

Positron and electron scattering on atoms and molecules—modified effective range theory revisited

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Abstract. New experiments on the very low-energy electron and positron scattering allow to verify the old question on applicability of modified effective range theory (MERT). We perform it using an analytical solution of the Schrödinger equation with the long-range polarization potential. In this work two atomic (He, Ar) and molecular (H₂, CH₄) target are studied using this approach. Total cross sections were used for obtaining parameters characterizing the scattering phase shifts related to the short-range interaction potential; differential cross sections were used for comparison. Differently from previous works, we conclude that MERT with few (2-3) partial waves applies very well up to energies of few eV in all four targets studied. For positrons, reliable experimental data indicate occurrence of zeros in the *s*-wave phase shifts for all four targets. This should be recognized as Ramsauer-Townsend minima.

1 Introduction

The modified effective range theory (MERT) for positron and electron scattering has been proposed half a century ago [1,2]. It was frequently used [3] to extrapolate experimental cross sections down to zero energy in series of the wavevector *k* powers. In an extensive study [4] it was shown that MERT series can be applied only in the very low energy range (below 1 eV in noble gases).

In [5,6] we proposed a different approach to MERT: the scattering phase shifts were obtained using Mathieu's functions, the analytical solutions of the Schrödinger equation with the long-range polarization potential. Whereas the effective range expansion (series of *k*) was introduced exclusively for a short-range part of the interaction potential. Such approach allowed to extend the applicability of MERT up to few eV. At present we use this alternative MERT to perform an extensive analysis of electron and positron scattering on light atomic and molecular targets (He, H₂, Ar, CH₄) using different sets of total cross sections (TCS). Argon (Ar) and methane (CH₄) show Ramsauer-Townsend (R-T) minimum for electron scattering [7,8]. While

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for positrons all four targets show a rise of TCS in the zero-energy limit but the existence of R-T minimum was not clear so far [9].

2 Modified effective range theory

We start with the radial part of the Schrödinger equation describing the relative motion of the particle in the polarization potential field

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{(R^*)^2}{r^4} + \frac{2\mu E}{\hbar^2} \right] \Psi_l(r) = 0, \quad (1)$$

where $\Psi_l(r)$ denotes the radial wave function, l is the angular momentum quantum number and E is the relative energy of the particle. For convenience we introduce some characteristic units R^* and E^* , where $R^* \equiv \sqrt{\alpha e^2 \mu / \hbar^2}$ denotes the characteristic length of the r^{-4} potential, and $E^* = \hbar^2 / (2\mu R^{*2})$ is the characteristic energy. Here α is the polarizability of the target, e is the elementary charge, μ is the reduced mass and \hbar is the Planck constant. The Schrödinger equation (1) can be transformed into Mathieu's differential equation of the imaginary argument and solved analytically [1, 2, 5, 6]. For $r \ll R^*$, when the polarization potential dominates over centrifugal potential and the constant energy term, behavior of $\Psi_l(r)$ is given by

$$\Psi_l(r) \stackrel{r \rightarrow 0}{\sim} r \sin \left(\frac{R^*}{r} + \phi_l \right), \quad (2)$$

where ϕ_l is a short-range phase, which is determined by the short-range part of the interaction potential. For $E = 0$ and $l = 0$ the solution (2) becomes exact at all distances, and from its asymptotic behavior at large distances one can easily determine the value of the s -wave scattering length

$$A = -R^* \cot(\phi_0). \quad (3)$$

At large distances: $r \gg R^*$, $\Psi_l(r)$ must take the form of the scattered wave

$$\Psi_l(r) \stackrel{r \rightarrow \infty}{\sim} \sin \left(kr - l\frac{\pi}{2} + \eta_l \right), \quad (4)$$

where $k = \sqrt{2\mu E} / \hbar$. Using the analytical solutions one can find the following relation between the phase shift η_l and the short range phase ϕ_l [1, 2]

$$\tan \eta_l = \frac{m^2 - \tan^2 \delta_l + B \tan \delta_l (m^2 - 1)}{\tan \delta_l (1 - m^2) + B(1 - m^2 \tan^2 \delta_l)}, \quad (5)$$

where $\delta_l = \frac{\pi}{2}(\nu - l - \frac{1}{2})$, $B = \tan(\phi_l + l\pi/2)$, and m and ν are parameters, that are determined from the analytical solutions of the Mathieu's differential equation [5].

