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Modified effective range analysis of low energy electron and positron scattering on CO_2

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Abstract. Analytical solutions for the modified effective range problem have been applied to positron and electron scattering on carbon dioxide in the low (below 10 eV) energy range. For positrons, the solution with three partial waves reproduces very well experimental results up to the positronium formation threshold; the *s*-wave contribution rises in the limit of zero energy and the *p*-wave contribution reaches a very broad maximum at about 0.5 eV. For electron scattering, the present solution shows a sharp rise of the *s*-wave contribution in the limit of zero energy, explained by earlier calculations as a virtual negative ion state. The *p*-wave shows a resonant structure at about 5 eV corresponding to an experimentally well known $^2\Pi_u$ shape resonance. An additional maximum in the *p*-wave contribution is observed at about 1-2 eV. The latter feature would explain resonant-like scattering observed recently in high-resolution vibrational excitation measurements [M. Allan, Phys. Rev. Lett. 87 (2001) 033201].

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1. Introduction – experiments and theory

Knowledge of cross sections for electron scattering on CO_2 is of basic importance for understanding operation of high power infrared lasers; CO_2 is also the main factor in human-induced greenhouse effect. The low-energy electron scattering total cross section is characterized by a strong rise in the limit of zero energy, with the total cross sections reaching as much as [1] $60\text{x}10^{-20}\,\text{m}^2$ at 0.1 eV and presence of a shape $2\Pi_u$ resonance at about 3.8 eV, observed as a maximum in the total cross section [2,3], with a big part (about 1/3, see [4]) coming from the vibrational excitation.

While early calculations using a semiempirical polarization potential [5,6] agreed pretty well with the electron-scattering experiment in a large (0.1-10 eV) energy range, ab-initio theories covering this energy range have been developed only recently [7,8,9]. The low energy rise has been attributed [10,11] to a virtual Σ_g state. The recent measurements of the vibrational excitation showed the presence of resonant enhancements also in the 1-2.5 eV energy range [12].

Positron scattering on CO_2 was studied experimentally by few groups (see the discussion below). For the theory, Gianturco and Paioletti [13] applied the density-functional method for short-range interaction effects in order to obtain elastic and rotational excitation cross sections in the 0.5-7 eV energy range and Gianturco and Mukherjee [14] used the body-fixed vibrational close-coupling scheme to obtain the elastic and the vibrational excitation cross sections in the same energy range. The weak point of theoretical calculations is that different

models were separately applied to positron and electron projectiles and for the very low and resonance energy regions in electron scattering.

The present work gives an analysis of positron and electron scattering on CO_2 in the framework of the modified effective-range theory (MERT) [15]. It is based on the analytical solution for scattering from a polarization potential with short-range effects introduced through parametrization of the phase shifts [16]. The analysis uses experimental total cross sections at energies below the threshold for electronic excitation (or positronium formation for positrons). In the this energy range (apart from resonances) the total cross section, measured with a few per cent error, approximates well the integral elastic cross section (usually measured with much bigger uncertainty and by normalized methods).

2. Choice of experimental data

For electron scattering the time-of-flight experiments in the very-low-energy range [1, 3] merge well with the electrostatic-beam experiment in the region of a few eV [2]. These three sets of data, weighted by their uncertainties form recommended values given in [4], are used for the present analysis.

Positron-scattering total cross sections were measured down to 0.5 eV by Hoffman et al. [17] with an apparatus using a long (109 cm) scattering cell, with rather small apertures (1.2 mm radius at the entrance and 2.4 mm at the exit) and a longitudinal guiding magnetic field (16 G at 2 eV collision energy) [18]. First measurements by Sueoka and collaborators [19] were performed down to 1 eV using 67.5 mm long scattering cell (we quote the geometrical length and not the "effective" 79.7 mm length) with 4 mm radius apertures and 9 G guiding field. The more recent data [20] (quoted also in [21]) were performed down to 0.3 eV with 1.8 G guiding field and 3 mm radius apertures; at 1 eV those data are by 10% lower than the value of Kwan et al. [22] and 20% higher than the early set [19].

