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A new ab initio method of calculating Z_{eff} and positron annihilation rates using coupled-channel T-matrix amplitudes

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Abstract. We present a new ab initio theoretical formulation to calculate Z_{eff} and hence the positron annihilation rates directly from the onshell and offshell (half) scattering amplitudes. The method does not require any explicit use of the scattering wave function and is formally exact within the framework of the well established Lippmann-Schwinger equation. It could serve as an effective tool as all the T-, K-, and S-matrix formulations, yield directly the scattering amplitudes; not the wave function. Numerical test of the method is presented considering sample static calculations in positron-hydrogen and positron-helium systems.

PACS. 03.65.Nk Scattering theory – 34.85.+x Positron scattering – 71.60.+z Positron states – 78.70.Bj Positron annihilation

1 Introduction

Positron, being an antiparticle, interacts intimately (short-range interaction) with atomic electrons due to the absence of any restriction imposed by the Pauli Exclusion principle. Thus their annihilation studies, namely, the *Positron annihilation spectroscopy* and *Positronium annihilation lifetime spectroscopy* have emerged as two front line research areas, as they are expected to provide a more detail account of their close interactions with the target and bear the potential of various modern technological applications [1–3].

Normally, the theoretical study of annihilation rate requires the evaluation of the scattering wave function which contains the short-range information of the scattering process [4–6]. However, it is of fundamental importance to note that most scattering calculations (T-, K-, S-matrix) yield directly the scattering amplitudes which reflect only the asymptotic behavior of the wave function. Thus, these calculations can not provide any information for the annihilation process. Consequently, attempts were made to use the scattering amplitudes to evaluate the annihilation parameters [7,8]. Rhyzikh and Mitroy [7] presents a method of calculating Z_{eff} in e^+-H scattering through the evaluation of the transition amplitude for $e^+ + \mathrm{H} \rightarrow 2\gamma + p$ calculated employing the scattering T-matrix results. Gribakin [8] employs an approximate method of evaluating the Z_{eff} from on-shell T-matrix elements. Here, we present a new ab initio theoretical formulation based on the integral equation formalism, whereby we express Z_{eff} directly in terms of T-matrix elements and facilitate its calculation exactly from the on-shell and half-onshell T-matrix scattering amplitudes (without any explicit use of the scattering wave function). Defining a new Z-matrix we present the Z_{eff} in a coupled-channel form exactly similar to the known T-matrix formulation. The introduction of Z-matrix facilitates the partial wave representation of the coupled equations which are useful for analytical and numerical evaluations.

Theoretically, the positron annihilation rates (Λ) are expressed in terms of Z_{eff}, the *effective* number of target electrons available to the incoming positron as [4–6,8]:

$$\Lambda = \pi r_0^2 c Z_{\mathit{eff}} N \ \mathrm{s}^{-1} \tag{1}$$

and Z_{eff} is defined in terms of the scattering wave function $|\psi_k^+\rangle$ as [4–6]

$$Z_{\mathit{eff}}(\mathbf{k}) = \left\langle \psi_k^+ | \sum_{j=1}^{N} \delta(\mathbf{r}_j - \mathbf{x}) | \psi_k^+ \right\rangle \tag{2}$$

where r_0 is the classical electron radius; c is the speed of light; $4\pi r_0^2 c$ is the non-relativistic electron-positron annihilation rate; $\pi r_0^2 c$ is the same for the spin-averaged case of two-gamma annihilation (which excludes electron-positron triplet state contribution and considers only singlet state annihilation). N is the number density of atoms or molecules in the medium; δ is the Dirac δ-function; $\mathbf{x}$ and $\mathbf{r}_j$ are the positron and the electron co-ordinates.

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$$\langle\psi_k^+|\Delta|\psi_k^+\rangle = \langle k\phi_n|\Delta|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k''\frac{\langle k\phi_n|T|k''\phi_{n''}\rangle\langle k''\phi_{n''}|\Delta|k\phi_n\rangle}{E-E_n''-i0} + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k''\frac{\langle k\phi_n|\Delta|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T|k\phi_n\rangle}{E-E_n''+i0} + \frac{1}{(2\pi)^6}\sum_{n''}\sum_{m''}\int d^3k_1''\int d^3k_2''\frac{\langle k\phi_n|T|k_1''\phi_{n''}\rangle\langle k_1''\phi_{n''}|\Delta|k_2''\phi_m''\rangle\langle k_2''\phi_{m''}|T|k\phi_n\rangle}{(E-E_n''-i0)(E-E_m''+i0)}. \quad (11)$$

Here we present a new formulation whereby the *r.h.s.* of equation (2) is represented exactly by the onshell and half-offshell coupled-channel T-matrix scattering amplitudes, thus facilitating the evaluation of Z_{eff} without any explicit use of the scattering wave function. When a positron collides with a target, it can have direct as well as rearrangement scattering. So, we present our formulation in two different sections consisting of (I) direct (elastic and inelastic) scattering and (II) direct plus rearrangement (positronium formation) scattering.

