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CHARGE TRANSFER IN HIGH-ENERGY ATOMIC COLLISIONS

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Abstract: In the framework of the distorted-wave Born approximation (DWBA), a simple analytic expression is obtained for electron capture cross sections in high-energy collisions. Reasons for the striking agreement between theory and experiment are presented.

1. Introduction

The theory of charge transfer in high-energy atomic collisions has remained an intriguing problem over a long period of time. Extensive reviews of this subject can be found in articles by McDowell and Coleman (1970), Mapleton (1972), Bransden (1972), and by Massey and Gilbody (1974). Different methods have been used to predict electron transfer cross sections, but the success in explaining cross sections does not by itself constitute a criterion of the validity of a theory. In fact, Greider and Dodd (1966) have pointed out that the DWBA is questionable as a first approximation to rearrangement scattering. In this note, we show that the conditions for the validity of DWBA are considerably relaxed in the high-energy limit.

2. The formalism

The differential cross section for the capture of a target electron by a positive ion is

$$\frac{d\sigma}{d\Omega} = \frac{\mu_i \mu_f}{(2\pi\hbar^2)^2} \frac{k_f}{k_i} \left| T_{fi} \right|^2 \tag{1}$$

where k_i and k_f are the initial and final relative momenta of the colliding particles in the initial and final states, μ_i and μ_f being their respective reduced masses. In DWBA, the prior form of the transition amplitude is given by

$$T_{fi} = \int d\vec{r}_a \, d\vec{r}_b \; \chi^{(-)*}_{k_f}(\vec{r}_f) \, \varphi^*_f(\vec{r}_b) \, V_i \, \varphi_i(\vec{r}_a) \, \chi^{(+)}_{k_i}(\vec{r}_i) \tag{2}$$

In eq. (2), $\vec{r}_a$ and $\vec{r}_b$ are respectively the co-ordinate vectors of the electron relative to the residual particle (target minus electron) and to the positive ion. $\varphi_i(\vec{r}_a)$ and $\varphi_f(\vec{r}_b)$ represent the bound states of the electron in its initial and final system. $\chi^{(+)}_{\vec{k}_i}(\vec{r}_i)$ and $\chi^{(-)}_{\vec{k}_f}(\vec{r}_f)$ describe the relative motion of the colliding particles in the initial and final states, $\vec{r}_i$ and $\vec{r}_f$ being the respective channel vectors. The Coulomb interaction between the positive ion and the residual particle (target minus electron) is explicitly utilized in constructing the distorted wave functions $\chi^{(+)}_{\vec{k}_i}(\vec{r}_i)$ and $\chi^{(-)}_{\vec{k}_f}(\vec{r}_f)$. The perturbation causing the transition is therefore

$$V_i = Z^{(f)}_{eff} \frac{e^2}{r_b} \tag{3}$$

where $Z^{(f)}_{eff}$ is the effective charge of the positive ion, and V_i denotes the Coulomb interaction between the electron and the positive ion.

In momentum space, eq. (2) reads

$$T_{fi} = \int d\vec{p}_i \, d\vec{p}_f \; \psi^{(-)*}_{\vec{k}_f}(\vec{p}_f) \, \psi^{(+)}_{\vec{k}_i}(\vec{p}_i) \; \tilde{\phi}^*_f\left(\frac{M_2}{M_2+m}\vec{p}_f - \vec{p}_i\right) \; \phi_i\left(\vec{p}_f - \frac{M_1}{M_1+m}\vec{p}_i\right) \tag{4}$$

where we have introduced the Fourier transforms

$$\psi^{(+)}_{\vec{k}}(\vec{p}) = (2\pi)^{-3/2} \int d\vec{r} \; e^{-i\vec{p}\vec{r}} \; \chi^{(+)}_{\vec{k}}(\vec{r}) \tag{5}$$

and

$$\phi_i(\vec{p}) = (2\pi)^{-3/2} \int d\vec{r} \; e^{-i\vec{p}\vec{r}} \; \varphi_i(\vec{r}) \tag{6}$$

The function $\tilde{\phi}_f(\vec{p})$ is defined by

$$\tilde{\phi}_f(\vec{p}) = (2\pi)^{-3/2} \int d\vec{r}_b \; e^{-i\vec{p}\vec{r}_b} \; V_i(r_b) \, \varphi_f(\vec{r}_b) \tag{7}$$

M_1, M_2 and m refer to the masses of the target, the projectile and the electron respectively.