The new apparatus constructed at Trento laboratory [23] uses a 10 mm long scattering cell with 0.75 mm apertures radii and 9 G guiding field. The positron scattering data for CO_2 extending down to 0.1 eV [24] rise quickly in the low-energy limit and form the highest set. As we discussed in detail for N_2 measurements [25], the use of large apertures in the scattering cell combined with high magnetic fields can lead to a strong underestimation of the total cross section in the low energy limit. At sufficiently low energies, when the cyclotronic radius of positrons in the magnetic field equals or is smaller than the scattering cell exit apertures, all positrons scattered into the forward cone (up to 90º scattering angle) are recaptured by the magnetic field and guided to the detector. Assuming an isotropic differential cross section and no inelastic processes present, the measured total cross section would then amount to 50% of the real value. Such a "half-value" collision energy equals to 0.8 eV in the experiment of [17], 1.1 eV in experiment of Sueoka and Mori [19], 0.026 eV in their repeated experiment [26], and as little as 0.0045 eV in the Trento experiments [25].

A second possible source of error in the absolute magnitude of total cross sections in the low energy limit can be the energy scale shift. In the Trento apparatus, detailed procedures both with a retarding field analyzer [27] and using the N_2 and Ar positronium thresholds [25] were applied, so a possible error in the energy scale is within ±0.1 eV. Note also that the energy resolution of the Trento apparatus is about 150 meV, as proved by observation of sharp resonant structures in He at 1.4-2.1 eV [28]. For all these arguments we believe that the cross sections from Trento laboratory can be considered presently the most reliable set for positron scattering.

3. Analytical solution for modified effective range approximation

As already stated by O'Malley et al. [29] the zero energy limit in electron and positron scattering should be well approximated by the modified effective range theory. In this theory scattering is assumed to be due to polarization potential solely and the short-range effects are introduced by an effective range R_0.

Electron scattering on noble gases has been extensively evaluated in the framework of MERT by Buckman and Mitroy [30] who used five-parameter expansion in series of momentum k for the s and p-wave phase shifts. Electron scattering on non-polar molecules (H_2, N_2, CO_2) was studied, among others by Fabrikant [31]. In all these studies an upper limit for MERT analysis was confined to energies below 1 eV (0.2 eV for CO_2). In a recent work [16] we have applied analytical solutions for scattering on the polarization potential to extend the applicability of MERT to higher energies. We obtained MERT expansion by developing the parameter characterizing the short range interaction into series of k . We tested this scheme for positron scattering on Ar and N_2 up to 2 eV - the parameters of the short range potential were obtained by fitting recent experimental total cross sections [25].

We resume here the main notions. The radial Schrödinger equation for a particle moving in the polarization potential $V(r) = -\alpha e^2/2r^4$ is

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2}\right) - \frac{\alpha e^2}{2r^4} - E\right]\Psi_l(r) = 0, \tag{1}$$

where μ is the reduced mass, α is the static dipole polarizability, E is the relative energy of the particles, and $\Psi_l(r)$ denotes the radial wave function for the partial wave l. With appropriate change of variables, the Schrödinger equation (1) can be transformed into Mathieu's differential equation of the imaginary argument [32], and solved analytically in terms of the continued fractions (see e.g. [16]). At small distances where the polarization potential dominates over centrifugal potential and the constant energy term, the asymptotic behaviour of $\Psi_l(r)$ is described by

$$\Psi_l(r) \xrightarrow{r\to 0} r\sin\left(R^*/r + \phi_l\right) \tag{2}$$

where $R^* = e/\hbar\sqrt{\alpha\mu}$ describes a typical length related to the polarization interaction, and ϕ_l is some short-range phase, that depends on the short-range part of the potential. For l=0 the short range phase determines the s-wave scattering length: a = - R*cot ϕ_0.

