Applicability of Modified Effective-Range Theory to positron-atom and positron-molecule scattering

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We analyze low-energy scattering of positrons on Ar atoms and N₂ molecules using Modified Effective-Range Theory (MERT) developed by O'Malley, Spruch and Rosenberg [Journal of Math. Phys. 2, 491 (1961)]. We use formulation of MERT based on exact solutions of Schrödinger equation with polarization potential rather than low-energy expansions of phase shifts into momentum series. We show that MERT describes well experimental data, provided that effective-range expansion is performed both for s- and p-wave scattering, which dominate in the considered regime of positron energies (0.4 - 2 eV). We estimate the values of the s-wave scattering length and the effective range for e⁺-Ar and e⁺-N₂ collisions.

Electron (and positron) scattering on atoms at very low energies is dominated by polarization forces. Modified effective range theory (MERT) was developed by O'Malley, Rosenberg and Spruch [1, 2] for low-energy scattering of charged particles on neutral polarizable systems in general. O'Malley [3] applied MERT for electron scattering on noble gases, in particular in the region of Ramsauer-Townsend minimum, using early total [4] and momentum transfer [5] experimental cross sections. Haddad and O'Malley [6] used three parameter MERT fit for s-wave phase-shift in electron-argon scattering and Ferch, Granitza and Raith [7] - for Ramsauer minimum in methane. Higher-order terms in MERT, resulting from short-range components of polarizability, were introduced by Ali and Fraser [8]. MERT analysis for Ne, Ar, Kr up to 1 eV was carefully revisited by Buckman and Mitroy [9] who used five-parameter fit for s-wave and p-wave shifts.

Applicability of MERT to low-energy positron scattering was already hypothesized in [2]. However, first measurements of total cross sections for positron scattering at low energies on noble atoms come only from seventies [10, 11]. The most systematic data for noble atoms, extending down to 0.3 eV were done in WSU Detroit lab, using positrons from a short-lived C⁹¹¹ radioisotopic source, with about 0.1 eV energy resolution [11]. Those data indicated clearly a rise of the cross section in the zero energy limit in gases, like He, Ar, H₂, Kr, Xe, CO₂, see [11]. Unfortunately, subsequent experiments [12, 13] used Ne²² source and thick W-vanes positron moderator, thus worsening energy resolution and not allowing to make reliable measurements below 1 eV. To gain in signal, large apertures and strong guiding magnetic fields were used, leading to underestimation of cross sections - some data showed even a fall in the limit of zero energy for highly polarizable targets, like C₆H₆ [14].

Only two of the most recent set-ups reached energies below 1 eV with good signal-to-noise ratio. In San Diego annihilations rates in Ar and Xe were measured, showing a steep rise below 1 eV [15]. In Trento total cross sections in Ar and N₂ were measured [16] with angular resolution better by a factor of 30 than in some previous experiments [12]. Both laboratories confirm the early observations from WSU Detroit on the rise of positron cross sections in the zero-energy limit. Such a rise is also predicted by ab-initio theories [17], see [16] for detailed comparison. A phenomenological attempt to apply MERT-like fit for low-energy cross sections in benzene and cyclohexane was done by Karwasz, Pliszka and Zecca [18].

In the present paper we apply MERT to positron total cross sections on argon and nitrogen, using recent experimental data from Trento [16]. We use MERT model based on direct solution of Schrödinger equation with polarization potential as originally proposed by O'Malley, Spruch and Rosenberg [1]. Differently from earlier works, for the p-wave phase shift we consider not only the polarization potential but contribution from a general-type short range interaction. This allows us to extend the MERT applicability for positrons to energies above 1 eV. A clear indication on importance of p-wave scattering in this energy range comes from recent differential cross sections measurements in argon [19]. The present model introduces a second MERT parameter for the p-wave shift thus developing an approximation with two parameters for both s and p-wave phaseshifts. The first parameter is to be interpreted as a scattering length and the second as an effective range. We compare our MERT model with the expansion into momentum series valid at low energies and with ab-initio theories [17, 20].