The parameters ϕ_l entering the asymptotic formula (2), depend on energy, and can be expanded in powers of k . In our case it is more convenient to expand $\tan(\phi_l + l\frac{\pi}{2})$, entering formula (5):

$$\tan \left(\phi_l + l\frac{\pi}{2} \right) = B_l + \frac{1}{2} R^* R_l k^2 + \dots, \quad (6)$$

where $B_l \equiv \tan(\phi_l + l\frac{\pi}{2})|_{k=0}$. In the particular case of $l = 0$, B_0 can be expressed in terms of s -wave scattering length as: $B_0 = -R^*/A$. The lowest order correction in k

is quadratic, and can be interpreted as an effective range R_l for the partial wave l [1,2].

Previous MERT approach used approximate formulae for the s , p and d -wave phase shifts (η_l) [1,2,4]. At present we use an exact expression (5) for few first partial waves with the short-range phase shift (ϕ_l) expanded according to (6). The number of partial waves necessary to be treated by (5) can be estimated by comparing the energy of particle with the height of the centrifugal barrier $E_{max}(l) = \frac{1}{4}E^*l^2(l+1)^2$ for r^{-4} interaction [10]. The particle can penetrate the inner (short-range) part of the potential only when $E > E_{max}(l)$. In most cases, the elastic TCS can be describe considering only the contribution of s and p -wave and sometimes also d -wave phase shifts. The small phase shifts related to the higher partial waves, which can not overcome the repulsion of centrifugal barrier, can be taken into account using a following expression [1]

$$\tan \eta_l = \frac{\pi q^2}{8(l - \frac{1}{2})(l + \frac{1}{2})(l + \frac{3}{2})} + O(k^4). \quad (7)$$

This expression, valid for $l \geq 1$, is exact in the low-energy limit and this result can be also reproduced using the first-order Born approximation.

3 Positron experiments

Positrons constitute an alternative probe to electron scattering [11] – no exchange interaction acts for them. For electron TCS a good agreement exists (see [7,8,12,13]) while experiments on positron scattering date only to 70'ies of last century and are tedious. Early experiments from WSU Detroit [9] used a long (109 cm), curved scattering cell and a weak guiding magnetic field. The energy resolution was good (probably 0.1–0.2 eV) but the angular resolution was only moderate (in the range 10–20°). As shown by Buckman and collaborators [14] for Ar, the Detroit data can be brought qualitatively into agreement in the low energy limit with the recent TCS from Canberra [15] if a correction (by some +20°) is done. The recently developed Canberra apparatus [14,15] uses a strong magnetic field (500 G) so TCS have to be deconvoluted extrapolating the signal to the zero field.

Another early set-up, from Tokyo University [16] used a low magnetic field (3.6–27 G), 7 cm long scattering cell but wide (6–9 mm diameter) apertures. As a consequence the measured TCSs were underestimated in the low energy limit. As we showed in detailed analysis for benzene [17] and N₂ [18] those data can be brought into agreement with recent experiments if a correction for the angular resolution is performed.

The apparatus developed originally at Trento University [18] used 10 cm-long scattering cell length but narrow (1.5 mm diameter) apertures; the guiding field was about 9 G and the angular resolution error was negligible. The new configuration of the Trento apparatus [19] uses short (2.4 cm) cell and low counting rate (about 1 e⁺/s). However data [19] for H₂ obtained with this apparatus disagree with other experiments and recent theories, see [20]. The same machine was used in CH₄ [21].