At large distances $\Psi_l(r)$ must take the form of the scattered wave

$$\Psi_l(r) \xrightarrow{r\to\infty} \sin\left(kr - l\,\pi/2 + \eta_l\right) \tag{3}$$

where $k = \sqrt{2\mu E}/\hbar$ and phase-shifts η_l can be expressed in terms of the short-range phases:

$$\tan\eta_l = \frac{m^2 - \tan^2\delta + (m^2-1)\tan\left(\phi_l + l\,\pi/2\right)\tan\delta}{(1-m^2)\tan\delta + \tan\left(\phi_l + l\,\pi/2\right)(1 - m^2\tan^2\delta)} \tag{4}$$

Here, δ = π/2(ν-l-1/2), and m and ν are some parameters characterizing Mathieu functions of the imaginary argument (see [16] for details). The effective range is introduced by expanding of tan(ϕ_l +l π/2) in powers of k

$$\tan\left(\phi_l + l\,\pi/2\right) = A_l + \tfrac{1}{2}R^*R_l k^2 + \ldots, \tag{5}$$

where $A_l = \tan(\phi_l + l\pi/2)\big|_{k=0}$ The lowest order correction in k is quadratic, and can be interpreted as effective range R_l for partial wave l [33].

4. Application for positron and electron scattering on CO_2.

Using for the (spherical) polarizability of CO_2 the value obtained from electron-scattering electronic excitation experiments α=16.92 a_0^3 [34] we obtain $R^* = 4.113\ a_0$. For MERT fit for positrons we used all experimental data from Trento lab from 0.1 eV up to the positronium formation threshold (i.e. 6.8 eV). The experimental data can be approximated quite well assuming contributions just from two partial waves *s* and *p*. If MERT expansion is performed also for *d* wave, the agreement remains within the statistical error bar for the whole energy range considered, see figure 1. The *s*-wave partial wave cross sections rises in the limit of low energies and dominates over the *p*-wave contribution for energies below 0.2 eV; the *s*-wave contribution passes through zero at 2 eV. Parameters of the potential (zero-energy contributions A_l and the effective ranges R_l) for the three partial waves are given in table 1. Note the zero value for the *p*-wave zero-energy parameter A_1 and a negative value for the *s*-wave scattering length.

