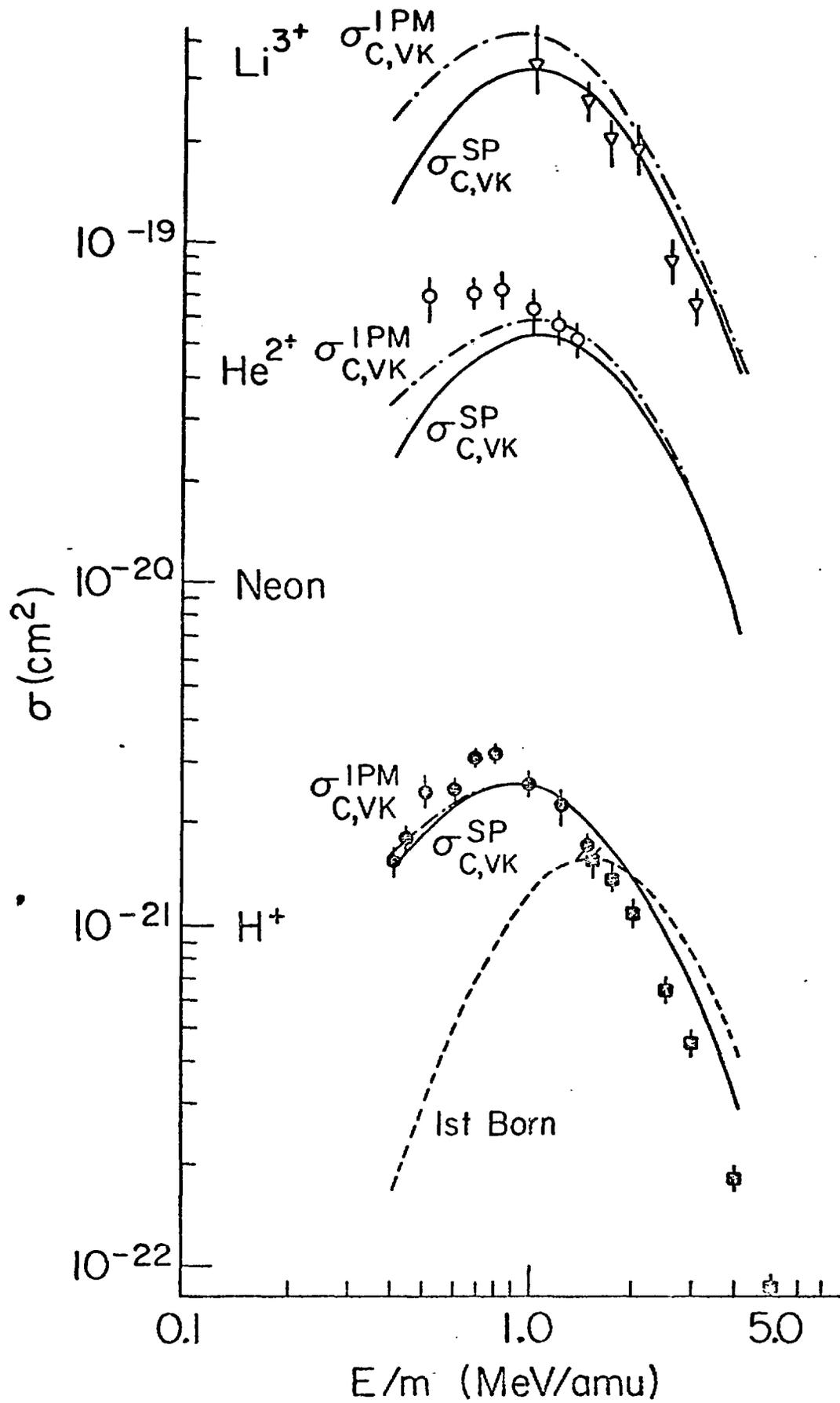
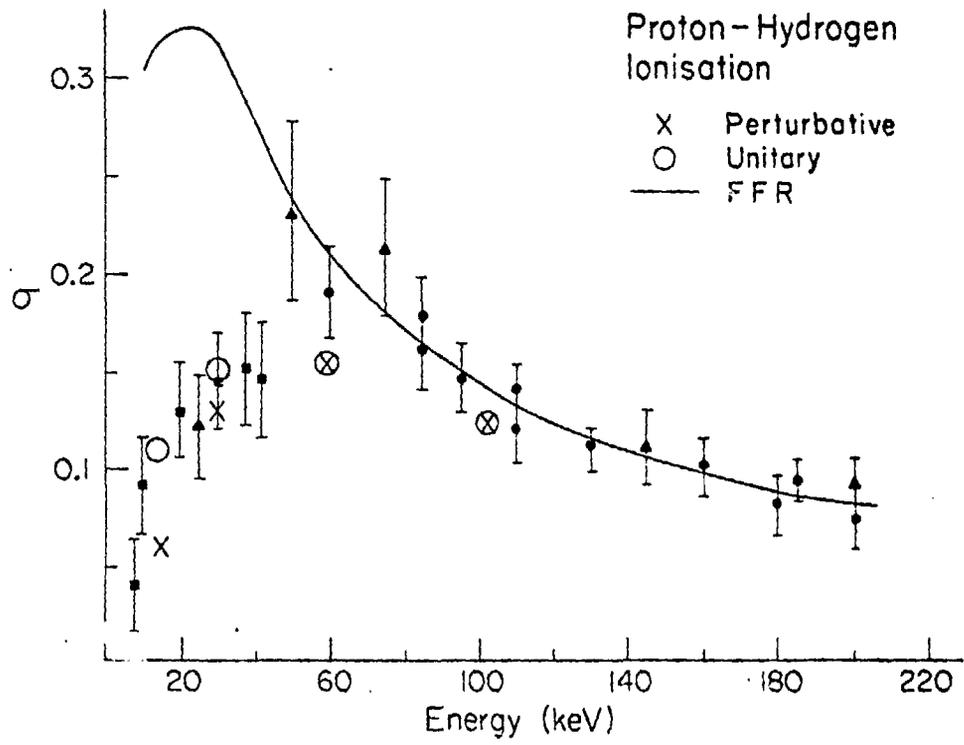