4 MERT results

4.1 Helium

The low polarizability ($\alpha = 1.407 a_0^3$ [22]) provides relatively high effective energy $E^* = 9.671$ eV. Therefore the d -wave needs a high energy of at least

Table 1. MERT fitting parameters: $A = -R^*/B_0$ (s -wave scattering length), B_1 (zero-energy contribution for p -wave), R_0 (s -wave effective range), and R_1 (p -wave effective range) for electron and positron scattering on helium.

| | $A(a_0)$ | B_1 | $R_0(a_0)$ | $R_1(a_0)$ |
|------------------------------|----------|-------|------------|------------|
| $e^- + \text{He}$ (Buckman) | 1.186 | -20 | 0.01 | -100 |
| $e^+ + \text{He}$ (Sullivan) | -0.45 | -0.05 | -1.54 | -0.78 |
| $e^+ + \text{He}$ (Karwasz) | -0.59 | -1.29 | -0.28 | 1.16 |

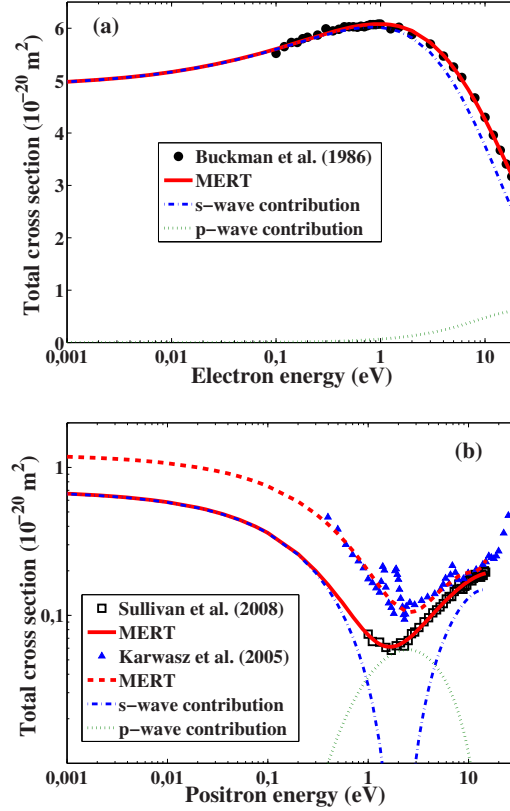


Fig. 1. Total cross sections for (a) electron and (b) positron scattering on helium. Experimental data are from Buckman et al. [23], Sullivan et al. [28] and Karwasz et al. [29]. In (b) the partial waves contribution is shown only for the data of Sullivan [28].

$E_{max}(l = 2) \approx 87 \text{ eV}$ to overcome the repulsion of the centrifugal barrier. Thus only two partial waves, s and p , are sufficient to explain TCS in whole energy range for elastic scattering of electrons ($E < 20 \text{ eV}$) and positrons ($E < 15 \text{ eV}$). The fitting was performed using unweighted least-square method; results for TCS are shown in Table 1 and Fig. 1.

For electron scattering TCS data of Buckman et al. [23] were used in current MERT analysis. The overwhelming contribution comes from the s -wave up to 20 eV. The derived scattering length A (numerically equal here to R^*) stays in a perfect accord with other experimental and theoretical results, see for example [7] and references therein. To validate our approach the parameters from Table 1 were used to calculate elastic differential cross sections (DCS). The comparison of calculations with some experimental results is shown in Fig. 2. The agreement in the whole 1.5–20 eV is to be judged as excellent.