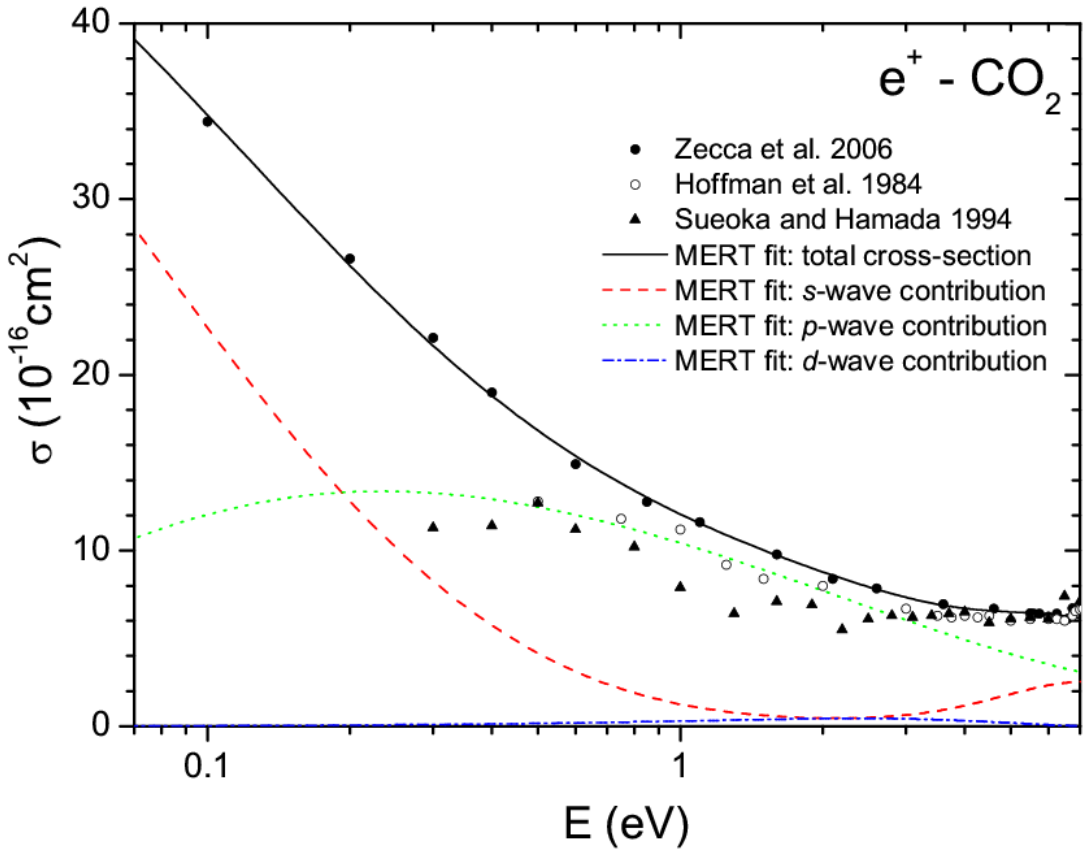

Fig. 1. MERT analysis for positron scattering on CO_2. Experimental data are: full circles – Zecca et al. [24], open circles – Hoffman et al. [17], triangles – Sueoka and Hamada [20]. Theoretical curves are: MERT fit for the total cross-section (solid line), and contributions from *s* wave (dash line), *p* wave (dot line) and *d* wave (dash-dot line).

	$a/R^*=-1/A_0$	A_1	A_2	R_0/R^*	R_1/R^*	R_2/R^*
$E^+ - CO_2$	- 1.120	- 0.0077	- 0.177	- 0.389	- 0.157	0.028
$e - CO_2$	- 1.616	- 6.250	- 0.406	- 0.266	2.780	0.131

Table 1. Positron and electron scattering parameters obtained by fitting MERT model to the experimental data.

For electron scattering we used the recommended data [4] from 0.1 to 2.0 eV: the fit with MERT expansion for two partial waves reproduced the set within experimental uncertainties, see fig.2. The obtained scattering length a =- 6.61a_0 agrees well with the value a=- 6.17a_0 predicted by Morisson [35] and the limits given by Fabrikant [31]: -7.2 $a_0 < a <$ -6.8a_0.

