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LETTER TO THE EDITOR

# On possible absorption effects in elastic scattering of electrons on molecules

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**Abstract.** Elastic cross sections for positron scattering on noble gases (Ar, Kr) at energies of a few tens of eV exhibit structures which have been attributed to absorption effects. Recent, precise measurements for Ar do not confirm the existence of such effects for electron scattering. Here, we show that previous measurements indicate the existence of an absorption effect for $e^- + H_2$ scattering around 60 eV. The reason for this can probably be ascribed to the $e^-$–$H_2$ total cross section partitioning scheme, which is more similar to the one for $e^+$–Ar than to the one for $e^-$–Ar.

Coupling between elastic and inelastic channels is a well identified phenomenon in the theory of electron scattering on atoms and molecules (cf Joachain 1975). Briefly, inclusion of an absorption potential into a complex scattering equation causes a reduction in the real (elastic) scattering amplitude (cf Jain 1986, Staszewska *et al* 1984). However, it has not been shown whether these two effects can compensate for each other, i.e. whether the total cross section can constitute an 'invariant' of scattering.

There are few experimental indications of coupling between different channels. Absorption and resonant phenomena are usually studied separately from elastic scattering, and absolute (non-normalized) values of cross sections can rarely be obtained. Positron scattering measurements are more difficult than their electron counterparts. The results are more noisy due to the low intensity and brightness of slow positron beams. Surprisingly, some evidence of channel-coupling has been observed in the energy dependency of positron–argon (Dou *et al* 1992a) and positron–krypton (Dou *et al* 1992b) differential cross sections. In argon, an abrupt drop (by a factor of 3 at 90° scattering angle) has been observed in the energy range 40–60 eV. The energy of this drop shifts to higher values for bigger scattering angles and is more visible for obtuse angles. Due to this shifting, the effect smoothes out in the total elastic or in the total scattering (absorption plus elastic) cross sections and has not been observed in such measurements (see Stein *et al* 1992).

What remains puzzling in the observations of Dou *et al* (1992a) is the energy range in which the drop occurs: no significant thresholds (like positronium formation or ionization) can be identified in this range. Between 30 and 60 eV the positronium-formation cross section gradually diminishes, while the ionization cross section reaches a maximum (see Stein *et al* 1992). In krypton, resonant-like peaks at 25 and 200 eV were observed in the differential elastic cross sections. Tentatively, they have been attributed to coupling of the elastic channel with the positronium-formation and ionization channels, respectively (Dou *et al* 1992b).

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In spite of the mentioned difficulties in handling positron beams, these structures have been evidenced outside the experimental uncertainties. It is important to note that the drop in elastic scattering for argon has not been noticed in the preliminary measurements of differential cross sections (Smith *et al* 1990). This is to be attributed to the normalization procedure which was performed separately for low and high energies. In order to evidence possible structures, the differential cross sections should be normalized at one energy only and the transmission efficiency of the analysing optics should be achromatic.

The same kind of measurements has been recently repeated for electron scattering on argon (Cvejanović and Crowe 1994). No rapid changes in the differential cross sections have been observed for any of the studied angles (60°, 90°, 120°) between 20 and 110 eV. The question arises of whether the coupling phenomena should be attributed exclusively to positron noble gases scattering. An intensive theoretical work aiming at the explanation of these structures is underway (see Cvejanović and Crowe 1994 for an updated list of references).

In the present paper we re-analyse the existing experimental data for electron–molecular hydrogen scattering in order to identify another possible system where these coupling effects are detectable. The leading indication for the choice of hydrogen refers to the partitioning scheme for this molecule, i.e. the percentile contribution of the elastic and inelastic channels to the total cross section.

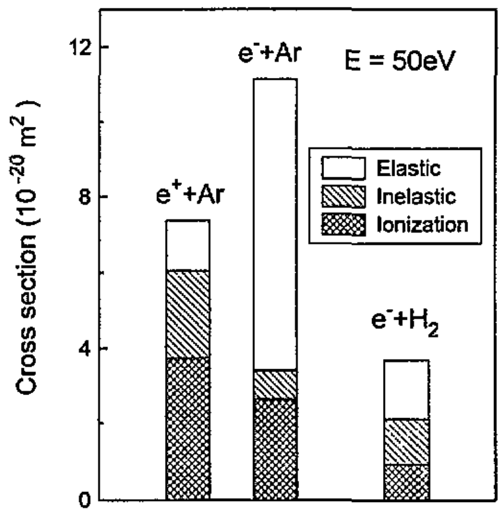


**Figure 1.** Partitioning scheme for electron and positron scattering on argon and hydrogen at 50 eV: $e^+ + Ar$, ionization from Knudsen *et al* (1990) corresponding to ionization + electronic excitation of Mori and Sueoka (1994); inelastic = positronium formation from Fornari *et al* (1983) corresponding to the 'lower limit' for positronium formation of Zhou *et al* (1994); elastic is that obtained by subtraction of the two above values from the total one (Stein *et al* 1992).

