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Electron impact excitation of positive ions — partial wave approach in Coulomb–eikonal approximation

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ABSTRACT.

The eikonal partial wave theory for the electron impact excitation of positive ions is formulated firstly and is demonstrated in the 1s→2s, 2p excitations of hydrogen–like ions.

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The eikonal approximation (EA) and eikonal related approximations have been reasonably successful in predicting intermediate–energy cross sections for electron–atom (ion) scattering processes (Walters 1984). In fact, the EA is a kind of the distorted wave model (DW) rather than that of the potential type one (Henry 1981, Qian *et al* 1989a). Great efforts have been dedicated to develope the eikonal type distorted model, in which a straight path integral of interaction potential appears as a phase of an exponential function. This phase integral term can be used to describe the distortion over the continuum projectile wave due to the interaction between the projectile and the bound electrons. Because of the additivity of the phase integral with respect to various interactions, it is provided with a favorable conditions for describing the multiple scattering from many electron targets in principle (Qian *et al* 1989b). However, as is well known, serious difficulties in handling the calculation of the phase integral terms have been an obstacle to extend the application of the EA to complex atoms (ions) and there has no alternative but to rely on analytic target wave functions of a restricted type for the process calculations. This is very severe drawback of EA, if not fatal, in its practical applications (Franco 1971, 1973, and Gien 1986).

But now this state of affairs has been changed. W. J. Qian and H. Narumi have particularly paid an attention to the fact that the product of the Coulomb interaction and its eikonal phase integral term, such as

$$\Gamma(r_{oj}) = exp[-\frac{i}{k_i}\int_{-\infty}^{z}\frac{1}{r_{oj}}dz] \qquad (1)$$

where z is parallel to incident wavevector $\mathbf{k_i}$ and $r_{oj}=|\mathbf{r}_o-\mathbf{r}_j|$, can be expressed by some expansion similar to the famous Laplace formula

$$r_{oj}^{-1}=\sum_{\lambda\mu}\frac{r_<^{\lambda}}{r_>^{\lambda+1}}\frac{4\pi}{2\lambda+1}Y_{\lambda\mu}^{*}(\hat{\mathbf{r}}_o)Y_{\lambda\mu}(\hat{\mathbf{r}}_j)\ . \tag{2}$$

where $r_>$ and $r_<$ are the larger and the smaller of r_0 and r_j, respectively, and $Y_{\lambda\mu}$ is the spherical harmonic function. Qian *et al* (1989) derived the following spherical harmonic expansion for the product term mentioned above

$$\frac{\Gamma(r_{oj})}{r_{oj}}=\sum_{\lambda\mu}\sum_{\lambda_0\mu_0}i^{\lambda-\lambda_0}J_{\lambda\lambda_0}(r_j,r_o)\Lambda(\lambda\mu,\lambda_0\mu_0)Y_{\lambda\mu}(\hat{\mathbf{r}}_j)Y_{\lambda_0\mu_0}^{*}(\hat{\mathbf{r}}_o) \tag{3}$$

with

$$J_{\lambda\lambda_0}(r_j,r_o)\begin{cases}=\dfrac{4\pi}{2\lambda+1}\dfrac{\Gamma(\frac{\lambda+\lambda_0+1-i\eta_i}{2})}{\Gamma(\frac{\lambda_0-\lambda+i\eta_i}{2}+1)}\dfrac{1}{\Gamma(\lambda+\frac{1}{2})}\dfrac{r_j^{\lambda}}{r_o^{\lambda+1}}(\frac{r_0}{2})^{i\eta_i}\\ \quad\times{}_2F_1(\frac{\lambda+\lambda_0+1-i\eta_i}{2},\frac{\lambda-\lambda_0-i\eta_i}{2},\lambda+\frac{3}{2};\frac{r_j^2}{r_0^2})\quad for\ r_0>r_j,\\ =\dfrac{4\pi}{2\lambda_0+1}\dfrac{\Gamma(\frac{\lambda+\lambda_0+1-i\eta_i}{2})}{\Gamma(\frac{\lambda-\lambda_0+i\eta_i}{2}+1)}\dfrac{1}{\Gamma(\lambda_0+\frac{1}{2})}\dfrac{r_0^{\lambda_0}}{r_j^{\lambda_0+1}}(\frac{r_j}{2})^{i\eta_i}\\ \quad\times{}_2F_1(\frac{\lambda+\lambda_0+1-i\eta_i}{2},\frac{\lambda_0-\lambda-i\eta_i}{2},\lambda_0+\frac{3}{2};\frac{r_o^2}{r_j^2})\quad for\ r_j>r_0.\end{cases} \tag{4}$$