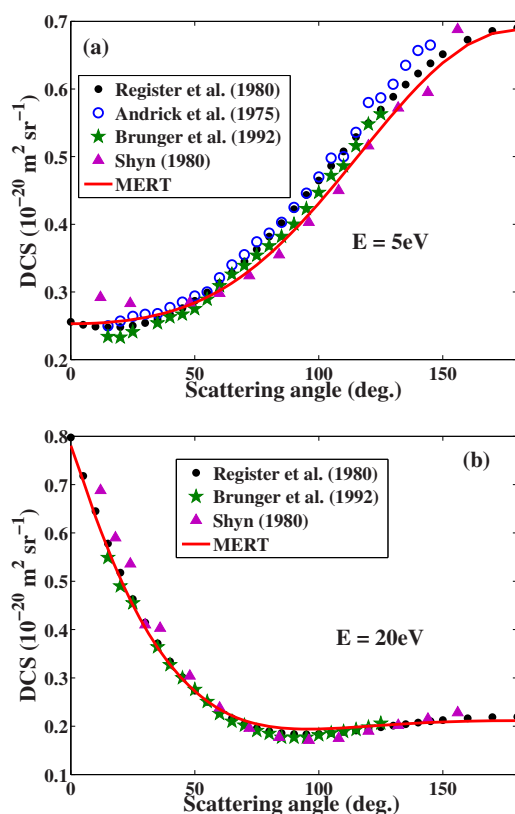


Fig. 2. Differential cross section versus the scattering angle at (a) 5 eV and (b) 20 eV for electron scattering on helium. Experimental data are from Andrick et al. [24], Shyn [25], Register et al. [26] and Brunger et al. [27].

For positrons, the agreement between MERT coefficients derived using TCS datasets of Jones et al. [28] and Karwasz et al. [29] is rather poor. Nevertheless both MERT fits indicate the presence of R-T minimum, at 2 eV and 3.2 eV, respectively.

4.2 Argon

Argon is a target with much higher polarizability ($\alpha = 11.23 a_0^3$ [22]) than helium. Hence it is necessary to include d -wave phase shifts using equation (5) in order to find a good fitting to experimental TCS data describing electron elastic scattering (energies $E \leq 10$ eV). Whereas for positrons, still only s and p waves are sufficient to reconstruct experimental TCS for energies below the positronium formation threshold ($E \leq 5$ eV). The results of fitting and derived MERT parameters are given in Fig. 3 and Table 2, respectively.

There is a very good agreement between MERT parameters calculated using the electron TCS data of Buckamn et al. [23] and Ferch et al. [3]. Moreover we have checked that the obtained scattering phase shifts for s , p and d waves agree very well for those given in Ref. [30] and further, calculated momentum transfer cross sections (MTCS) agrees fairly with swarm-derived ones from Ref. [31].

For positrons, two experimental datasets of Karwasz et al. [32] and Jones et al. [15] were used in the analysis. Obtained s -wave scattering lengths (see Table 2) stay in

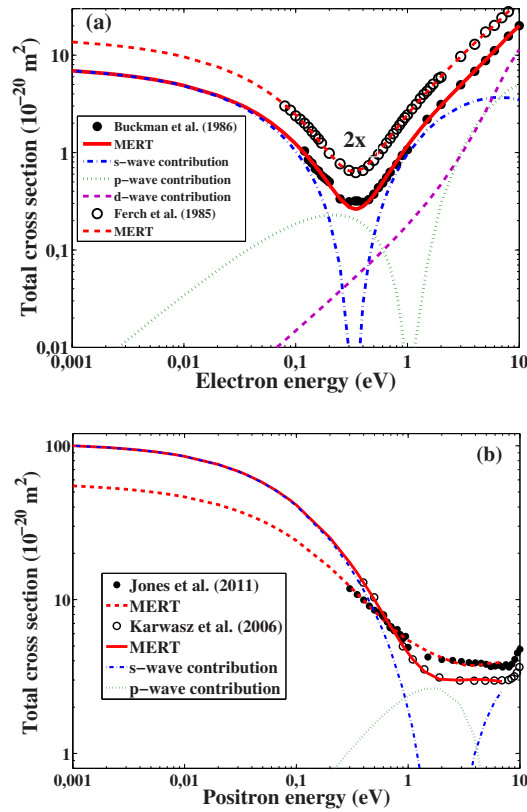


Fig. 3. Total cross sections for (a) electron and (b) positron scattering on helium. Experimental data are from Buckman et al. [23], Ferch et al. [3], Jones et al. [15] and Karwasz et al. [32]. The partial waves contributions are shown only for the data of Buckman [23] and Karwasz [32].