The analysis of the partitioning scheme for positron–argon scattering indicates clearly the difference of this system in respect to electron–noble gas collisions (see figure 1). For positrons, the scattering in the 20–100 eV range is highly dominated by inelastic processes. At 50 eV the ionization together with the excitation (Knudsen *et al* 1990, Mori and Sueoka 1994) contribute more than 50% of the total cross section. The positronium-formation channel (Fornari *et al* 1983, Zhou *et al* 1994) contributes about 30%. Without analysing the detailed dependence of the elastic cross section on energy (cf Stein *et al* 1992) the remaining 20% constitutes an upper limit for elastic scattering. This is quite opposite to electron scattering, in which the elastic cross section (cf de Heer *et al* 1979) amounts to 65% of the total cross section and exceeds by a factor three the absolute value for positron collisions. For positron scattering it seems plausible that, due to these relative proportions, even small changes in the inelastic channel influence visibly (outside the experimental error) the elastic cross section. This is not the case in electron–atom scattering; this fact could explain the negative result of the experiment by Cvejanović and Crowe (1994). In electron scattering on molecular hydrogen the proportions between elastic and inelastic parts are intermediate, with respect to $e^- + Ar$ and $e^+ + Ar$, around 1:1 at 50 eV (see figure 1).

Another particularity of molecular hydrogen relies on the fact that the total cross section reaches the maximum at a low energy (about 3 eV), and falls down monotonically above it. A number (up to 5) of partial waves must be used to fit the experimental differential cross sections even at 15 eV (Khakoo and Trajmar 1986). This allows us to use the high-energy, Born approximation as an analysing tool of existing experimental data.

Hydrogen partial cross sections have been studied in a number of independent experiments; so a set of reliable data can be chosen (cf Trajmar *et al* 1983). In particular, elastic scattering has been examined in most of the laboratories active in this field (see Brugner *et al* 1991 for the review). However, only the measurements of Nishimura *et al* (1985), those from Pasadena (Srivastava *et al* 1975, Khakoo and Trajmar 1986) and those of Shyn and Sharp (1981) cover the energy range from 10 to 100 eV. To our knowledge, only the latter two fulfil the condition of a one-point normalization.

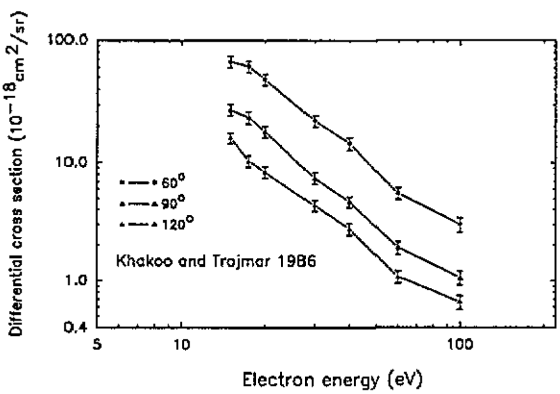


**Figure 2.** Elastic differential cross sections for electron scattering on $H_2$ (from Khakoo and Trajmar 1986). Absolute values were obtained by normalization to $e^- + He$ and $e^- + Ne$ values simultaneously. The error bars correspond to relative experimental uncertainties.

The differential cross sections from Khakoo and Trajmar (1986) as a function of the collision energy are shown in figure 2 for the same angles reported in the measurements of Dou *et al* (1992a). For all the three angles presented, one notices that the fall in the cross sections between 40 and 60 eV is more rapid than at lower energies. Due to the limited number of experimental points between 30 and 100 eV, this effect is not so clear as in the case of $e^+ + Ar$. A rough estimate of the drop in $H_2$ can be made by drawing a straight line between the 60 and 100 eV points. The drop looks to be of the order of 30%.

In order to perform a more convincing check, the differential cross sections of Shyn and

Sharp (1981) between 60 and 108° has been fitted by the Born formula (cf Joachain 1975)

$$\frac{d\sigma}{d\theta} = \frac{4V_0^2}{(\alpha^2 + 4k^2 \sin^2(\theta/2))^2} \tag{1}$$

for elastic scattering on a Yukawa potential (atomic units used)

$$V(r) = -V_0 \frac{e^{-r\alpha}}{r} \tag{2}$$

where $a = 1/\alpha$ is the 'range' and $V_0$ the 'strength' of the interaction. If the differential cross sections follow this formula, the plots of $(d\sigma/d\omega)^{-1/2}$ against energy should be straight lines, with the interception point on the $Y$ scale determined by the ratio $\alpha/V_0$; the ratios of the slopes should scale as $(\sin^2(\theta/2))^2$. As seen immediately from figure 3 for all considered angles, the data between 10 and 100 eV, with exclusion of the 60 eV points, follow equation (1). The differential cross sections at 60 eV are lower than would be expected from the regression line (note the inverted $Y$ scale). This effect is especially distinct at angles close to 90°.