In the high-energy limit the momentum wave functions $\psi^{(+)}_{\vec{k}_i}(\vec{p}_i)$ and $\psi^{(-)}_{\vec{k}_f}(\vec{p}_f)$ are strongly peaked around $\vec{p}_i = \vec{k}_i$ and $\vec{p}_f = \vec{k}_f$, respectively. If at these values of the momenta the functions ϕ_i and $\tilde{\phi}_f$ are not zero, one may replace the variables $\vec{p}_i$ and $\vec{p}_f$ in ϕ_i and $\tilde{\phi}_f$ by the values $\vec{k}_i$ and $\vec{k}_f$. The resulting expression for the transition amplitude becomes

$$T_{fi} = (2\pi)^3 \phi_i\left(\vec{k}_f - \frac{M_1}{M_1+m}\vec{k}_i\right) \tilde{\phi}^*_f\left(\frac{M_2}{M_2+m}\vec{k}_f - \vec{k}_i\right) \chi^{(-)*}_{\vec{k}_f}(\vec{r}=0) \; \chi^{(+)}_{\vec{k}_i}(\vec{r}=0) \tag{8}$$

The assumption used in deriving eq.(8) is that the momentum distribution of the bound states is much wider and more slowly varying than the spread of the scattering wave packets. If the bound state wave function has nodes, the peaking approximation becomes invalid in the vicinity of the nodes, but it should not affect the evaluation of the total cross section. In order to verify the nature of the spreading of the scattering wave packet, we used the representation of $\psi_{\vec{k}}(\vec{p})$ given by Bethe and Salpeter (1957), which is valid at high energies, and found that even after the subtraction of the delta function term, $\delta(\vec{k}-\vec{p})$, the remaining term is still very strongly peaked over $\vec{p} = \vec{k}$.

The transition amplitude, eq.(8), depends upon the value of the scattering wave functions at r = 0. At r = 0, these functions are dominated by the Coulomb repulsion between target and projectile. At these distances, the effect of the electron-ion interaction is negligible, and the question of the best auxiliary potential, which according to Greider and Dodd is important for the convergence of the DWBA, does not enter into eq.(8).

Inserting (8) into (1) and using the result that

$$\left| \chi_{\vec{k}}^{(\pm)}(\vec{r}=0) \right|^2 = \frac{2\pi\eta}{\exp(2\pi\eta)-1} \tag{9}$$

where η is the Sommerfeld parameter

$$\eta = Z_i Z_f \frac{e^2}{\hbar v} \tag{10}$$

with Z_i and Z_f representing the nuclear charges of the colliding particles and v their relative velocity, one obtains for the total cross section

$$\sigma = \sigma^{BK} \left[\frac{2\pi\eta}{\exp(2\pi\eta)-1} \right]^2 \tag{11}$$

where σ^{BK} is the Brinkman-Kramers cross section. The effect of screening on the estimate of the cross section was investigated in the case of proton-hydrogen atom collision. A screened Coulomb potential (Jackson (1962)) of the form

$$U(r) = \exp(-\alpha r)\, \frac{e^2}{r} \left(1 + \frac{\alpha r}{2}\right) \tag{12}$$

where α is twice the inverse Bohr radius, was used to calculate the scattering wave functions. It was found that at a proton energy of 100 keV, the cross section showed a 1% deviation from eq.(11).

In the one-electron approximation, the average Brinkman-Kramers cross section for an electron capture from a hydrogen-like target from an initial state with principal quantum number n_i into an empty hydrogen-like shell of principal quantum number n_f is given by (McDowell and Coleman, page 379)

$$\sigma^{BK} = \frac{2^{18}\pi k^8 K_i^5 K_f^5 n_f^2}{5\left[k^4 + 2k^2(K_i^2 + K_f^2) + (K_i^2 - K_f^2)^2\right]^5} \tag{13}$$

where

$$k = mv/\hbar$$

and

$$K_a = \frac{mc^2}{\hbar c}\,\frac{Z_{eff}^{(a)}e^2}{\hbar c}\,\frac{1}{n_a} \quad ; \qquad a = i, f \tag{14}$$