2 Positron annihilation considering the direct scattering channels

In this section, we consider the direct scattering of positrons from atomic (ϕ_n) targets where the total wave function is expanded as [9]:

$$\psi_k^+(\mathbf{x},\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = \sum_n F_n(\mathbf{x})\phi_n(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) \quad (3)$$

where F_n's are the expansion coefficients, representing the motion of the positron with momentum $\mathbf{k}$; $\mathbf{r}_j$ is the coordinate of the jth electron and $\mathbf{x}$ is that of the positron. The total Hamiltonian is partitioned as

$$H = H_d^0 + V_d \quad (4)$$

where H_d^0 is the unperturbed part of the total Hamiltonian in the direct scattering channel of the positron and the atom and V_d is the positron-atom interaction potential. The unperturbed and the total Hamiltonians satisfy the following eigen-value equations:

$$H_d^0|k\phi_n\rangle = E|k\phi_n\rangle \quad (5)$$

$$(H_d^0 + V_d)|\psi_k^+\rangle = E|\psi_k^+\rangle \quad (6)$$

where $E = k^2/2m - \mathcal{E}_A$ is the total energy; $\mathcal{E}_A$ is the binding energy of the initial target atom (ϕ_n); m and $\mathbf{k}$ are the reduced mass and the onshell momentum of the positron. With the eigen-value equations (5, 6) for the unperturbed and the total Hamiltonians, one can write the Lippmann-Schwinger equation for the scattering wave function $|\psi_k^+\rangle$ as [9,10]:

$$|\psi_k^+\rangle = |k\phi_n\rangle + \frac{1}{E-H_d^0+i0}V_d|\psi_k^+\rangle. \quad (7)$$

Using the closure relation $(2\pi)^{-3}\sum_{n''}\int d^3k''$ $|k''\phi_{n''}\rangle\langle k''\phi_{n''}| = 1$, and using the T-matrix definition: $V_d|\psi_k^+\rangle = T|k\phi_n\rangle$, in equation (7), we arrive at the expression for the total scattering wave function in terms of the T-matrix elements:

$$|\psi_k^+\rangle = |k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''=1}^{\infty}\int d^3k''\frac{|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T|k\phi_n\rangle}{E-E_n''+i0}. \quad (8)$$

The total scattering wave function can be evaluated from this equation [7]. However, we generally solve it for the scattering T-matrix amplitudes obtained by multiplying equation (8) by V_d and projecting with $\langle k'\phi_{n'}|$ and using the T-matrix definition: $V_d|\psi_k^+\rangle = T|k\phi_n\rangle$:

$$\langle k'\phi_{n'}|T|k\phi_n\rangle = \langle k'\phi_{n'}|V_d|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k''\frac{\langle k'\phi_{n'}|V_d|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T|k\phi_n\rangle}{E-E_n''+i0}. \quad (9)$$

Equation (9), in its one-dimensional partial-wave form (Eq. (18)), is exactly solved using the matrix inversion method [11]. Simultaneous equations are formed by replacing k' with various values of k'' on which the radial integral over dk'' is discretized. The solutions of the simultaneous equations give us the both-onshell ($\langle k'\phi_{n'}|T|k\phi_n\rangle$) and half-offshell ($\langle k''\phi_{n'}|T|k\phi_n\rangle$) T-matrix amplitudes for various values of k'', where $\mathbf{k},\mathbf{k}'$ are on shell momenta and $\mathbf{k}''$ are the off-shell ones. While the solutions for the onshell T-matrix elements reflect the asymptotic behavior of the wave function and provide the physical cross-sections, the half-offshell elements are usually thrown away. We understand that the latter might contain the short-range properties of the wave function and they together with the on-shell elements can lead to an exact evaluation of the Z_{eff}. We multiply equation (8) from left by $\sum_{j=1}^N \delta(\mathbf{x}-\mathbf{r}_j) = \Delta$, (say) and project it by $\langle\psi_k^+|$ to obtain:

$$\langle\psi_k^+|\Delta|\psi_k^+\rangle = \langle\psi_k^+|\Delta|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k''\frac{\langle\psi_k^+|\Delta|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T|k\phi_n\rangle}{E-E_n''+i0}. \quad (10)$$

