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ABSTRACT

The present review briefly presents the growing experimental as well as theoretical interests in recent years in the double-continuum wave functions and double-photoionization cross sections of two-electron systems. The validity of existing double-continuum wave functions is analysed and the importance of electronic correlations in both the initial as well as final states wave functions involved in the transition amplitude for double-photoionization process is demonstrated. At present, we do not have comprehensive and practical double-continuum wave functions which account the full correlation of two-electron in the continuum. Basic difficulties in making accurate theoretical calculations of double ionization by a single high energy photon especially in the vicinity of the threshold, where the correlation plays an important role, are discussed. Illuminating, illustrative and representative examples are presented in order to show the present status and the progress in this field. Future challenges and directions, in high-precision double-photoionization cross sections calculations, have been discussed and suggested.

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1 Introduction

The subject of various forms of double-continuum wave functions is of growing interest to theorists because it is needed to solve a very broad range of problems, for example, double-photoionization, photo double detachment of negative ions, inner-shell photoionization followed by Auger process, electron impact single ionization, inner-shell excitation by electron impact which leads to autoionization, threshold law, etc. To obtain a full solution of the Schroedinger equation for two-electron system in any coordinate system was practically not feasible until now. Asymptotic solution is feasible. Knowledge of accurate asymptotic double-continuum wave functions is indispensable in order to perform a reliable theoretical calculation employing an elaborate method. For example, the R-matrix[1] method requires accurate functions in the outer region, i.e. asymptotic region. Asymptotic wave functions are also used in deriving threshold law. Wannier hypothesis, which is built also in the Wannier-Rau-Peterkop (WRP)[2–4] theory, is that the probability for the double escape of two electrons is determined only by the long range interaction, i.e. the Coulomb interaction in the zone II and III as shown below.

I	II	III
Reaction zone	Coulomb zone	Outer zone

Due to this assumption only the asymptotic part of the wave function should be considered. *Rosenberg*[5], Rudge and *Seaton*[6], *Rudge*[7], *Peterkop*[8] and Burke et *al*[9] have investigated the asymptotic double-continuum wave functions. In the threshold law, the exponent of the excess energy depends only on the final state wave function, i.e. the asymptotic part of the double-continuum wave function.

Double photoionization consists in the absorption of a single photon by an atom or a molecule followed by a simultaneous ejection of two electrons. The interaction of a photon with each electron is independent from the others so that double photoionization is a forbidden process unless the electronic correlation is taken into account. If two electrons with small kinetic energies leave the residual positive ion, the motion is strongly influenced and controlled by their mutual repulsion due to the Coulomb interaction ($\frac{1}{r_{12}}$). The interaction leads to the exchange of energy and angular momentum over long distances and therefore implies a correlation between outgoing electrons. The final state consists of an ion and two continuum electrons i.e.

$$\gamma + X = X^{++} + e^- + e^- \tag{1}$$

For the He atomic system, extensive investigation[10–28] of double photoionization process has been made. For H^- system, Donahue et al.[29] have studied the double-photoionization cross-section in detail. For the H_2 system, Dujardin et al.[30] and Le Rouzo[31] have studied the double-photoionization cross section. Threshold law for the double photoionization has also been discussed[32–52]. In the case of complex atoms and molecules, the double photoionization (DPI) process can be divided into two classes (a) the normal Auger process via core ionization and (b) the resonant double Auger process via resonant core excitation. From a theoretical point of view, multi-electron atoms, molecules and ions are extremely difficult because of the core.

The main reasons for choosing double-continuum wave functions and double-photoionization of He, H^- and H_2 in this review are:

(1) Various forms of asymptotic double-continuum wave functions are

available but in the close vicinity of threshold of double *photoionization*[53–74], where full correlation plays an important role, accurate double continuum wave function was not obtained until now. Accurate double-continuum wave functions have been a long standing and challenging problem for theorists. Several possibilities are explored in this review.

(2) The double-photoionization has the advantage that this is dominated by electric dipole transition and the resulting final state is pure and well defined. In the case of He, H^- and H_2, the final state consists of nucleus and two outgoing electrons and hence there are no complications due to core and offers the best opportunity to test the validity of double-continuum wave function[75–79].

(3) A number of experimental observations and theoretical predictions of double photoionization cross *sections*[80–92] are available for two-electron systems but there is considerable discrepancy between experiment and theory which indicates that the probability for the DPI process in atoms, molecules and ions is significant because of electronic correlations. Electronic correlations have been extensively intestigated by Tiwary and his co-workers[93–133].

2 All existing double-continuum wave functions

2.1 Product of two Plane wave *functions*[10]

$$\Psi(r_1, r_2) = e^{ik_1 \cdot r_1} e^{ik_2 \cdot r_2} \tag{2}$$

2.2 Product of Plane wave and Spherical wave *functions*[10]

$$\Psi(r_1, r_2) = e^{ik_1 \cdot r_1} \frac{e^{ik_2 r_2}}{r_2} \tag{3}$$

2.3 Redmond wave *function*[5]

$$\Psi(r_1, r_2) = e^{ik_1.r_1} e^{ik_2.r_2} e^{i\gamma} \tag{4}$$

where, $\gamma = \frac{Z}{k_1} ln(k_1.r_1 + k_1 r_1) + \frac{Z}{k_2} ln(k_2.r_2 + k_2 r_2) + \frac{1}{k_{12}} ln(k_{12}.r_{12} + k_{12} r_{12})$

2.4 Product of two unscreened Coulomb wave *functions*[10]

$$\Psi(r_1, r_2) = N[\phi_{\epsilon_1}(r_1)\phi_{\epsilon_2}(r_2) + \phi_{\epsilon_1}(r_2)\phi_{\epsilon_2}(r_1)] \tag{5}$$

where,

$$\phi_\epsilon(r) = N' F_l(\frac{\eta_e}{k_e}, r) y_{lm}(r)$$

$$F_l(k, r) \approx (2kr)^l e^{ikr} {}_1F_1(i/k + l + 1, 2l + 2; -i2kr)$$

2.5 Brauner et al wave *function*[79]

$$\begin{aligned} \Psi(r_1, r_2) = e^{ik_1.r_1} {}_1F_1(\frac{i}{k_1}, 1; i(k_1.r_1 + k_1 r_1)) \\ e^{ik_2.r_2} {}_1F_1(\frac{i}{k_2}, 1; i(k_2.r_2 + k_2 r_2)) \\ e^{ik_{12}.r_{12}} {}_1F_1(\frac{i}{k_{12}}, 1; i(k_{12}.r_{12} + k_{12} r_{12})) \end{aligned} \tag{6}$$

