



# Screening corrections for the interference contributions to the electron and positron scattering cross sections from polyatomic molecules



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## ABSTRACT

An improvement of the screening-corrected Additivity Rule (SCAR) is proposed for calculating electron and positron scattering cross sections from polyatomic molecules within the independent atom model (IAM), following the analysis of numerical solutions to the three-dimensional Lippmann–Schwinger equation for multicenter potentials. Interference contributions affect all the considered energy range (1–300 eV); the lower energies where the atomic screening is most effective and higher energies, where interatomic distances are large compared to total cross sections and electron wavelengths. This correction to the interference terms provides a significant improvement for both total and differential elastic cross sections at these energies.

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## 1. Introduction

Electron and positron ( $e^-/e^+$ ) scattering processes from atoms and molecules have been a subject of interest during the last few decades. Recently this interest has considerably increased due to the relevance of these processes in radiation interaction models for biomedical applications [1]. Scattering experiments are complicated in general and difficulties determining absolute values as well as uncertainties connected with energy and angular resolution limitations require some complementary data from theory. In this context sufficiently accurate general calculation procedures, for a wide variety of targets, over a broad energy range, are extremely useful.

The lack of spherical symmetry makes *ab initio* calculations for electron and positron scattering cross sections by molecules almost unfeasible at intermediate and high energies, and therefore available theoretical methods rely on different approximate treatments. One of these techniques, the Independent Atom Model (IAM) [2–8], is particularly successful. The IAM treatment assumes that the molecules can be approximately substituted by their constituent atoms in their corresponding positions, which independently scatter incident electrons or positrons. One of the greatest advantages of this approach is the possibility of obtaining reliable

results for a large number of molecular species from the data of a reduced number of atoms. With this method, total elastic, inelastic and differential elastic cross sections can be easily obtained with reasonable accuracy within its energy range of applicability, typically above 100 eV.

An important limitation of the IAM treatment is that it ignores any multiple scattering of the projectile within the molecule, hence it's application only for relatively high incident energies (>100 eV). Some years ago, we proposed an approximated method to partially account for these effects, the screening corrected additivity rule (SCAR) [9,10], which extended the applicability of the IAM method down to lower energies, typically 20–30 eV.

In a recent letter [11] the IAM treatment for elastic scattering has been revisited, indicating the relevance of interference contributions arising from all the scattering centres in the molecule. These contributions were particularly important at small scattering angles, where experimental systems are unable to distinguish them. Nevertheless they contribute significantly to the integrated cross sections, and therefore it is crucial to use interference corrected values for Monte Carlo simulations [12] and for experimental data normalisation procedures [13]. However, as the AR procedure fails for energies below 100 eV by noticeably overestimating the cross section for decreasing energies, the effect of the interference terms in this range is not appreciable. In these conditions the SCAR procedure constitutes an excellent tool to evaluate the magnitude and consequences of interference terms at intermediate energies, below 100 eV.

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The main objective of this study is to revise the SCAR procedure in order to include these interference contributions. For this purpose, considering only elastic scattering for representative molecular targets will be enough, and therefore, following the scheme of our previous letter [1], we will solve a three-dimensional Lippmann–Schwinger equation for some multicentre potentials. Although we have compared these results for different molecular configurations based on C and H atoms for different interatomic distances, we will present here only data for the H<sub>2</sub> and CH<sub>4</sub> at their equilibrium geometries as they suffice to illustrate all the relevant results.

## 2. Review of interference and screening corrections

Assuming the IAM approximation, the molecular cross sections can be derived from the well known approximate expression [2] for multicenter dispersion

$$F(\theta) \approx \sum_{\text{atoms}} f_i(\theta) e^{i\mathbf{q} \cdot \mathbf{r}_i} \quad (1)$$

where  $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$  is the momentum transfer,  $\mathbf{r}_i$  are the atomic positions and  $f_i(\theta)$  are the atomic scattering amplitudes. As this corresponds to the independent scattering from each atom, the approximation is expected to be valid only for large interatomic distances compared to the wavelength associated to the incident projectile.

From the above molecular dispersion function, the differential elastic cross section is easily obtained by averaging its modulus squared  $|F(\theta)|^2$  over all the molecule orientations' [2,6], obtaining:

$$\begin{aligned} \frac{d\sigma_{\text{molecule}}^{\text{elastic}}}{d\Omega} &= \sum_{i,j} f_i(\theta) f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}} = \sum_i |f_i(\theta)|^2 \\ &+ \sum_{i \neq j} f_i(\theta) f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}} = \sum_i \frac{d\sigma_{\text{atom } i}^{\text{elastic}}}{d\Omega} + \frac{d\sigma^{\text{interference}}}{d\Omega} \end{aligned} \quad (2)$$

where  $q \equiv |\mathbf{q}| = 2k \sin \theta/2$ ,  $r_{ij}$  is the distance between  $i$  and  $j$  atoms,  $\sin qr_{ij}/qr_{ij} = 1$  when  $qr_{ij} = 0$ , and  $d\sigma^{\text{interference}}/d\Omega$  represents the  $\sum_{i \neq j}$  interference contribution to the molecular differential cross section.

Hereafter, we will consider only elastic processes, which are enough for our purposes, and hence a real scattering potential for each atom (no imaginary inelastic part) will be used to obtain the atomic scattering amplitudes  $f_i(\theta)$ . In these conditions the total cross section will be coincident with the corresponding integral elastic cross section.