Let us briefly review the effective-range expansion for 1/r⁴ interaction. We divide the interaction potential between charged particle and neutral atom into the long-range part: \( V_p(r) = -\alpha e^2/(2r^4) \) with \( \alpha \) denoting the atomic polarizability and \( e \) the charge, and the short-range part: \( V_s(r) \) describing forces acting at distances comparable to the size of atoms. In the relative coordi-
nate the motion of particles is governed by
\[
\left[ \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} + \frac{(R^*)^2}{r^4} + k^2 \right] \Psi(r) = 0, \tag{1}
\]
where \( \Psi(r) \) denotes the radial wave function for \( l \)-th partial wave, \( \hbar k \) is the relative momentum of the particles, \( R^* \equiv \sqrt{\alpha e^2 \mu / \hbar^2} \) denotes a typical length scale related with the \( r^{-4} \) interaction, and \( \mu \) denotes the reduced mass. In Eq. 1, we do not include \( V_c(r) \), which is replaced by appropriate boundary condition at \( r \to 0 \). The Schrödinger equation with polarization potential can be solved analytically [1, 21, 22] (see Appendix for details). At small distances \( (r \ll R^*) \) behavior of \( \Psi(r) \) is governed by
\[
\Psi(r) \sim \frac{1}{kr} \sin \left( \frac{R^*}{r} \phi + \delta \right), \tag{2}
\]
where \( \phi \) is a parameter which is determined by the short-range part of the interaction potential. For \( r \gg R^* \), \( \Psi(r) \) takes the form of the scattered wave
\[
\Psi(r) \sim \frac{1}{kr} \sin (kr - l \frac{\pi}{2} + \eta), \tag{3}
\]
with the phase shift \( \eta \)
\[
\tan \eta = \frac{m^2 - \tan \delta^2 + B \tan \delta (m^2 - 1)}{\tan \delta (1 - m^2) + B (1 - m^2 \tan \delta)}, \tag{4}
\]
where we use similar notation as in Ref. 1. Here \( B = \tan (\phi + l \frac{\pi}{2}) \), \( \delta = \frac{\pi}{2} (\nu - l - \frac{1}{2}) \), and \( m \) and \( \nu \) are parameters obtained from the analytic solution of the Mathieu’s differential equation (see Appendix). To introduce effective range we expand \( B \) around zero energy: \( B(k) = B(0) + \frac{1}{2} R_0 R^* k^2 + \ldots \). The second term can be interpreted as correction due to the finite range of the interaction, with \( R_0 \) representing the effective range.

In the zero-energy limit expansion of MERT in series of momentum \( k \) is useful. In the particular case of \( l = 0 \), \( B(0) \) can be expressed in terms of \( s \)-wave scattering length \( a_s \): \( B(0) = -R^*/a_s \), and expansion of \( \cot \eta_0 \) at \( k = 0 \) yields 1, 22
\[
q \cot \eta_0(q) = -\frac{1}{a} + \frac{\pi}{3a^2} q^2 + \frac{4}{3a} \ln \left( \frac{q}{4} \right) q^2 + \frac{R_0^2}{2(R^*)^2} q^2 + \frac{20}{9a} - \frac{\pi^2}{3a^3} - \frac{8}{3a^2} \psi \left( \frac{7}{2} \right) \right] q^2 + \ldots \tag{5}\]
where \( a = a_s / R^* \), \( q = k R^* \) and \( \psi \left( \frac{7}{2} \right) \) denotes the digamma function 22. We apply similar procedure for \( p \)-wave. In this case, however, we expand directly \( \tan \eta_1 \) given by Eq. 1
\[
\tan \eta_1 = \frac{\pi q^2}{15} + \frac{q^3}{90} - \frac{83 \pi q^4}{23625} - \frac{4}{1350} \ln \left( \frac{q}{4} \right) q^5 - \frac{R_1}{18 \beta R^*} q^5 + \frac{15 \pi - 15 \pi^2}{20256} - \frac{1488}{20256} + \frac{120 b \psi \left( \frac{7}{2} \right)}{20256} q^5 + \ldots \tag{6}\]
Here, \( b = B(0) \) for \( l = 1 \), and \( R_1 \) denotes the effective range for \( p \)-wave. For higher partial waves we retain only the lowest order term in \( k \), which is sufficient to describe the scattering in the considered regime of energies
\[
\tan \eta_l \approx \frac{\pi q^2}{8 (l - \frac{1}{2})(l + \frac{1}{2})(l + \frac{3}{2})}, \quad l \geq 2 \tag{7}\]

Let us turn now to positron scattering. We compare the total cross-section measured in experiment for Ar and N\(_2\) 14, 16 with predictions of the theoretical model based on the effective-range expansion. In our approach the effects of the short-range potential are included both for \( s \)- and \( p \)-wave giving the leading contribution to the scattering in the considered regime of energies. Thus, our model contains four unknown parameters: the scattering length \( a \) and the effective range \( R_0 \) for \( s \)-wave, and the zero-energy contribution \( b = B(0) \) and the effective range \( R_1 \) for \( p \)-wave.