Table 2. MERT fitting parameters for argon.

| | $A(a_0)$ | B_1 | B_2 | $R_0(a_0)$ | $R_1(a_0)$ | $R_2(a_0)$ |
|-----------------------------|----------|-------|-------|------------|------------|------------|
| $e^- + \text{Ar}$ (Buckman) | -1.51 | -0.44 | 0.21 | -0.38 | 0.06 | 0.30 |
| $e^- + \text{Ar}$ (Ferch) | -1.50 | -0.49 | 0.27 | -0.40 | 0.10 | 0.36 |
| $e^+ + \text{Ar}$ (Karwasz) | -5.52 | -3.82 | — | 0.71 | 3.19 | — |
| $e^+ + \text{He}$ (Jones) | -4.11 | -3.67 | — | -1.47 | 1.97 | — |

agreement with other published results spanning the range of $-2.8 a_0$ to $-5.3 a_0$ (see [33] and references therein). However the existence of the R-T minimum is indicated only by the fit to data of Karwasz et al. and we have checked that the derived scattering phase-shifts on the basis of this experiment are in good accord with the theoretical results of McEachran et al. [34] obtained within the polarized-orbital approximation.

4.3 Molecular hydrogen

In molecular hydrogen the polarizability is $\alpha = 5.314 a_0^3$ [22]. As a result the d -wave contribution is small compared to s and p waves for energies $E < 10$ eV, both for electrons and positrons. In Fig. 4(a) we compare the present MERT fit with recommended TCS [13] for electrons. The agreement using only two partial waves is

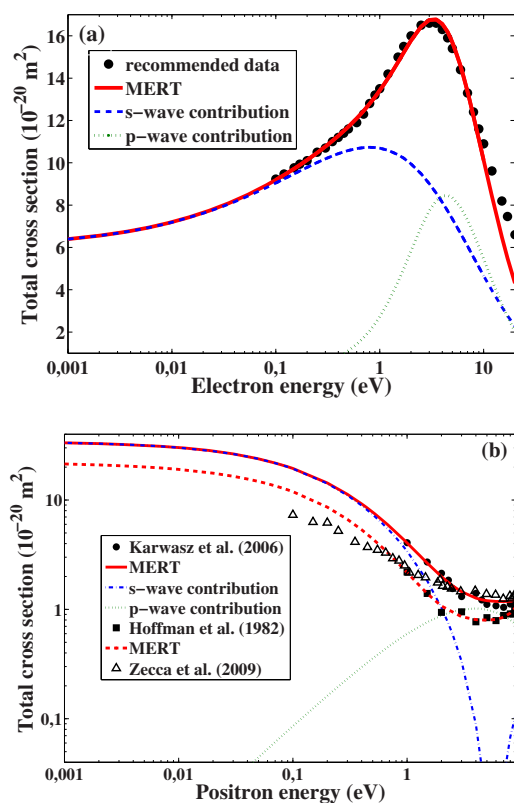


Fig. 4. Total cross sections for (a) electron and (b) positron scattering on molecular hydrogen. Recommended data for electrons are from [13]. Positron experimental data are from Hoffman et al. [35], Karwasz et al. [32] and Zecca et al. [19]. In (b) the partial waves contribution is shown only for the data of Karwasz.

Table 3. MERT fitting parameters for molecular hydrogen.

| | $A(a_0)$ | B_1 | $R_0(a_0)$ | $R_1(a_0)$ |
|--|----------|-------|------------|------------|
| $e^- + \text{H}_2$ (Landolt-Bornstein) | 1.30 | 0.38 | -0.90 | 1.75 |
| $e^+ + \text{H}_2$ (Karwasz) | -3.13 | -1.99 | -0.12 | -0.90 |
| $e^+ + \text{H}_2$ (Hoffman) | -2.51 | -1.94 | 0.29 | -2.51 |

very good. The s -wave contribution dominates up to about 1 eV; at the cross sections maximum (3-4 eV) both the s -wave and p -wave are important.

For positrons, MERT fits to the pioneer data of Hoffman et al. [35] and more recent experiment of Trento [32] give quite similar results for parameters describing the zero-energy contribution of s - and p -waves (see A and B_1 in Table 3). Both sets indicate also the existence of R-T minimum. No reasonable four-parameter fit was possible for the data from Ref. [19] (see Fig. 4(b)) obtained with new configuration of Trento apparatus.