$$\Lambda(\lambda\mu,\lambda_0\mu_0)=\delta_{\mu\mu_0}[(2\lambda+1)(2\lambda_0+1)]^{\frac{1}{2}}$$
$$\times\sum_{\alpha=0}^{\infty}i^{\alpha}(2\alpha+1)\begin{pmatrix}\lambda&\alpha&\lambda_0\\0&0&0\end{pmatrix}\begin{pmatrix}\lambda&\alpha&\lambda_0\\-\mu&0&\mu_0\end{pmatrix}b_{\alpha}(\eta_i) \tag{5}$$

$$b_\alpha(\eta_i) = \frac{\pi^{\frac{1}{2}}\Gamma(1+i\eta_i)}{4\Gamma(-i\eta_i)} \frac{\Gamma(\frac{\alpha}{2} - i\frac{\eta_i}{2})}{\Gamma(\frac{\alpha}{2} + i\frac{\eta_i}{2} + \frac{3}{2})} , \qquad (\eta_i \equiv \frac{1}{k_i}). \tag{6}$$

In Eqs. (3)~(5), the λ and λ_0 are called, respectively, the multipolarity of the bound states and that of the continuum states. In Eq. (4), ${}_2F_1(a,b,c;z)$ is hypergeometric function which is an absolutely convergent function of r_0 and r_j in the case of Re(c−a−b)>0. The usual notation for the Wigner 3−j coefficient is used in Eq. (5). When $\eta_i \to 0$, Eq. (3) is reduced to Eq. (2), as is expected. One can readily see that the expression of Eq. (3) together with Eqs. (4), (5) and (6) provide an essential basis of the eikonal partial wave theory, just as Eq. (2) does for the Born's partial wave treatment.

In fact, in our Coulomb−eikonal approximation (CE), the direct scattering amplitude for an electron colliding with a hydrogenic ion in initial state a and exciting it to final state b is

$$f(\mathbf{k}_i, \mathbf{k}_f) = -\frac{1}{2\pi} < \xi_f^{(-)}(\mathbf{r}_0, \mathbf{r}_j) \left| \frac{\Gamma(r_{oj})}{r_{oj}} \right| \xi_i^{(+)}(\mathbf{r}_o, \mathbf{r}_j) > \tag{7}$$

with

$$\xi_i^{+}(\mathbf{r}_0, \mathbf{r}_j) = \varphi_a(\mathbf{r}_j) F_{\mathbf{k}_i}^{(+)}(Z_i, \mathbf{r}_0) \tag{8a}$$

$$\xi_f^{(-)}(\mathbf{r}_0, \mathbf{r}_j) = \varphi_b(\mathbf{r}_j) F_{\mathbf{k}_f}^{(-)}(Z_f, \mathbf{r}_0) \tag{8b}$$

where $F_{\mathbf{k}_i}^{(+)}(Z_i, \mathbf{r}_0)$ and $F_{\mathbf{k}_f}^{(-)}(Z_f, \mathbf{r}_0)$ are Coulomb wave functions with outgoing and ingoing boundary conditions in the field of an ion with charge $Z_i = Z$ and $Z_f = Z-1$, respectively, and $\varphi_a(\mathbf{r}_j)$ and $\varphi_b(\mathbf{r}_j)$ are the initial and final hydrogenic bound states.

Combining Eqs. (3) and (8) with (7), adopting an approach similar to that of Burgess *et al* (1970, 1974), the excitation cross section Q for the transition between two levels $n_a l_a - n_b l_b$ by a beam of unpolarized electrons is given by the partial wave expansion

$$Q(n_a l_a \rightarrow n_b l_b) = \frac{16\pi}{2l_a + 1} \frac{1}{k_i^2} \sum_{l_i l_f} \sum_{LM} \left| \sum_{\lambda\lambda_0} f_{\lambda\lambda_0} D_{\lambda\lambda_0} \right|^2 \tag{9}$$

where $k_i l_i$ ($k_f l_f$) are respectively the wave and orbital angular momentum quantum numbers of the colliding electron before (after) the collision. The coefficients $f_{\lambda\lambda_0}$ resulting from the angular integral are given as

$$f_{\lambda\lambda_0} = \sum_{\mu\mu_0} i^{\lambda-\lambda_0} \wedge(\lambda\mu,\ \lambda_0\mu_0) < l_b l_f LM \left| Y_{\lambda\mu}(\hat{\mathbf{r}}_i) Y^*_{\lambda_0\mu_0}(\hat{\mathbf{r}}_o) \right| l_a l_i LM > \tag{10}$$