For the investigated regime of positrons energies, \( q = k R^* \) can take values larger than unity, therefore for \( s \)- and \( p \)-wave we do not use expansions (5)-(6) valid for \( q \lesssim 1 \), but we rather applied the initial formula (1) for the phase shift, performing only finite-range expansion for the parameter \( B \). In this case, values of \( \nu \) and \( m \) has to be evaluated numerically, using the approach described in the Appendix.

For the calculations we use experimental values of the polarizability: \( \alpha = 11.33 \alpha_0^3 \) and \( \alpha = 11.54 \alpha_0^3 \) (atomic units), for Ar and N\(_2\), respectively 22. Table I contains values of the characteristic distance \( R^* \) and the characteristic energy \( E^* = k^2/(2 \mu R^*) \) for the polarization potential, and the values of four parameters: \( a \), \( b \), \( R_0 \), \( R_1 \) which were determined by fitting our model to the experimental data.

In the case of N\(_2\) the size of the molecule scaled by \( R^* \) is much larger than for Ar, therefore we restricted our effective-range analysis to lower energies, fitting the model to experimental data with \( E \lesssim 0.8 E^* \). In this regime the contribution of the effective-range correction in \( p \)-wave is rather small, and one does not get reliable results for this parameter from the fitting procedure. Thus, for N\(_2\) we considered only three parameters \( a \), \( b \) and \( R_0 \) accounting for effects of the short-range part of the potential.

Fig. II shows the experimental data for the total scattering cross-section for Ar as a function of positron collision energy. They are compared with: the MERT theoretical curve which best fits the experimental data, its low-energy expansion given by Eqs. 5-6, and the results of McEachran et al. 17. The total cross-section is presented in units of \( R^* \), while the energy is scaled by \( E^* \). In the inset we additionally present contributions of the \( s \) and \( p \) waves to the total scattering cross-section. Similar results but for the scattering of positrons on N\(_2\) are illustrated in Fig. 2.

We note the good agreement between our model and the results of McEachran et al. 17 at low energies. Obtained value of the scattering length \( a_s = -5.58 \alpha_0 \) agrees well with the calculations of McEachran et al. 17.
TABLE I: Characteristic distance $R^*$, characteristic energy $E^*$ and four fitting parameters: $a_s$ (s-wave scattering length), $R_0$ (s-wave effective range), $b$ (zero-energy contribution $B(0)$ for $p$-wave) and $R_1$ ($p$-wave effective range) for Ar and N$_2$.

|       | $R^*(a_0)$ | $E^*(eV)$ | $a_s/R^*$ | $b$       | $R_0/R^*$ | $R_1/R^*$ |
|-------|------------|-----------|------------|-----------|-----------|-----------|
| Ar    | 3.351      | 1.211     | -1.665     | -5.138    | 0.3165    | 2.281     |
| N$_2$ | 3.397      | 1.179     | -2.729     | -12.65    | 0.8186    | —         |

FIG. 1: Total cross-section for the scattering of positrons on argon versus the energy. Depicted are: experimental data (squares), the theoretical fit based on effective-range expansion (solid line), its low-energy part given by Eqs. 5-7, and the theoretical results of McEachran et al. (dashed line). The inset shows in addition the s- and p-wave cross-sections. Data are scaled by the characteristic distance $R^*$ and the characteristic energy $E^*$ of the polarization potential.

FIG. 2: The same as Fig. 1 but for the scattering of positrons on N$_2$.