Approximation (11) should remain valid as long as the electron cloud does not get deformed during the collision with the ion, i.e., if

$$\pi\eta \lesssim 1 \tag{15}$$

3. Comparison with experiment

The total cross section for electron capture at high energies is obtained by summing σ^{BK} in eq. (13) over all values of n_f and by inserting the result in eq. (11). For a proton incident on hydrogen, the condition $\pi\eta \lesssim 1$ means that (11) should be valid for proton energies exceeding 250 keV. In figs. 1 and 2, the theoretical predictions are shown for the reaction

$$H^+ + H(1s) \longrightarrow \sum_{n,\ell} H(n\ell) + H^+$$

Also plotted are the experimental results for protons incident on H_2 multiplied by 0.5. It is, however, not obvious that the hydrogen molecule could be considered as equivalent to two independent hydrogen atoms. Tuan and Gerjuoy (1960) showed that in the high-energy limit the ratio of charge transfer from atomic hydrogen to charge transfer from H_2 tends towards a value between 0.6 and 0.7. In spite of the scatter in the experimental points, we can see from the figures that a scaling factor between 0.6 and 0.7 will improve the agreement between the high-energy DWBA (11) and the measured capture cross sections.

In order to avoid the problem of scaling factors, we investigated the nonresonant electron capture in proton-helium collisions:

$$H^+ + He(1s^2) \longrightarrow \sum_{n,\ell} H(n\ell) + \sum_{n',\ell'} He^+(n'\ell')$$

In this reaction the high-energy approximation (11) should be valid for proton energies exceeding 1000 keV. We note that the simultaneous transfer of one He electron and the Coulomb excitation of the remaining electron is not included in DWBA, but as a second-order process it should not be important at high impact energies. By comparison with correlated two-electron wave functions, Bransden and Sin Fai Lam (1966) found that the single-electron wave function which belongs to $Z_{eff}^{(i)} = 1.6875$ is adequate for the calculation of electron capture in helium. We therefore used this effective charge to calculate the intrinsic momentum κ_i. The calculated cross sections are compared with the experimental cross sections in table 1.

4. Conclusion

The non-relativistic high-energy DWBA approximation (11) reproduces very well the experimental situation in the energy ranges under consideration. This agreement is, of course, no proof for the reliability of the theory. Nevertheless, it should be realized that the DWBA capture rate in the case of 10.5 MeV protons on He is in accordance with the result of more advanced scattering methods as described by Begum et al. (1973). The high-energy electron transfer is not only a test for the correctness of the scattering theory used in a calculation, but it simultaneously probes the asymptotic tail of the momentum distribution of the bound electron. Since Hartree-Fock calculations are not very sensitive to the asymptotic region of the electron momentum distribution, the reliability of theoretical capture cross sections for complex targets will be obscured at high energies.

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TABLE 1

Total cross sections σ^{BK} (eq.(13)) and σ (eq.(11)) for electron capture by protons from helium.

E	σ^{BK}	σ	σ(experiment)	
1.063	11.3^{-5}†	1.22^{-5}	$(2.9\pm0.4)^{-5}$	a)
2.45	11.8^{-7}	2.91^{-7}	$(3.2\pm0.4)^{-7}$	a)
2.99	3.81^{-7}	1.08^{-7}	$(1.2\pm0.1)^{-7}$	a)
5.41	12.4^{-9}	4.97^{-9}	$(5.4\pm0.6)^{-9}$	a)
6.45	4.42^{-9}	1.93^{-9}	$(2\pm0.4)^{-9}$	b)
10.5	2.52^{-10}	1.32^{-10}	$(1.2\pm0.4)^{-10}$	b)

Proton energy E in MeV, cross sections in 10^{-16} cm^2.

†The ~~sub~~superscript indicates the power of ten by which the number is to be multiplied.

a) Welsh et al. (1967)

b) Berkner et al. (1965)

FIGURE CAPTIONS

Fig. 1: Total cross sections for electron capture by protons from atomic hydrogen. Curve 1: Impulse approximation (Coleman and McDowell 1965). Curve 2: Continuum distorted wave method (Salin 1970). Curve 3: High-energy DWBA limit (eq.(11)). Curve 4: Brinkman-Kramers approximation (eq.(13)). Experimental results: ▣ Barnett and Reynolds 1958, △ Welsh et al. 1967, ▲ Schryber 1968, ○ Williams 1967, ● Toburen et al. 1968.