In Eq. (10) we have chosen a representation for the overall wave function in which the coupled angular momenta $l_a l_i LM$ and $l_b l_f LM$ are good quantum numbers, where L is the total angular momentum and M is its azimuthal number. By employing standard tensor operator methods (Edmonds 1957), we get

$$f_{\lambda\lambda_0} = \sum_{\alpha=0} i^{\lambda_0+\alpha-\lambda} (-1)^{l_b+l_f+L+M} \prod{}^2(\lambda_0\alpha\lambda) \prod(l_a l_i L l_b l_f L) b_\alpha(\eta_i) \frac{1}{4\pi}$$

$$\times \begin{pmatrix} \lambda & \alpha & \lambda_0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_b & \lambda & l_a \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_f & \lambda_0 & l_i \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & \alpha & L \\ M & 0 & -M \end{pmatrix} \begin{Bmatrix} l_a & l_i & L \\ \lambda & \lambda_0 & \alpha \\ l_b & l_f & L \end{Bmatrix} \tag{11}$$

where $\prod(j_1, j_2, \cdots) = (2j_1+1)^{\frac{1}{2}}(2j_2+1)^{\frac{1}{2}} \cdots$. When $\eta_i \to 0$, f_{λ_0} is reduced to the coefficient f_λ which have been evaluated by Percival (1957) for the Born partial wave theory. The conventional symbol for the 9–j coefficient is used here.

The values of D_{λ_0} depend only on radial functions of atomic bound electron and incident external electron, i.e.,

$$D_{\lambda_0}(n_b l_b k_f l_f; n_a l_a k_i l_i) = \int F_{k_f l_f}(Z_f|r_0) y_{\lambda_0}(r_0) F_{k_i l_i}(Z_i|r_0) dr_0 \tag{12}$$

$$y_{\lambda_0}(r_0) = \int P_{n_b l_b}(r_j) J_{\lambda_0}(r_0, r_j) P_{n_a l_a}(r_j) dr_j \tag{13}$$

where $P_{n_a l_a}$ and $P_{n_b l_b}$ are the radial wavefunctions of the initial and final states of the atomic system, $F_{k_i l_i}(Z_i|r_0)$ and $F_{k_f l_f}(Z_f|r_0)$ represent the spherical Coulomb waves of the initial and final continuum states of the projectile with $Z_i = Z$ and $Z_f = Z-1$. In the present paper we do not consider the effect of exchange temporarily.

The Coulomb–eikonal predictions of the integrated cross sections for 1s→ 2s e–He^+excitation are shown in Fig. 1, plotted versus incident– electron energy E_i in eV, ranging from just above the threshold to 1000 eV, and compared with other theoretical data and available experiment. Curve CE is the present CE prediction. The conventional Coulomb–Born cross section lies above the observation curve everywhere and has a finite non–zero value at threshold although there remains a discrepancy of almost a factor of two or more at threshold between theory and experiment (Dolder *et al* 1973). As is expected, Curve PG (plane–wave Glauber) goes smoothly to zero at threshold. Whereas the present results provide apparent improvement near threshold, exhibit better behaviour at intermediate energy range and tend to the Coulomb–Born results in the limit of high incident energy. As far as we know, this work is the first attempt that the long–range interaction between the projectile and the nucleus are taken into account properly for both incident and final channel under the eikonal framework. In our calculations we take $Z_i = Z$, $Z_f = Z-1$, so our theory can be regarded as Coulomb–projected eikonal model as contrasted with Coulomb–projected Born which was proposed by Geltman (1971) firstly. The inclusion of the Coulomb potential is responsible for the non–zero–threshold cross section. Furthermore, the CE approximation assumes the distortion effect due to the charge cloud of the target ion on the basis of the CB approximation. This phase distortion appears as an oscillating term that lead to decrease the prediction as compared to CB, and for this reason, to improve the results at intermediate projectile energies ($E_i < 500$ eV) as well as the behaviour near threshold significantly.

Fig. 2 shows various theoretical data of $1s \rightarrow 2p$ excitation in e–He^+ collision. The long–dashed curve labeled CBⅡ is the unitarized Coulomb–Born approximation, neglecting exchange effect. The double dot–dashed curve labeled PG is the Glauber prediction neglecting Coulomb–distortion. Curve CG represents the Coulomb–modified Glauber prediction. Both PG and CG show zero value cross section at threshold (Thomas 1978). Our present result shows reasonable data which lies between curves PG and CBⅡ for the most part. Judging by appearance, the curve CBⅡ without exchange provide 'best' agreement with experimental data

(Dashchenko *et al* 1974). But this is no more than a coincidence since the inclusion of exchange goes so far as to produce unreasonable deviation from the expected values conversely. It was reported that the eikonal cross sections are increased when the exchange amplitudes are taken into account in the case of electron– hydrogen elastic scattering (Foster *et al* 1976, Onaga *et al* 1987). Presumably it should be possible for CE to improve the agreement by including the exchange effect for the case of electron impact excitation.