APPENDIX A

To solve radial Schrödinger equation 11 we substitute $r = \sqrt{R^*e^{-z}/\sqrt{k}}$ and $\Psi(r) = \psi(r)\sqrt{R^*/r}$, which yields the Mathieu’s modified differential equation 24, 28

$$\frac{d^2\psi}{dz^2} - [a - 2q \cosh 2z] \psi = 0. \quad (A1)$$

where $a = (l + \frac{1}{2})^2$ and $q = kR^*$. Two linearly independent solutions $M(z)$ and $T(z)$ can be expressed in the following form 22, 28

$$M_{\nu}(z) = \sum_{n=-\infty}^{\infty} (-1)^n c_n(\nu) J_{2n+\nu}(2\sqrt{q} \cosh z), \quad (A2)$$

$$T_{\nu}(z) = \sum_{n=-\infty}^{\infty} (-1)^n c_n(\nu) Y_{2n+\nu}(2\sqrt{q} \cosh z), \quad (A3)$$

which defines them for $z > 0$. Here, $\nu$ denotes the characteristic exponent, and $J_{\nu}(z)$ and $Y_{\nu}(z)$ are Bessel and Neumann functions respectively. Substituting the ansatz $A2$ and $A3$ into $A1$, one obtains the recurrence relation:

$$[(2n + \nu)^2 - a] c_n + q(c_{n-1} + c_{n+1}) = 0, \quad (A4)$$

which can be solved in terms of continued fractions. To this end we introduce $h^+_n = c_n/c_{n-1}$ and $h^-_n = c_{-n}/c_{-n+1}$ for $n > 0$, which substituted into $A4$ gives the continued fractions $h^+_n = -q/(qh^+_n + dn_m)$ and $h^-_n = -q/(qh^-_{n+1} + dn_n)$ with $d_n = (2n + \nu)^2 - a$. In practice to find numerical values of the coefficients $c_n$ we set $h^+_m = 0$ and $h^-_m = 0$ for some, sufficiently large $m$ and calculate $h^+_n$ and $h^-_n$ up to $n = 1$. Characteristic exponent has to determined from Eq. $A4$ with $n = 0$.

Asymptotic behavior of $M_{\nu}(z)$ and $T_{\nu}(z)$ for large $z$ follow immediately from asymptotic expansion of Bessel
functions

\[ M_\nu(z) \xrightarrow{z \to \infty} \frac{2}{\pi^{1/4}} e^{-z/2} s_\nu \cos \left( \frac{e^z \sqrt{q} - \frac{\pi}{2} \nu - \frac{\pi}{4}}{2} \right) \]  
(A5)

\[ T_\nu(z) \xrightarrow{z \to \infty} \frac{2}{\pi^{1/4}} e^{-z/2} s_\nu \sin \left( \frac{e^z \sqrt{q} - \frac{\pi}{2} \nu - \frac{\pi}{4}}{2} \right) \]  
(A6)

where \( s_\nu = \sum_{n=-\infty}^{\infty} c_n(\nu) \). To obtain asymptotic behavior for large and negative \( z \) one has to join solutions \( M_\nu(z) \) and \( T_\nu(z) \), with another pair of solution \( M_\nu(-z) \) and \( T_\nu(-z) \) at \( z = 0 \). [22] This yields

\[ M_\nu(z) \xrightarrow{z \to -\infty} \frac{2}{\pi^{1/4}} e^{z/2} s_\nu \cos \left( \frac{e^z \sqrt{q} + \frac{\pi}{2} \nu - \frac{\pi}{4}}{2} \right) \]  
(A7)

\[ T_\nu(z) \xrightarrow{z \to -\infty} -\frac{2}{\pi^{1/4}} e^{z/2} s_\nu \sin \left( \frac{e^z \sqrt{q} + \frac{\pi}{2} \nu - \frac{\pi}{4}}{2} \right) 
- \cot \pi \nu (m^2 - 1) \cos \left( \frac{e^z \sqrt{q} + \frac{\pi}{2} \nu - \frac{\pi}{4}}{2} \right) \]  
(A8)

Finally we write the wave function \( \Psi(r) \) in the form

\[ \Psi(r) = \sin(\phi + \frac{\pi}{2} \nu + \frac{\pi}{4}) \sqrt{\frac{R^*}{r}} M_\nu \left( \ln \sqrt{\frac{R^*}{kr}} \right) 
+ \cos(\phi + \frac{\pi}{2} \nu + \frac{\pi}{4}) \sqrt{\frac{R^*}{r}} T_\nu \left( \ln \sqrt{\frac{R^*}{kr}} \right) \]  
(A9)

where \( \phi \) is a parameter which appear in the small \( r \) expansion. [3]. Now, the behavior of \( \Psi(r) \) at small and large distance described by Eqs. [22-24], can be readily obtained from asymptotic expansions [A5-A8].

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