By integrating Eq. (2) the total molecular cross section can be written as:

$$\sigma_{\text{molecule}}^{\text{total}} = \sum_{\text{atoms}} \sigma_{\text{atom } i}^{\text{total}} + \sigma^{\text{interference}} \quad (3)$$

where  $\sigma^{\text{interference}}$  represents the integration of the above differential interference contribution. It must be noted that this contribution would not be present in (3) if this expression were directly obtained from (1) by applying the optical theorem. This latest procedure is known as the 'Additivity Rule' (AR) and is widely described in literature [5–7,9,14–23]. As discussed in [11], the appropriate expression is Eq. (3), and the discrepancy relies on the approximate nature of Eq. (1) which doesn't fulfil the optical theorem. It has also been shown that interference terms are only relevant at small angles and their integrated contribution ( $\sigma^{\text{interference}}$ ) is non negligible even at high energies [11].

At intermediate energies (10–100 eV), where atomic cross-sections are not small compared to interatomic distances in the

molecule, the IAM approximation fails since the atoms can no longer be considered as independent scattering centres and multiple scattering within the molecule is not negligible. Approximate methods revealed that important corrections are needed by the IAM method for these energies [8,9,19,21,24,25] and it has been shown [9] that the energy range for which these corrections are relevant depends on the size of the molecule: around 10% for N<sub>2</sub> and CO up to 200 eV, for CO<sub>2</sub> up to 300 eV, and for benzene up to 600 eV.

Representative molecular cross-section calculations are based on a corrected form of the IAM treatment known as the SCAR (Screening Corrected Additivity Rule) procedure, which approximately accounts for these multiple scattering effects. All the details for this procedure have been extensively described elsewhere [9,10,26] and therefore they are only briefly mentioned here.

Basically, within the SCAR procedure the integral molecular cross sections (both elastic and inelastic), ignoring interference contributions, are expressed as:

$$\sigma_{\text{molecule}}^{\text{total}} = \sum_{\text{atoms}} s_i \sigma_{\text{atom } i}^{\text{total}} \quad (4)$$

where the  $s_i$  screening coefficients reduce the contribution of each atom to the total molecular cross section ( $0 \leq s_i \leq 1$ ). The calculation of these coefficients requires some simple closed expressions [9,26] based only on data about position and the total cross section  $\sigma_{\text{atom } i}^{\text{total}}$  of each atom in the molecule. This procedure is applicable to any arbitrary molecular geometry and size [27]. Note that only elastic processes are considered in this study and therefore the total cross section and the integral elastic cross section are coincident.

As far as the differential elastic cross sections are concerned, the SCAR procedure distinguishes two contributions, one from the direct scattering cross section ( $\sigma_D$ ) which is related to the angular distribution given by the single scattering differential cross section, and the re-dispersed cross section ( $\sigma_{\text{molecule}}^{\text{elastic}} - \sigma_D$ ) which corresponds to an assumed isotropic angular distribution. The latter contribution approximately accounts for re-dispersion processes inside the molecule. After estimating their relative weight by means of the  $s_i$  screening coefficients and the aforementioned angular distributions of the atomic elastic cross sections [9] the resulting expression is

$$\frac{d\sigma_{\text{molecule}}^{\text{elastic}}}{d\Omega} \cong (1 - X_S) \frac{\sigma_{\text{molecule}}^{\text{elastic}} - \sigma_D}{4\pi} + \left[ 1 + X_S \left( \frac{\sigma_{\text{molecule}}^{\text{elastic}}}{\sigma_D} - 1 \right) \right] \frac{d\sigma_D}{d\Omega} \quad (5)$$

where  $\sigma_D$ ,  $X_S$  and  $d\sigma_D/d\Omega$  are defined by

$$\sigma_D = \sum_{\text{atoms}} s_i^2 \sigma_{\text{atom } i}^{\text{total}} \quad (6)$$

$$\frac{d\sigma_D}{d\Omega} = \sum_i s_i^2 \frac{d\sigma_{\text{atom } i}^{\text{elastic}}}{d\Omega} + \sum_{i \neq j} v s_i s_j f_i(\theta) f_j^*(\theta) \frac{\sin qr_{ij}}{qr_{ij}} \quad (7)$$

$$X_S = \frac{\int_0^{45^\circ} \frac{d\sigma_D}{d\Omega} \sin \theta d\theta}{\int_0^{180^\circ} \frac{d\sigma_D}{d\Omega} \sin \theta d\theta} \quad (8)$$

As seen from Eq. (7), the direct contribution of the scattering is a screening version of Eq. (2). The first summation operator in (7) accounts for each atomic contribution, reduced by a  $s_i$  factor, whereas the second one represents the reduced interference terms.

We should note that applying the AR, i.e. ignoring the integral  $\sigma^{\text{interference}}$  contributions but including them in the differential cross section values, Eqs. (6) and (7) can be in conflict. In order to avoid this contradiction we introduced an additional reducing factor ( $v$ ) applied to the positive values of  $d\sigma^{\text{interference}}/d\Omega$  in order to ensure that  $\int d\Omega (d\sigma^{\text{interference}}/d\Omega) = 0$ . This additional condition was called the 'normalised' SCAR treatment. Most of the recent

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