Fig. 2: Total cross sections for electron capture by protons from atomic hydrogen. Details as in fig. 1.

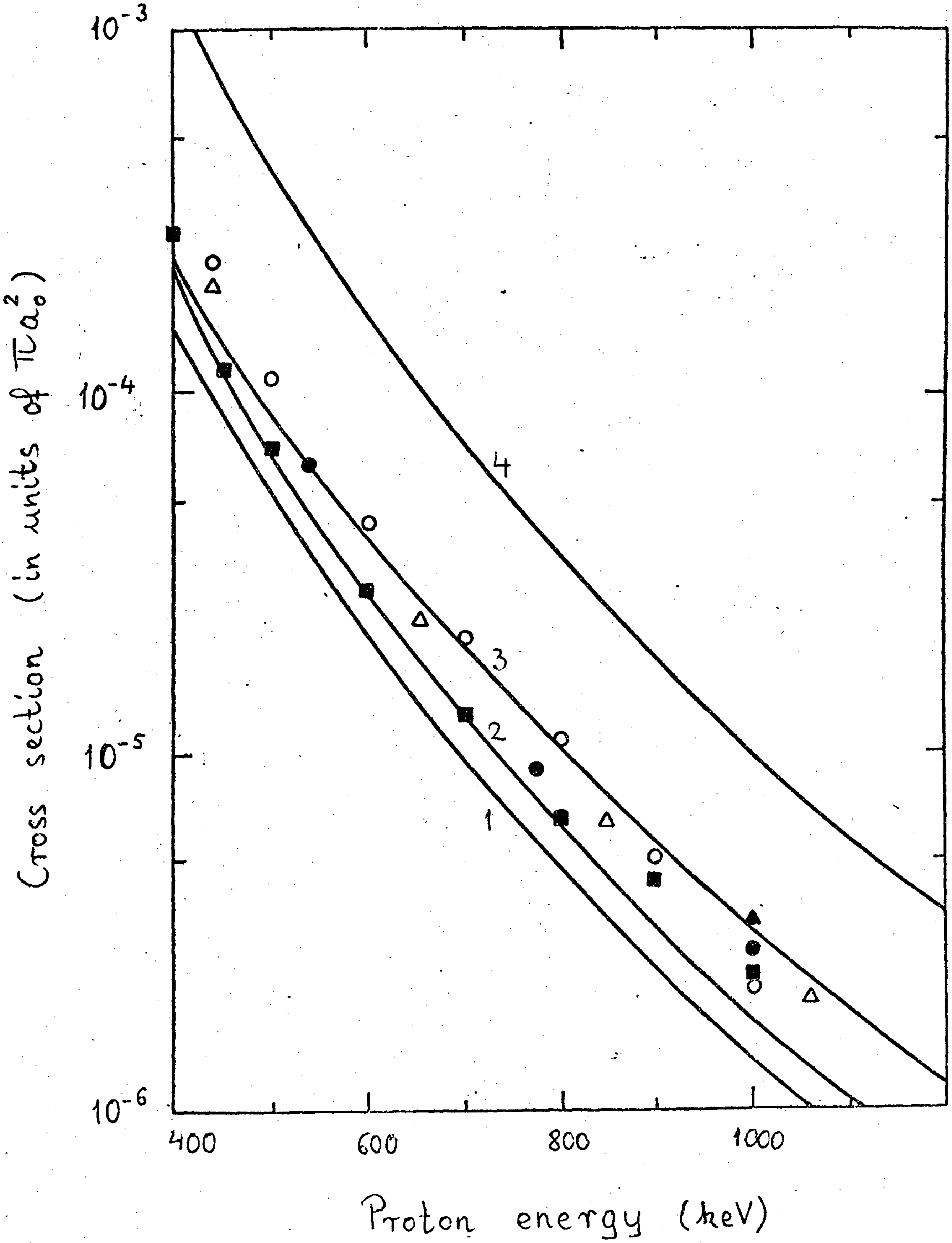
10^{-3}
10^{-4}
10^{-5}
10^{-6}
4
3
2
1
400
600
800
1000
Cross section (in units of πa_0^2)
Proton energy (keV)