2.6 Altick monopole wave *function*[75]

$$\begin{aligned} \Psi \approx \rho_1^{\frac{i}{k_1}} e^{ik_1\rho_1} \rho_2^{\frac{i\zeta}{k_2}} e^{ik_2\rho_2} \\ + \rho_2^{\frac{i}{k_1}} e^{ik_1\rho_2} \rho_1^{\frac{i\zeta}{k_2}} e^{ik_2\rho_1} \end{aligned} \tag{7}$$

$$[(\rho_1\rho_2)^{-\zeta_1}(1-\frac{\zeta_1\rho_1}{\zeta_2\rho_2}/1-\frac{\zeta_1}{\zeta_2})^{\zeta_1-\zeta_2}]$$

2.7 Altick dipole wave *function*[76]

$$\begin{aligned}\Psi \approx \rho_1^{\frac{i}{k_1}} e^{ik_1\rho_1}\rho_2^{\frac{i\zeta}{k_2}} e^{ik_2\rho_2} f_{l_1l_2}(y) \\ +\rho_2^{\frac{i}{k_1}} e^{ik_1\rho_2}\rho_1^{\frac{i\zeta}{k_2}} e^{ik_2\rho_1} \\ [(\rho_1\rho_2)^{-\zeta_1}(1-\frac{\zeta_1\rho_1}{\zeta_2\rho_2}/1-\frac{\zeta_1}{\zeta_2})^{\zeta_1-\zeta_2}]g_{l_1l_2}(y)\end{aligned} \tag{8}$$

2.8 Peterkop wave *function*[8]

$$\Psi \approx A(\Omega)R^{-n_0}e^{iS_f+i\gamma} \tag{9}$$

where Ω = a set of five angular variables

and

$$\gamma = \omega(\Omega)lnR + \beta(\Omega)$$

$$R = \sqrt{(r_1^2 + r_2^2)}$$

2.9 Rau wave *function*[3]

$$\Psi_{\epsilon\to 0} = \chi(R)e^{iCR^{\frac{1}{2}}(1+a\beta^2+\frac{b}{16}\gamma^2)} \tag{10}$$

where

$$\chi(R) = R^{-(a+b+9/4)}$$

$$a = (-1 + 2\mu)/8$$

$$b = (-1 + i2\rho)/4$$

$$c = \sqrt{(}8z_0)$$

$$\mu = \frac{1}{2}((100z - 9)/(4z - 1))^{\frac{1}{2}}$$

$$\rho = \frac{1}{2}((9 - 4z)/(4z - 1))^{\frac{1}{2}}$$

2.10 Rudge-Seaton wave *functions*[6]

$$\Psi_{\epsilon=0} \approx BR^{(n-\frac{5}{2})}e^{iAR^{\frac{1}{2}}} \tag{11}$$

$$\Psi_{\epsilon\neq 0} \approx (-i)^{\frac{1}{2}}(\frac{k^3}{R^5})^{\frac{1}{2}} f(kr_1 sin(\alpha), kr_2 cos(\alpha)) \tag{12}$$
$$e^{i(kR+\zeta(r_1 r_2,\alpha))/k} ln(2kR)$$

2.11 Burke et al wave *function*[9]

In the new R-matrix theory, two continuum electrons are expanded in terms of a continuum R-matrix basis. In addition, a two-dimensional R-matrix

propagator approach is developed that enables the internal region to be subdivided and highly excited target states that extend out to large distances to be treated. Analytical forms of this double continuum wave function as well as application of this function to double photoionization process are not available in the literature.

2.12 Double-continuum wave functions in the entire space

Asymptotic wave functions are not adequate at small distances. One needs wave functions which are valid in the entire configuration space, i.e. double-continuum wave functions which can be obtained solving the Schroedinger equation for two-electron systems without imposing any constraints but unfortunately this is not feasible. For this reason, we will describe several possible models which are valid in different physical situations.

Models without correlations: Independent particle

At very high incident energies, two ejected electrons are very far away from the residual ion, one can argue that two escaping electrons do not experience Coulomb force. Under this situation, one can describe two electrons by a product of two plane waves. A product of two plane waves gives the threshold law which differs completely from the experimental threshold law. No matter how far or how fast electrons are, they always experience Coulomb force. Hence, this model is the crudest model and is used in the first Born approximation. Since electrons always experience Coulomb force, such a widely used model is the product of two Coulomb wave functions. This model has been used in the calculation of double photoionization cross section of helium and hydrogen molecule. Since this model does not contain correlation, hence it gives linear threshold law which disagrees with experiment. Another possible physical situation may occur at an intermediate

energy range that one electron is slow and another fast. The slower electron may screen the fast one. In this case, one electron can be described by the Coulomb wave function and the faster one can be described by the plane wave. This model also gives the threshold law which disagrees with the experiment. For reliable calculations of double photoionization cross section, one needs correlated double-continuum wave function especially in the vicinity of the threshold where electron correlations play an extremely important role in order to obtain accurate results. Such wave functions are not available in the literature.

Recently, Burke et al.[9] have developed a new R-matrix formulation to handle double-continuum wave functions but there were no results available until now. Other possibilities, which will be feasible in the near future, are a combination of the standard R-matrix with (1) Altick asymptotic wave function, (2) hyperspherical function, (3) screened Coulomb function and (4) distorted wave function with dynamic screening.

3 Threshold Laws

There has been growing interest in the extensive theoretical and experimental investigations of threshold laws for escape processes, for example, double photoionization, electron impact ionization, etc. in atoms, molecules and ions because these laws provide answers of many fundamental questions in physics. A number of theoretical and experimental studies of these laws have been made for different escape processes. As we have mentioned earlier in this review, our main emphasis will be to study double photoionization threshold law in atoms, ions and molecules, i.e.

$$h\nu + X \rightarrow X^{++} + e^- + e^- \tag{13}$$

where X stands for atom or molecule or ion.

This requires a solution of three charged particles with Coulomb forces acting between them. The final state of reaction (13) consists of $X^{++} + e^+ + e^+$ where there are two attractive Coulomb forces , each electron being attracted by residual ion X^{++} and one Coulomb repulsive force, electron-electron interaction ($\frac{1}{r_{12}}$). If we ignore the repulsive force, the quadratic dependence on E would be reduced to a linear dependence on E. If the double-continuum electrons are represented by a product of two Coulomb wave functions, one can expect a linear threshold law because only two attractive Coulomb forces have been taken into account. Complication arises when three charged particles with Coulomb interaction are considered because of the electron correlation. To represent the final two-electron into the continuum as a product of single particle functions is only an approximation and even then there are different choices. For example, one could argue that in the neighbourhood of the threshold, as two electrons escape, there is some discrepancy in how the energy is partitioned between them, so that the slower one sees the full Coulomb field of the residual ion and the faster sees a completely screened and therefore neutral field. In this case, the final state is a product of a Coulomb wave function and a plane wave function and then there is only one ($\frac{1}{k}$) factor, so that

$$\sigma^{2+} \propto \epsilon^2 \tag{14}$$

Different assumptions on the relative screening in the escape process lead to different threshold laws. A successful threshold theory provides information on the mutual dynamic screening and mutual Coulomb repulsive interaction.