It is important to note that our evaluation of the cross sections are in progress through formal procedure, and the techniques involved can be applied to many–electron atomic system easily. In conclusion, we expect that our formalism will be able to open a good vistas of the eikonal theory. We are now extending the present model to some fundamental ionic processes of interest over wide range of ionic species.

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Captions

Fig. 1: Various theoretical predictions of the $1s \rightarrow 2s$ excitation cross sections (in units of $10^{-2}\pi a_0^2$) plotted vs incident electron energy E_i in eV. Curve CE is the present Coulomb–eikonal results; short dashed curve CBI, the Coulomb–Born results; the long dashed CBII, the unitarized Coulomb–Born predictions; the dot–dashed curve CG, the Coulomb modified Glauber results (Thomas 1978); the double dot–dashed curve PG, the Glauber results ignoring Coulomb distortion (Narumi *et al* 1975); ··· experimental points.

Fig. 2: Same as Fig. 1, but for $1s \rightarrow 2p$ excitation for He^+.

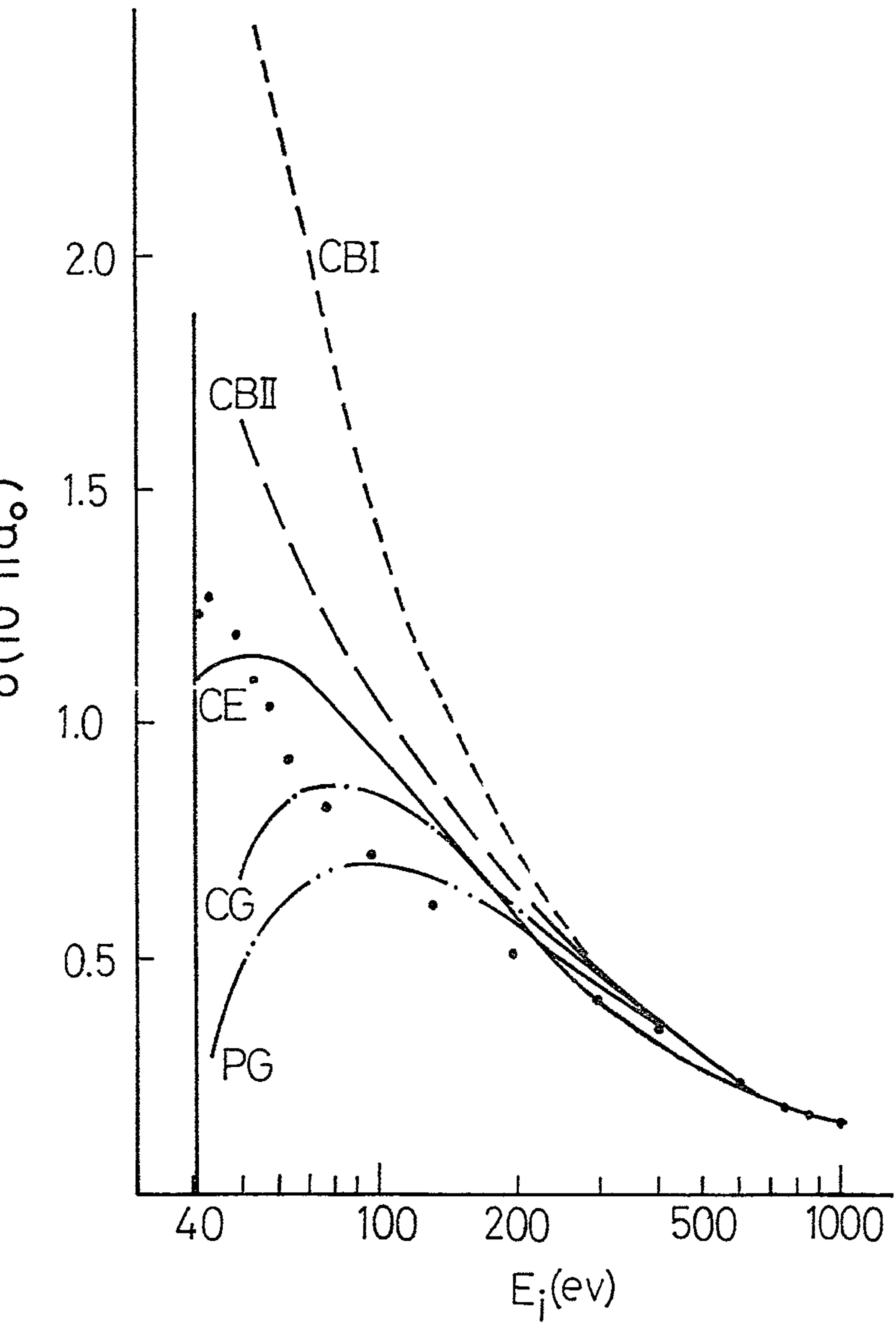

Fig. 1

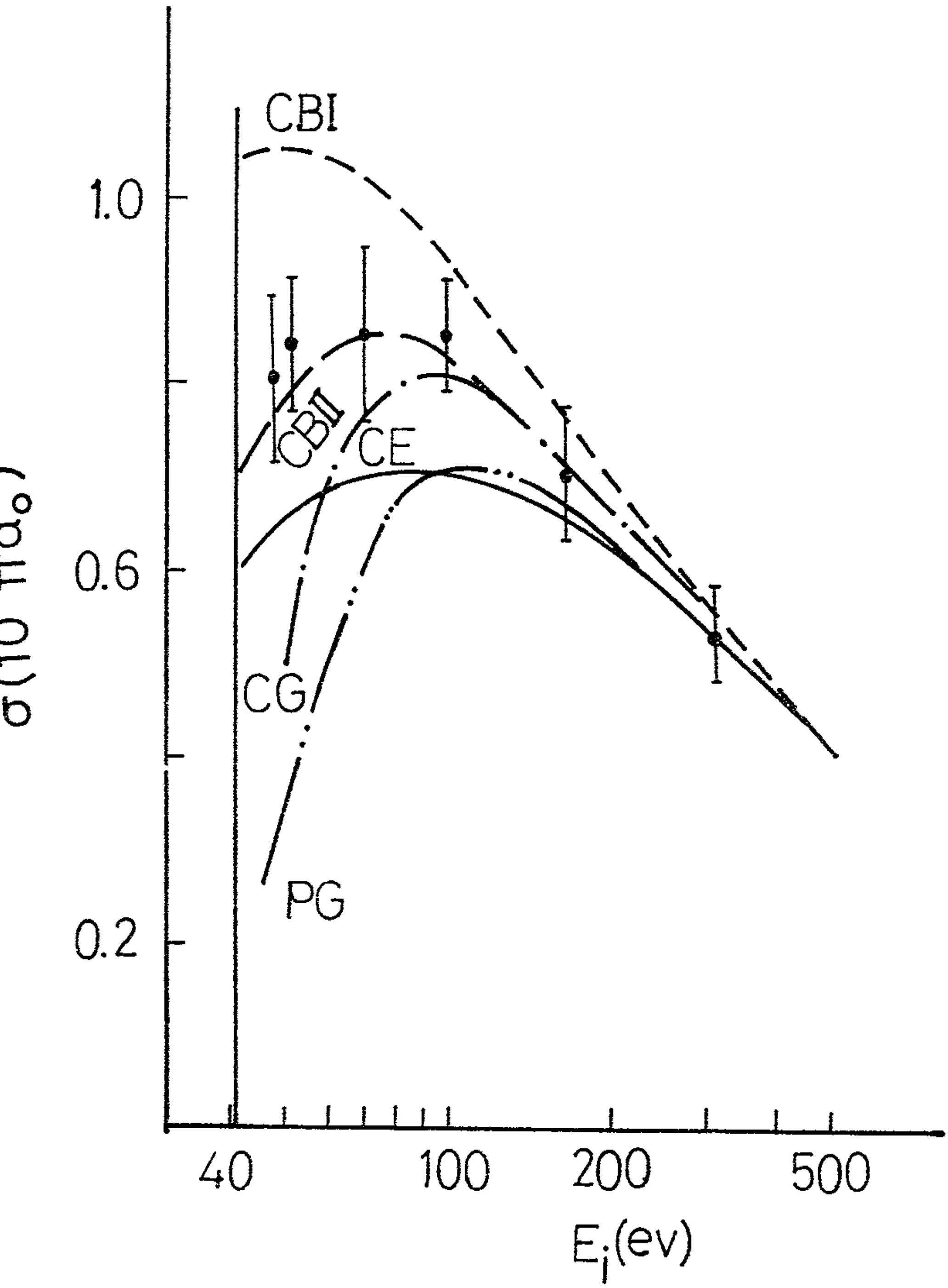

Fig. 2

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