Fig. 1

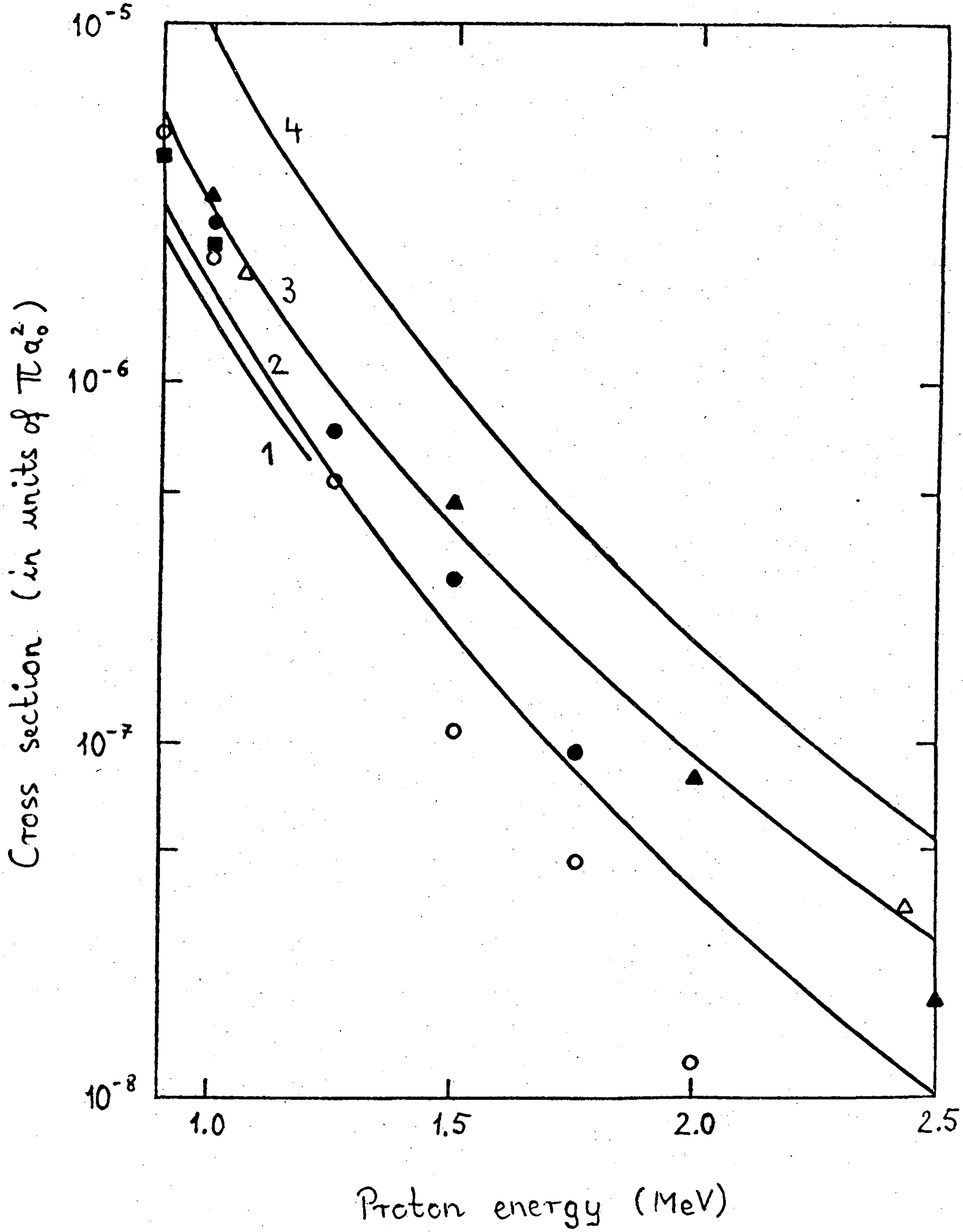
10^-5
10^-6
10^-7
10^-8
Cross section (in units of πa₀²)
1
2
3
4
1.0
1.5
2.0
2.5
Proton energy (MeV)

Fig. 2