The double photoionization threshold law is

$$\sigma^{2+} \propto \epsilon^{\beta} \tag{15}$$

where $\epsilon = \epsilon_1 + \epsilon_2$ = excess energy available to two-continuum electrons.
$= (E_\gamma - I^{2+})$ if the residual ion is in the ground state
$_\gamma$ = incident photon energy
I^{2+} = double ionization threshold
and $\beta = exponent = 1.056$
or

$$\sigma^{2+} = \sigma_0 \epsilon^{\beta} \tag{16}$$

where σ_0 is the constant of proportionality and $\sigma_0 = \sigma^{2+}$ at $\epsilon = 1$ eV
where exponent β depends only on the final state wave function i.e. the double-continuum wave function. It reflects that the accuracy of double-continuum wave function can be tested calculating the exponent, i.e. β offers the best opportunity to test the accuracy of the final state wave function. The question is how the accuracy of the initial state wave function plays an important role in obtaining reliable double photoionization cross section. One can argue that σ_0 depends on the accuracy of the ground state wave function. Another question that immediately arises is: does σ_0 depend only on the initial state or both initial and final states wave functions? There are many questions which one can ask. Byron and Joachain[10] have calculated the double photoionization cross sections using the correlated wave function for the ground state and uncorrelated wave function for the final state. Their results are not in agreement with the recent experiment which indicates that the correlation in the final state is necessary. Le Rouzo has performed a similar calculation for the DPICS of hydrogen molecule. His result is

in good agreement with the experimental data of Dujardin et al. He has obtained the linear threshold law which is valid up to about 10 eV above the threshold. Tiwary[19-23] has performed a calculation of DPICS of He using the correlated initial state wave function and the partially correlated final state wave function and obtained in good agreement with experimental data in the intermediate and high energy range but in the vicinity of the threshold the situation is unsatisfactory. This may be due to the lack of full correlation in the final state wave function because the correlation is extremely important in the neighbourhood of the threshold. Carter and Kelly[24] have calculated the DPICS of He using the many-body perturbation theory (MBPT). They have obtained good agreement with the experiment. Since their approach is a non-wave function approach it is difficult to draw to any definite conclusion.

3.1 Experimental Test of WRP

Threshold Law for Double-photoionization of He

Very recently, Kossmann et al have performed an extensive experimental investigation of the threshold law for the cross section of double photoionization of He. Figure 3a represents experimental results of Kossmann et al for the threshold cross section of double photoionization of He from threshold to 83 eV photon energy. Figure 3b exhibits the same data but smaller and enlarged energy scale. The solid line in both figures represents in a limited energy range a least square fit of the experimental data by the power law of equation (16) . Because of the small difference between a linear threshold law ($\beta = 1$) and the expected $\beta = 1.056$ non- linear threshold law, it appears from figure 3 that the linear threshold law is valid for the double

photoionization of He. A quantitative analysis of results clearly shows that WRP threshold law is valid because theoretical $\beta = 1.056$ and experimental $\beta = 1.05 + 0.002$ clearly demonstrate that it is indispensable to include full correlations in both initial as well as final states involved in the transition in order to obtain reliable results.

3.2 Double-photoionization of He ($^1S^e$)

Double photoionization of noble gas atoms has been of great interest to both experimentalists as well as theorists because double-electron photoionization in noble gases gives fundamental information on the electronic correlation. Helium, which is the simplest noble gas atom is more interesting because there are no complications due to core in the double photoionization process. A number of experiments and calculations have been carried out for the DPI of He. Figure 1 displays all available experimental as well as theoretical ratio of double to single photoionization cross sections. For the first time, Byron and Joachain performed a calculation for the DPI of He using uncorrelated wave functions for both ground as well as the final states and correlated wave function for the ground state and uncorrelated product of two Coulomb wave functions with effective charge 2 for both outgoing electrons for the final state (reaction is shown below).

$$h\nu + He \rightarrow He^{++} + e^- + e^- \qquad (17)$$

Results of DPI of He with uncorrelated wave functions, for both initial and final states involved in the transition amplitude, are extremely small, which indicate that the probability of the DPI process is very poor without correlations. Results with almost fully correlated wave function for the

ground state and uncorrelated wave function for the final state are in excellent agreement with the first experiment of Carlson (see figure 1). The agreement suggests that the correlation is important in the initial state, not in the final state. The recent experimental observations of Holland et al.[12] disagree considerably throughout the energy range of consideration with the experimental data of Carlson[11] and the theoretical prediction of Byron and Joachain[10]. This experimental result suggests that correlation, probably, is equally important in both initial and final states involved in the transition. Results of Holland et al. are in accord with the experimental points of Schmidt et al. at low energies and tend to lie lower than the curve of Wight and Van der Weil[14].

Brown[15] has reevaluated the DPI cross section of He using a Hylleraas type wave function without decomposition into partial waves and Coulomb function for the final state. His results favour the oldest experimental data and the theoretical results of Byron and Joachain. Amusia et al have also investigated this problem in the limit of high, non-relativistic photon energies. Their method leads to a greatly overestimated cross section in the energy range of recent measurements. *Yurev*[17] and Varnavshikh and *Labzovskii*[18] have performed the calculations for the DPI cross section of He in the threshold energy region using perturbation and variational methods respectively. Their results are in qualitative agreement with each other, but are limited to the low-energy range (not shown in the figure). *Tiwary*[19] has performed calculations for the DPI cross section of He using the position and momentum dipole matrix elements. Tiwary has employed almost fully correlated wave function for the ground state and the partially correlated wave function of Altick for the final state to evaluate dipole matrix elements. The values obtained from the length formulation tend to lie higher than those obtained using the velocity formulation. Both differ considerably from the first experimental observations and first theoretical predictions and tend to lie close

to the recent reliable experimental curve of Holland et al. especially in the high energy range. There is considerable discrepancy between theoretical results of Tiwary and experimental data of Holland et al in the vicinity of the threshold. This clearly indicates that (1) inclusion of correlation in the final state is important, (2) partial correlation is not adequate to obtain accurate results in the vicinity of the threshold i.e. two outgoing electrons are very slow. The effect of correlation decreases with increase of incident photon energy. It seems to be plausible because when escaping electrons are slow, they have enough time to develop correlations. Carter and Kelly have performed calculations for the DPI cross section of He using the many-body theory (MBPT) incorporating full correlation in both initial and final states. Their results are in good agreement in the entire energy range with the most recent and reliable experimental data of Holland et al.