4.4 Methane

In MERT calculations for CH_4 we used the value of polarizability $\alpha = 19.0 a_0^3$ suggested by Ref. [36]. Such high value provides very low $E^* = 0.72$ eV and

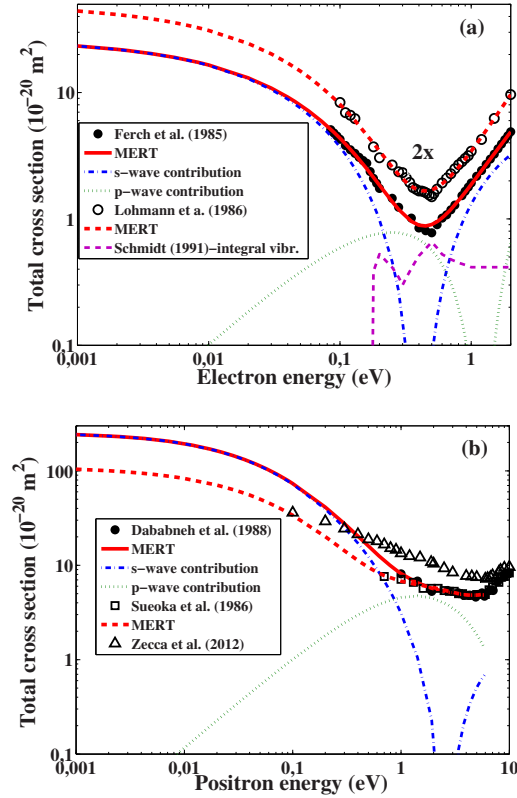


Fig. 5. Total cross sections for (a) electron and (b) positron scattering on methane. Experimental data are from Ferch et al. [37], Lohmann and Buckman [38], Sueoka et al. [39], Dababneh et al. [40] and Zecca et al. [21].

Table 4. MERT fitting parameters for methane.

| | $A(a_0)$ | B_1 | $R_0(a_0)$ | $R_1(a_0)$ |
|--------------------------------|----------|-------|------------|------------|
| $e^- + \text{CH}_4$ (Ferch) | -2.76 | -0.68 | -0.34 | 0.36 |
| $e^- + \text{CH}_4$ (Lohmann) | -2.69 | -0.67 | -0.85 | 0.50 |
| $e^+ + \text{CH}_4$ (Sueoka) | -5.65 | -2.82 | -1.22 | -3.05 |
| $e^+ + \text{CH}_4$ (Dababneh) | -8.55 | -2.44 | -0.25 | -4.49 |

$E_{max}(l = 2) \approx 6.45$ eV. Moreover, in order to obtain integral elastic cross sections the vibrational excitation, which constitutes about 30% of TCS at 0.4 eV, has to be subtracted. We used vibrational cross sections derived from swarm drift coefficient [36].

In this work we limit our MERT analysis to energies $E \leq 2$ eV where the chosen vibrational excitation cross section data are available. We found that in this energy range only two partial waves are sufficient to reconstruct experimental TCS for electrons given in Ref. [37] and [38]. MERT coefficients derived from both sets (see Table 4) are in very good agreement. Moreover these two sets give similar minima in MTSC of about 0.3×10^{-20} m² at 0.3 eV (not shown).

For positrons, the Tokyo [39] and Detroit [40] data give very similar MERT parameters for the p -wave (i.e. B_1 and R_1) but as far as only data of Ref. [40] give a zero

in the s -wave shift (i.e. the true R-T minimum), the data from Ref. [39] show only a minimum in this shift (not shown in Fig. 5). Again, no four-parameter fit worked for the data Ref. [21] obtained with new configuration of Trento apparatus.

5 Conclusions

In this work we showed the applicability of modified effective range theory (MERT) for modeling electron and positron elastic scattering cross sections in a wide variety of different atoms and non-polar molecules. Using only few partial waves within the potential barrier of the targets it is possible to reproduce integral, differential and momentum transfer cross sections being in very good agreement with some available experimental results. In particular case of positron scattering, we showed that the current model predicts the Ramsauer-Townsend minimum for all studied targets. These results present the potential of MERT to parameterize scattering phase-shifts from zero energy up to a threshold of the first inelastic channel using only few coefficients of the effective range expansion. However the effective-range parameters can be strongly affected by measurement uncertainties of the experimental data. Hence more measurements in the low-energy domain are needed in order to get final reliable parameterization.

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