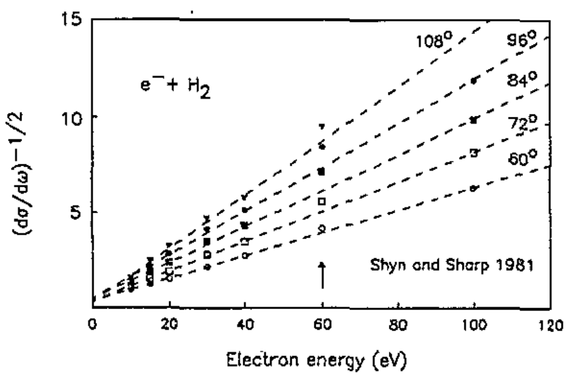


**Figure 3.** Plot of $(d\sigma/d\omega)^{-1/2}$ in $(10^{-20}\ m^2\ sr^{-1})^{-1/2}$ units against energy. Data from Shyn and Sharp (1981). First-order regression lines are drawn through the 10–40 eV and 100 eV points. Notice that the 60 eV points depart from the regression values lines towards lower values of the cross sections.

The regression lines intercept the $Y$ scale at $0.43 \pm 0.06$ (an average value for all angles between 12° and 96°). The slopes of the straight lines scale as $(\sin(\theta/2))^2$ within 12%. The magnitude of the 60 eV drop at 90°, evaluated from the regression procedure, would amount to 37%, so it is surely outside the experimental error stated by Shyn and Sharp (8% disregarding the normalization uncertainty).

*The parameters of the scattering potential derived from the fit are* $V_0 = 1.23$ au (which corresponds to an 'effective' atomic charge) and the range $a = 1.3$ au.

What is somehow surprising, in respect to positron measurements, is that this feature in the differential cross section is also visible in the integrated elastic cross sections, as given by the authors of the measurements. As seen from figure 4 the integrated cross sections of both Shyn and Sharp (1981) and of Khakoo and Trajmar (1986) follow an $1/E$ energy dependence between 10 and 30 eV, as predicted by the Born approximation (cf Joachain 1975), but they fall below it, starting from 40 eV. Above 100 eV the dependence once more obeys the Born approximation. Again, more conclusive statements will be possible when new measurements, with a better energy coverage, are available.

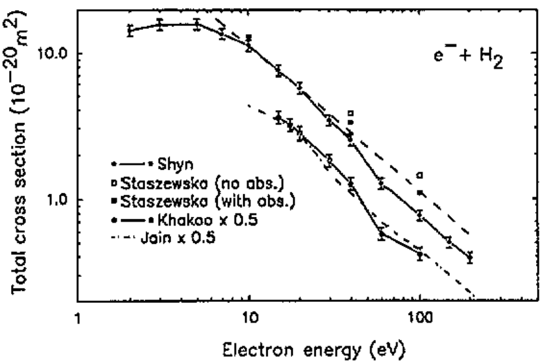


**Figure 4.** Integrated elastic cross sections for $e^- + H^2$ scattering: full circles, Shyn and Sharp (1981); open circles, Khakoo and Trajmar (1986); the error bars correspond to integration errors; chain curve, optical potential calculations of Jain and Baluja (1992); full squares, optical model without absorption (Staszewska *et al* 1984); open squares, the same model with absorption. The broken curve indicates the $1/E$ dependence drawn through the 20 eV point.

It may be relevant to note that a similar shoulder-like structure was predicted theoretically by Jain and Baluja (1992) in complex-optical potential (i.e. including absorption) calculations, even if the exact magnitude and the position of the structure do not completely agree with the experiment. The structure does not appear if no absorption is allowed (see data of Staszewska *et al* 1984, in figure 4).

Based on partitioning schemes, several other targets (for example $CH_4$ or Na) are good candidates for the observation of the coupling effects in the elastic channel. Nevertheless, the available measured data for the differential elastic cross sections in the energy range from a few tens to a few hundreds of eV are very sparse. A check on these molecules will be possible when new data become available.

One of us (GK) became familiar with the problem during his stay at Wayne State University at Detroit. The cordial hospitality of Professors T S Stein and W E Kauppila and the financial support from the Kosciuszko Foundation is acknowledged.

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