3.3 Double-photoionization of $H^-(^1S)$

Double photoionization of H^- negative ion by single photon impact has been measured by Donahue et al^{29} using a crossed-relativistic beam technique with sufficient energy resolution and close enough to threshold to yield an exponent of excess energy in the threshold law. Intercepting them with laser photons Doppler shifts the photon energy in the frame of the ion to energies greater than 14.35 eV require for double detachment.

$$h\nu + H^-(^1S) \rightarrow H^+ + e^- + e^- \tag{18}$$

The threshold cross section data are shown in figure 4.
The data can be fitted quite accurately to the form

$$\sigma(E) = A(E - E_t)^m + B \tag{19}$$

The fit results are

$$A = 38.5 + 1.5$$

,

$$B = 0.68 + 0.05$$

Although Donahue et al noted that they can also fit to an alternative result such as

$$\sigma(E) = A(E - E_t)(A + DSin(Cln(E - E_t) + F)) + B \qquad (20)$$

The results of the fit are given details by Donahue et al.

The experimental arrangement suffers, unfortunately, from a spurious two electron signal which sets in at energies slightly lower than 14.35 eV. This uncertainty in the threshold position, coupled with undetermined parameters prevents an unambiguous discrimination between the two results. Laboratory experiments on double detachment of negative ions can overcome some of these problems but results of sufficient accuracy in the close vicinity of the threshold are still unavailable.

3.4 Double-photoionization of $H_2(^1\Sigma_g^+)$

It is interesting to both experimentalists as well as theorists to extend the studies of the double photoionization of helium atomic system to another system with only two electrons with molecular symmetry, i.e., hydrogen molecule, although molecular hydrogen will be more complicated because of more degrees of freedom i.e. vibrations and rotations. For the first time, Dujardin et al^{30} have measured the cross section of double photoionization of hydrogen molecule by single photon impact

$$h\nu + H_2 \rightarrow H^+ + H^+ + e^- + e^- \qquad (21)$$

using the photoion-photoion coincidence (PIPICO) method in the energy range 47.5 eV to 140 eV. Le Rouzo treated this problem exactly in the same way as Byron and Joachain treated the double-photoionization (DPI) of helium atomic system. Le Rouzo[31] performed calculations for the DPI of hydrogen molecule in the length and velocity forms using almost fully correlated wave function for the ground state and product of two unscreened Coulomb wave functions for the final state. Figure 5 displays the experimental observations of Dujardin et al. and the theoretical prediction of Le Rouzo. It is seen from the figure that there is an excellent agreement between experiment and theory. Figure 6 displays the double-photoionization of molecular hydrogen in the threshold region. Figure 7 exhibits comparison of the cross sections derived from the molecular threshold law (dashed curve) with the R-averaged one (solid curve) over the whole photon energy range.

This suggests that it would be interesting to perform more refined experiments and calculations with full correlations in both the initial as well as final states involved in the transition. It would also be interesting to see the effect of two-centre wave function for the final state in the case of hydrogen molecule. It is well known that the exponent of excess energy depends only on the asymptotic part of the final state wave function and molecular threshold law modified due to vibrations. The product of two unscreened Coulomb wave functions gives linear threshold law and hence the result of Le Rouzo obeys the linear threshold law which disagrees with experiment.

3.5 Threshold triple differential cross section of double-photoionization of two-electron systems

The threshold triple differential cross section (TDCS) for the double-photoionization (DPI) of two-electron systems by impact of light is very sensitive to the electron-electron correlations. Most recently, Pont et al[69] have applied two different methods to the calculation of TDCS for double-photoionization of helium. In one method, the 3C method, the final state is described by a product of 3 Coulomb continuum wave functions, while in the other method, the 2SC method, the final state is described by a product of 2 screened Coulomb wave functions employing effective charge.
Figures 8 and 9 show the theoretical results of Pont et al.along with the data of Lablanquie et al[51], for both(a) equal and (b) and (c) unequal energy sharing. The different plots have been rescaled so that the TDCS has the same value at its maximum for all sets of data in a given case. The agreement between the (rescaled) results of the 2SC calculation and the length-gauge version of the 3C calculation is good in all cases apart from the two unequal energy sharing cases at higher excess energy. Finally, it is seen that the qualitative agreement between the results of the 2SC calculation and experimental data is rather poor; the 2SC results lie, for the most part, well outside the error bars of the experiment.

4 Conclusions and Future Directions

Great experimental and theoretical advancement has been made in the case of double photoionization (DPI) of two-electron systems but there is considerable discrepancy in the close vicinity of the threshold where correlations play an extremely important role. To obtain accurate double-continuum wave function in the vicinity of threshold is still a challenging problem for the theorists. Kossmann et al have measured the slope (σ_1)

for the DPI of He but there is no theory to evaluate the slope directly. Dynamic screening i.e. energy dependent screening is crucial especially when two slow electrons are escaping the positive ion but there is no method available to include the dynamic screening in the Coulomb wave function, Altick wave function, distorted wave function or any other wave functions. Unscreened Coulomb wave functions give a linear threshold law which disagrees with experiment. This suggests that a method should be developed to incorporate dynamic screening. In the case of even the simplest H_2, the DPI process has not been extensively investigated either experimentally or theoretically. There is one experimental result and one theoretical calculation with Coulomb wave function. Agreement is excellent between experiment and theory but this may be fictitious. The agreement reflects that the DPI of H_2 should be reinvestigated. In the case of He many body perturbation theory, which includes full correlations in both initial and final states, yields results which are in good agreement with the recent experiment. It clearly indicates that it is indispensable to incorporate full correlation of equal amount in both states involved in the transition in order to obtain reliable results. Angular distribution and energy sharing of two escaping electrons have not been studied but these can offer the opportunity to test the validity of a theoretical model as the exponent of excess energy does in the threshold law.

It is clear that there are numerous difficulties in obtaining the accurate double-continuum wave functions which play an extremely important role in reliable double-photoionization cross sections. However, we would like to make some constructive and fruitful suggestions for obtaining correlated double-continuum wave functions which may be the future directions:

(1) a new R-matrix developed by Burke et *al*[9] may be very useful for the double-continuum wave function (DCWF), (2) the standard R-*matrix*[1] may

be combined with the Altick asymptotic DCWF and hyperspherical DCWF, (3) solving the Schroedinger equation including the higher terms of the Neumann series, (4) developing some new ideas and techniques which provide to include the dynamic screening in the Coulomb, Altick and distorted wave functions and finally (5) developing some sophisticated numerical procedure to describe two continuum electrons in the entire configuration space.
In short, our knowledge of high-precision double-continuum wave function as well as double-photoionization cross section of atoms, molecules and ions, particularly for heavy atoms, molecules and ions, is by no means complete. Comprehensive and painstaking work needs to be done and the field will continue to grow, develop and flourish. The future holds many challenges for both experiment and theory.