Fig 1
P. 113



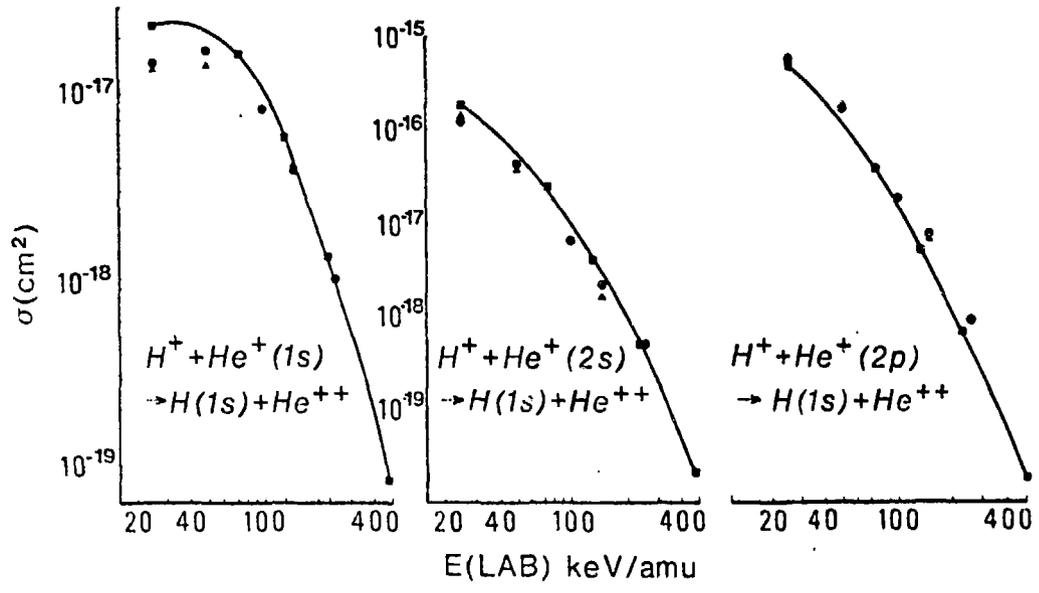


Fig. 11
Rambold

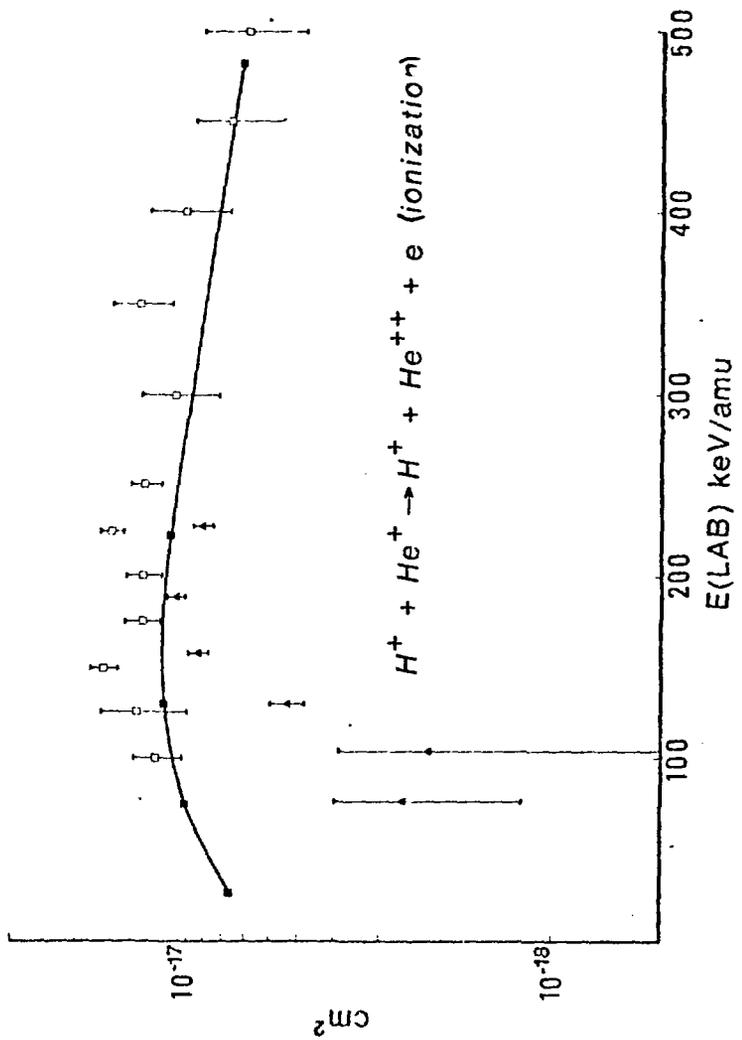


Fig 1
Reading
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