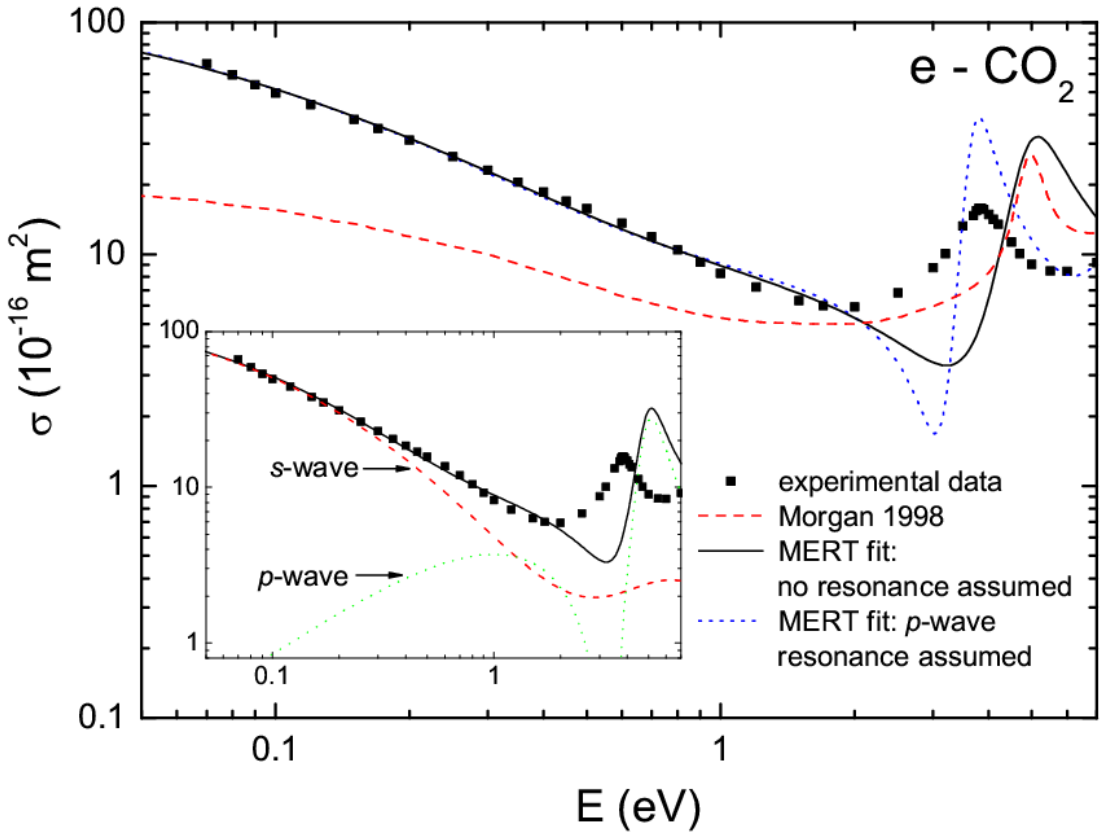

Fig. 2. MERT analysis for electron scattering on CO_2. Depicted are: recommended experimental data from review [4] (squares), multistate calculation of Morgan [11] (dash line), and theoretical fits with MERT expansion for two (solid line) and three (dot line) partial waves. For the latter calculation we assumed *p*-wave resonance at the experimentally observed peak. The inset shows in addition the *s*-wave and *p*-wave contributions to the MERT fit with two partial waves.

Differently from previous MERT approaches and in agreement with experiments, our MERT model predicts the existence of a shape resonance in *p*-wave channel at 5 eV. This is slightly higher than the peak in the experimental total cross section but also the calculation by Morgan [11] overestimates the energy of the shape resonance, see fig. 1. The shape resonance appears in the regime where the *d*-wave contribution can be significant, therefore we have

also tried a fit with MERT for three partial waves fixing additionally the position of the resonance at the experimentally observed value. Parameters of such a fit are given for sake of comparison with positron parameters in table I. This demonstrates the compatibility of MERT expansion for small energies and the existence of the *p*-wave shape resonance.

Our MERT analysis shows also a peculiar behaviour of the *p*-wave shift just below the shape resonance. The *p*-wave cross section changes quickly just below the resonance, reaching another maximum at 1 eV. We hypothesize that this maximum is responsible for a resonance-like enhancement of the vibrational excitation observed between 1 and 2.5 eV by Allan [12].

6. Conclusions

We show that the recently developed scheme based on analytical solutions and MERT expansion gives very good agreement with experimental data both for positron and electrons. For positrons the agreement extends up to the threshold for positronium formation. For electrons, the fit performed in the low energy range (below 2 eV) predicts the existence of a shape resonance at 5 eV, and an additional enhancement in the *p*-wave channel at about 1 eV. The obtained position of the resonance is slightly higher than the experimentally observed peak at 3.8 eV, and is close to the theoretical value of [11]. The agreement with the experiment can be improved, as far as the position of the resonance is concerned, using three partial waves in MERT expansion. Summarizing, the present MERT calculations reproduces well the observed cross section for both type projectiles. In the case of positron scattering MERT shows a sharp rise of the total cross section in the limit of zero energy; in the case of electrons it shows a similar rise in the zero-energy limit plus a shape resonance at about 5 eV.

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