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FIGURE CAPTION

Figure 1. The ratio of cross sections $\frac{He^{++}}{He^{+}}$

Experimental curves


, Holland et al


, Wight and Van der Wiel


, Schmidt et al


, Carlson

Theoretical curves

——— , Tiwary obtained from momentum matrix elements

—•••—, Tiwary obtained from position matrix elements

—•— , Byron and Joachain with almost full correlation in the ground state

– – – – , Byron and Joachain with no correlation in both initial and final states

—••— , Brown

— — —, Amusia et al

—•••• —, Carter and Kelly

Figure 2. Yield of very low energy electrons following photon impact on He

Figure 3a. Double-photoionization cross sections of He from threshold to 83 eV photon energy

• • • • , Experimental data of Kossmann et al

——— , Least squire fit

Figure 3b. Same as Figure 3a with smaller and enlarged energy scale

Figure 4. Double detachment cross sections for H^-

– – , Experiment of Donahue et al

——— , best fit by power and law and modulated linear law in figures 4a) and 4b) respectively

Figure 5. Double photoionization of molecular hydrogen

• • • • , Experiment of Dujardin et al

——— , R-averaged theoretical results of Le Rouzo

Figure 6. Double photoionization of molecular hydrogen in the threshold region

– – –, Molecular threshold law matched onto the exact theoretical result at point P

Figure 7. Comparison of the cross sections derived from the molecular threshold law (dashed curve) with the R-averaged one (solid curve) over the

whole photon energy range.

Figure 8. Polar plots of coplanar TDCS.
Electron 1 emerges along the polarization axis (see arrow) , and E = 4.0 eV, with (a) E1 = E2 = 2.0 eV; (b) E1 = 3.3 eV, E2 = 0.7 eV; and (c) E1 = 0.7 eV, E2 = 3.3 eV. Experimental data are from Ref.(51). Solid and dashed lines are from velocity and length gauge version of 3C theory, respectively, and the plotted line is from 2SC theory. Plots have been rescaled so that TDCS has same value at its maximum.

Figure 9. Same as figure 8 but with E = 18.6 eV and (a) E1 = E2 = 9.3 eV; (b) E1 = 15.6 eV, E2 = 3.0 eV; and (c) E1 = 3.0 eV, E2 = 15.6 eV.

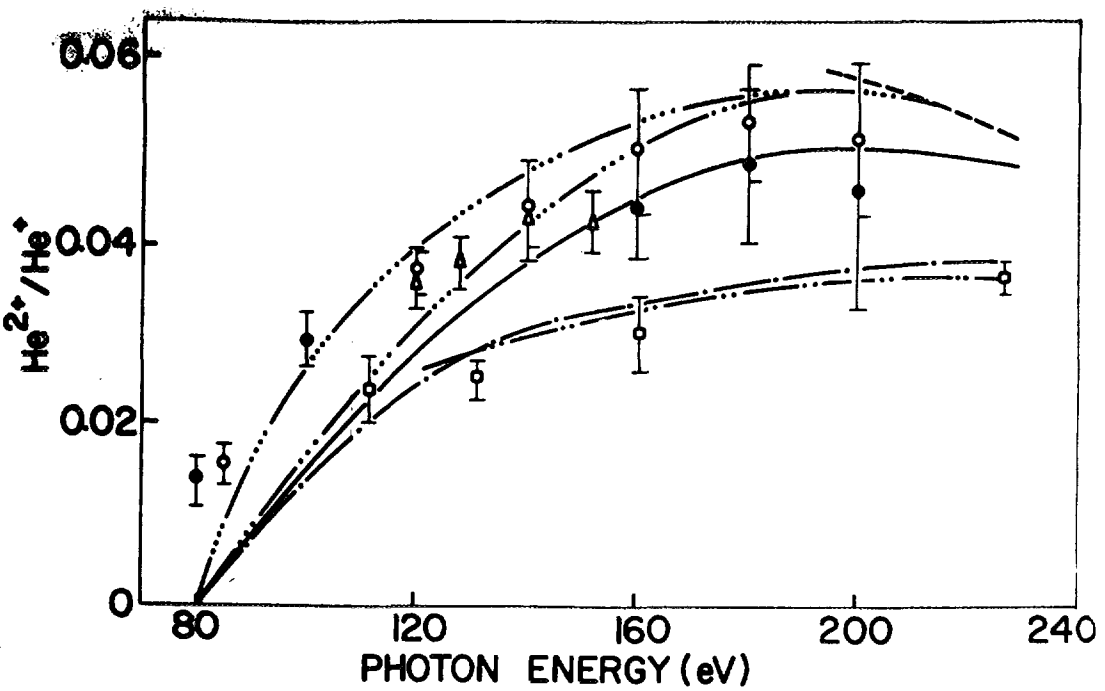
0.06
0.04
0.02
0
He^{2+}/He^{+}
80
120
160
200
240
PHOTON ENERGY (eV)

Fig. 1

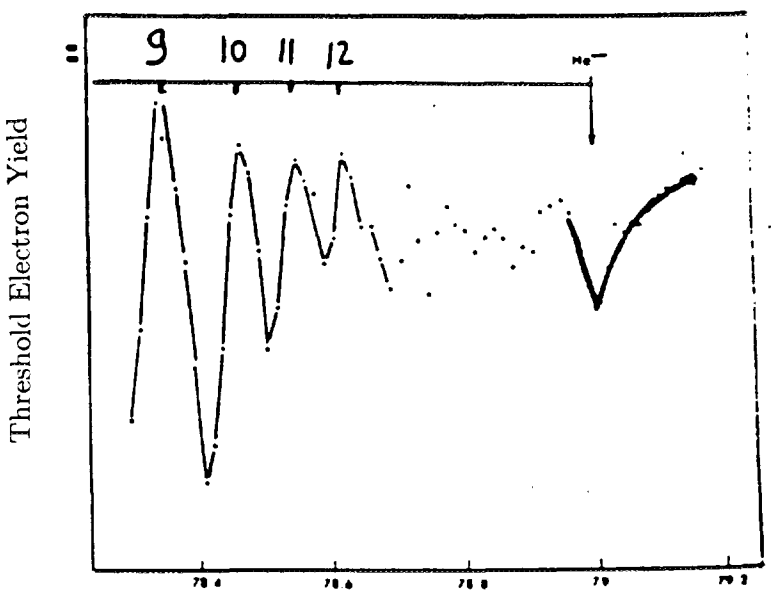
9
10
11
12
Threshold Electron Yield
Photon Energy (eV)

Fig. 2

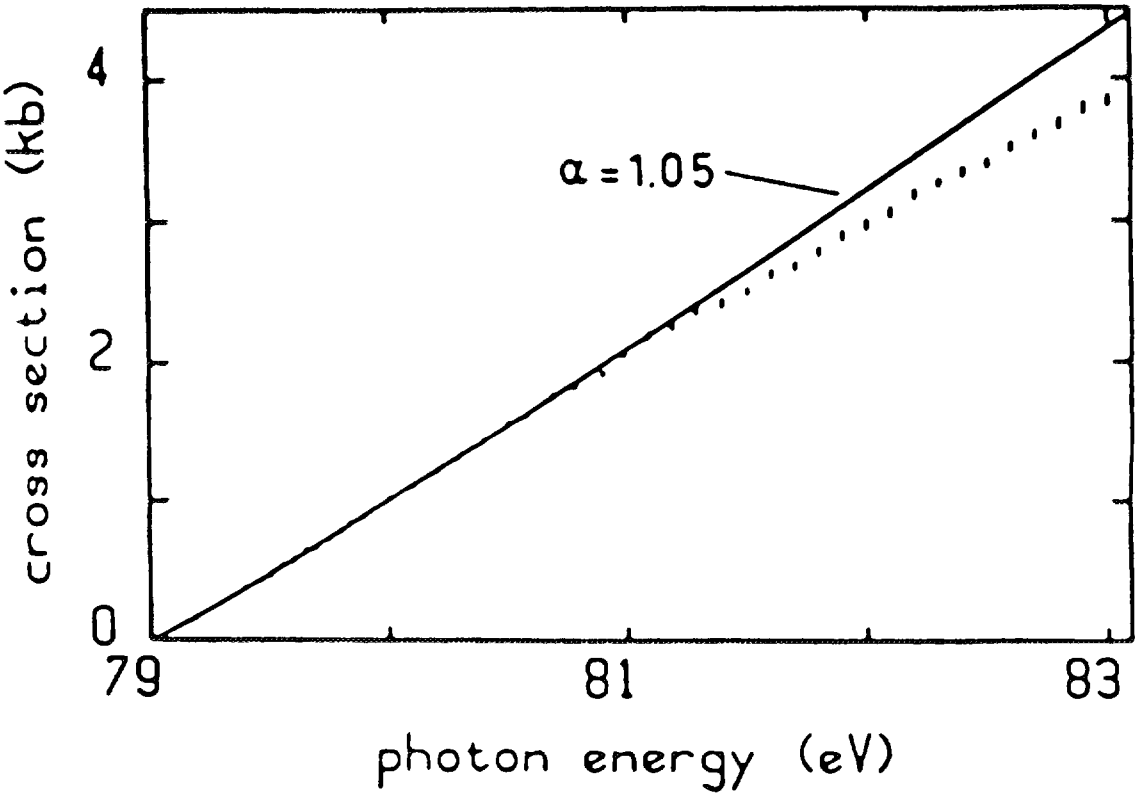
cross section (kb)
4
2
0
α = 1.05
79
81
83
photon energy (eV)

Fig. 3a

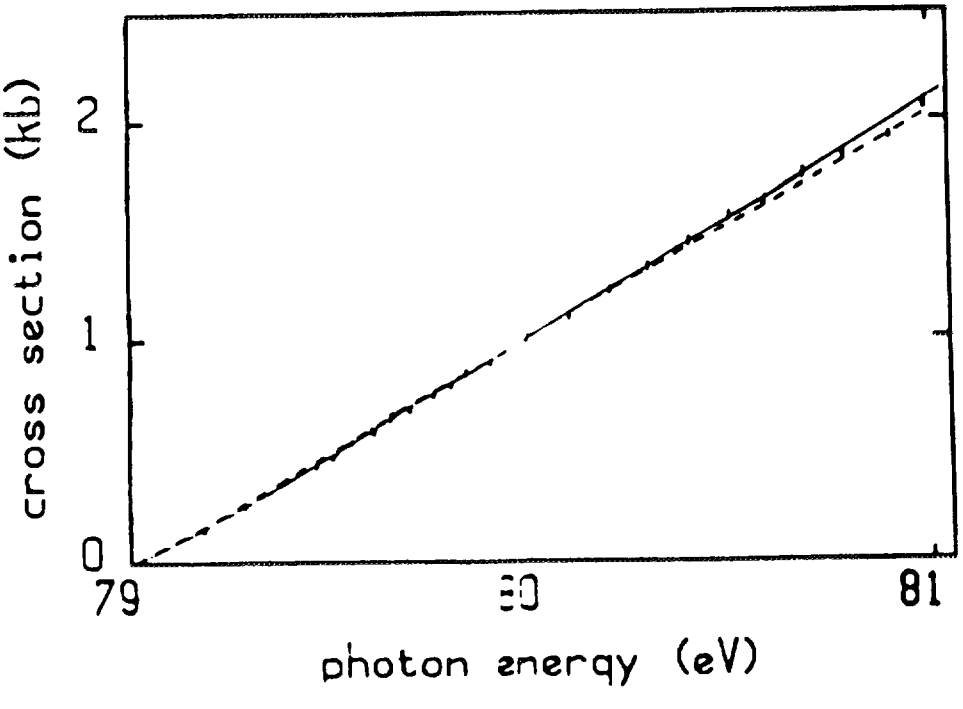
cross section (kb)
2
1
0
79
81
photon energy (eV)

Fig. 3b

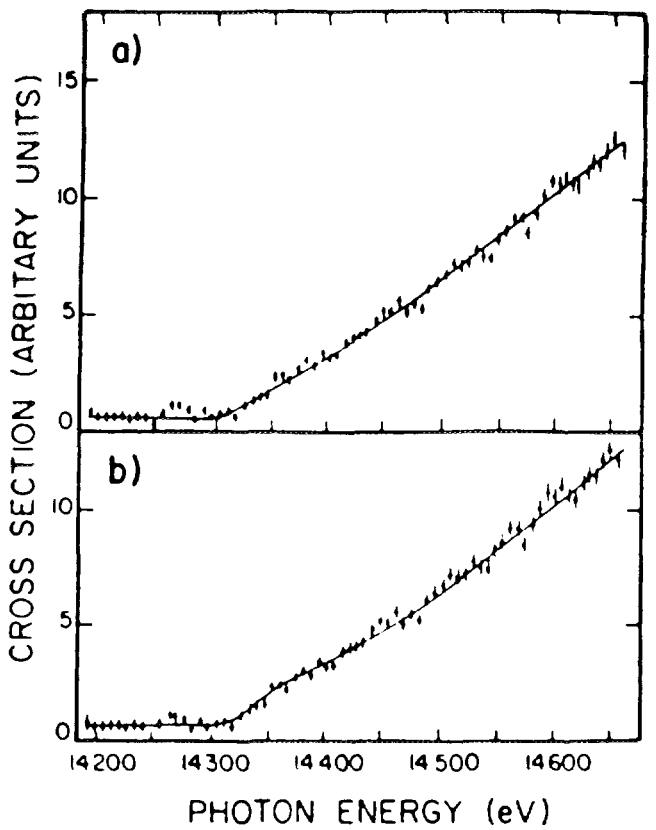
a)
b)
CROSS SECTION (ARBITARY UNITS)
15
10
5
0
10
5
0
14200
14300
14400
14500
14600
PHOTON ENERGY (eV)

Fig. 4

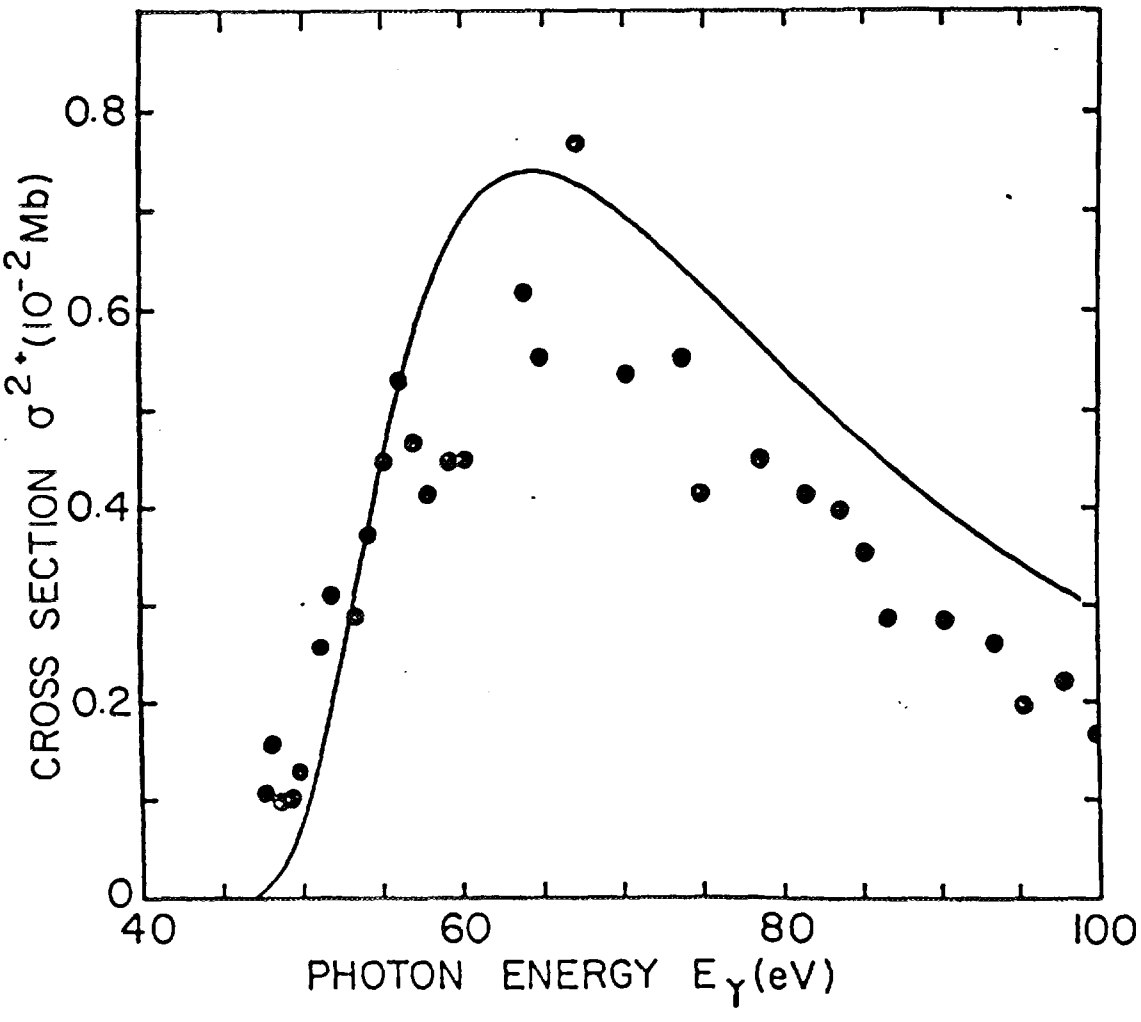
0.8
0.6
0.4
0.2
0
CROSS SECTION $\sigma^{2+}(10^{-2}Mb)$
40
60
80
100
PHOTON ENERGY E_γ(eV)

Fig. 5

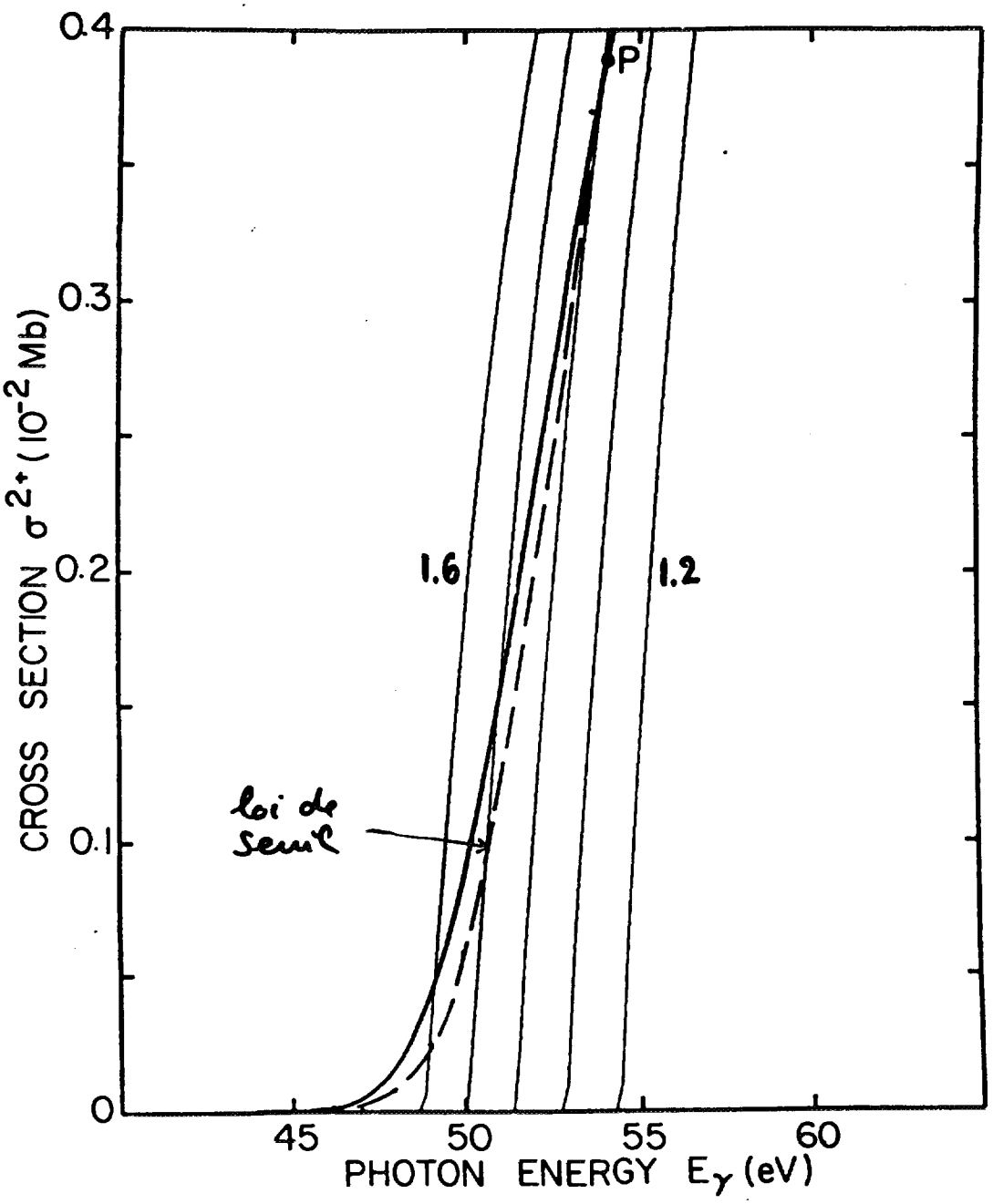
0.4
0.3
0.2
0.1
0
CROSS SECTION σ^{2+} (10^{-2} Mb)
P
1.6
1.2
loi de Seaton
45
50
55
60
PHOTON ENERGY E_γ (eV)

Fig. 6

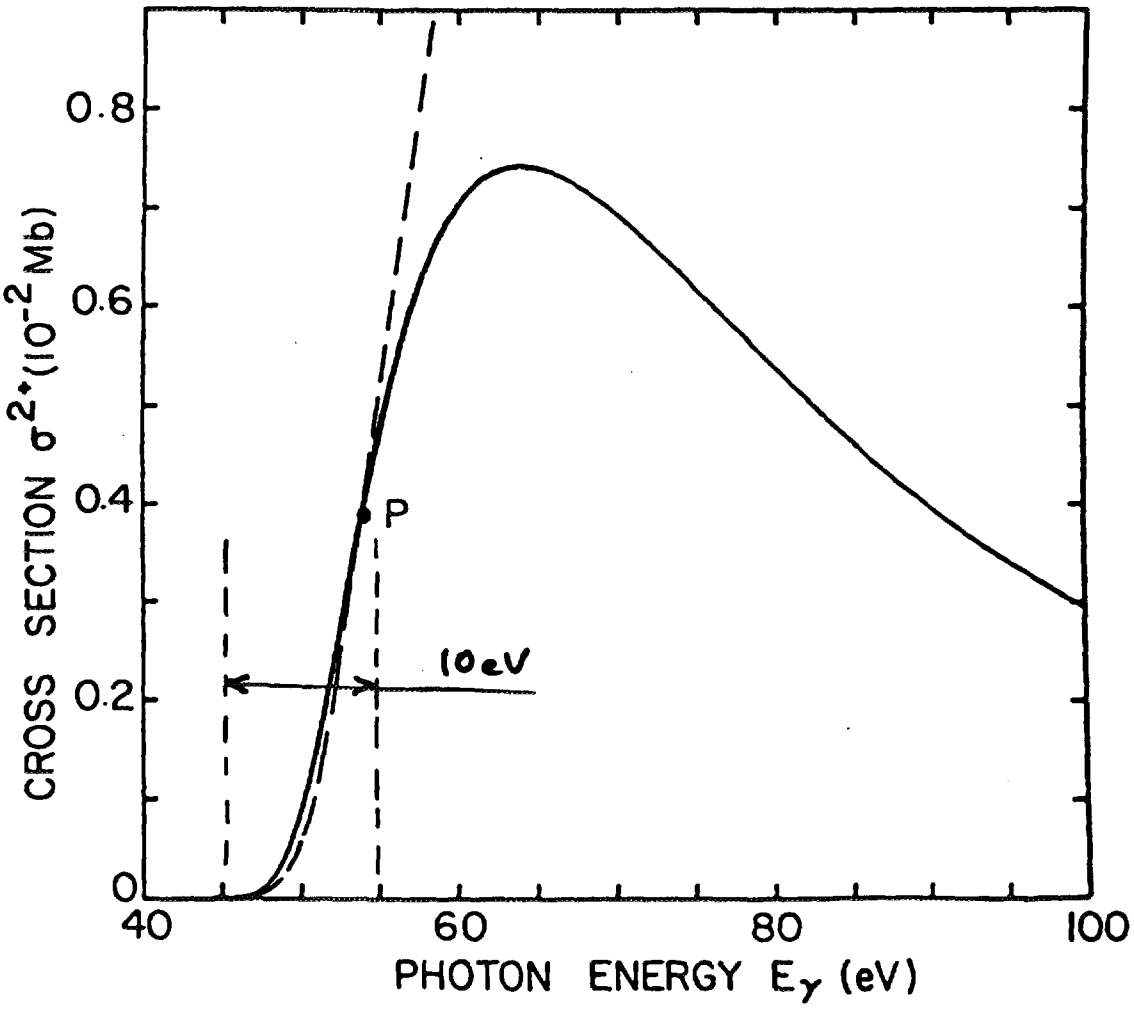
0.8
0.6
0.4
0.2
0
CROSS SECTION $\sigma^{2+}(10^{-2}$Mb)
P
10eV
40
60
80
100
PHOTON ENERGY E_γ (eV)

Fig. 7

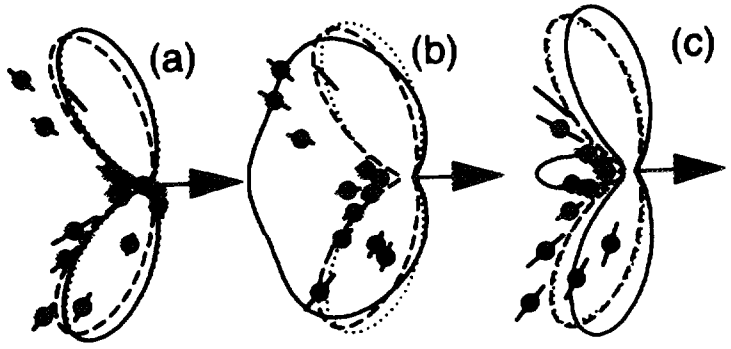

Fig. 8

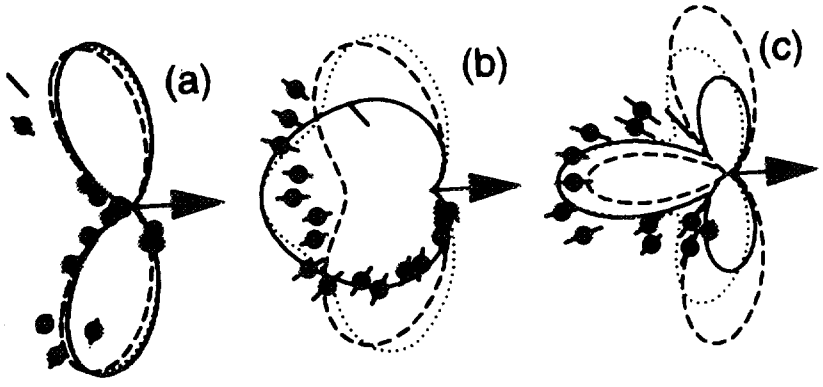

Fig. 9