At this stage, to calculate Z_{eff}, which is equivalent to $\langle\psi_k^+|\Delta|\psi_k^+\rangle$ (see Eq. (2)), we have two options: (i) using equation (8), substitute for $\langle\psi_k^+|$ in the *r.h.s.* of (10) or (ii) evaluate $\langle\psi_k^+|\Delta|k\phi_n\rangle$ separately and substitute in equation (10). The first case leads to a complicated equation as follows:

see equation (11) above.

$$\langle k'\phi_{n'}|X|k\phi_n\rangle = \sum_J \sum_M \sum_L \sum_{M_L} \sum_{L'} \sum_{M_{L'}} \langle L'l', M_{L'}m_{l'}|JM\rangle Y^*_{L'M_{L'}}(\hat{\mathbf{k}}')\langle Ll, M_L m_l|JM\rangle Y_{LM_L}(\hat{\mathbf{k}}) X_J(n'l'L'k', nlLk) \quad (17)$$

This equation, although can be solved numerically, needs an extra effort to evaluate the principal value part of the last term, which contains a product of two singularities arising out of the product of Greens functions. We, therefore, look for the evaluation of $\langle k\phi_n|\Delta|\psi_k^+\rangle$ by projecting equation (8) with $\langle k\phi_n|\Delta$:

$$\langle k'\phi_{n'}|\Delta|\psi_k^+\rangle = \langle k'\phi_{n'}|\Delta|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k'' \frac{\langle k'\phi_{n'}|\Delta|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T|k\phi_n\rangle}{E - E''_n + i0}. \quad (12)$$

We solve this equation exactly (which is a very straight forward numerical summation) and substitute the complex conjugate of $\langle k'\phi_{n'}|\Delta|\psi_k^+\rangle$ in equation (10) to get Z_{eff}. However, like the T-matrix equation, we solve them in their one-dimensional partial wave form. To arrive at the corresponding partial wave equations for (12) and (10), we define the matrices D and Z as:

$$\Delta|\psi_k^+\rangle = D|k\phi_n\rangle \quad (13)$$

$$\langle\psi_k^+|D = \langle k\phi_n|Z \quad (14)$$

and rewrite equations (12) and (10) formally in terms of them:

$$\langle k'\phi_{n'}|D|k\phi_n\rangle = \langle k'\phi_{n'}|\Delta|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k'' \frac{\langle k'\phi_{n'}|\Delta|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T|k\phi_n\rangle}{E - E''_n + i0} \quad (15)$$

and

$$\langle k\phi_n|Z|k\phi_n\rangle = \langle k\phi_n|\bar{D}|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k'' \frac{\langle k\phi_n|\bar{D}|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T|k\phi_n\rangle}{E - E''_n + i0} \quad (16)$$

where $\bar{D}$ is the complex conjugate of D. Using a partial wave decomposition of the form:

see equation (17) above

where, $X \equiv T, V, D, \Delta$, or Z; n, l are the principal and orbital quantum number of the target and L is the orbital quantum number of the moving positron in the initial state; primed quantities denote the same for the final state. With the above expansion, the scattering T-matrix equation and the above two equations for the D- and Z-matrices reduce to:

$$T_J(\tau', k'; \tau, k) = V_J(\tau', k'; \tau k) + \frac{m''}{4\pi^3}\sum_{\tau''}\int dk''k''^2 \frac{V_J(\tau', k'; \tau'', k'')T_J(\tau'', k''; \tau, k)}{k^2_{\tau''} - k''^2 + i0} \quad (18)$$

$$D_J(\tau', k'; \tau, k) = \Delta_J(\tau', k'; \tau k) + \frac{m''}{4\pi^3}\sum_{\tau''}\int dk''k''^2 \frac{\Delta_J(\tau', k'; \tau'', k'')T_J(\tau'', k''; \tau, k)}{k^2_{\tau''} - k''^2 + i0} \quad (19)$$

$$Z_J(\tau', k'; \tau, k) = \bar{D}_J(\tau', k'; \tau k) + \frac{m''}{4\pi^3}\sum_{\tau''}\int dk''k''^2 \frac{\bar{D}_J(\tau', k'; \tau'', k'')T_J(\tau'', k''; \tau, k)}{k^2_{\tau''} - k''^2 + i0} \quad (20)$$

where $\tau \equiv (nlL)$ and $\tau' \equiv (n'l'L')$; m'' is the reduced mass of the projectile in the intermediate state (here, $m'' = m = 1$ in au). We suppress the suffix d from V_d for convenience.

In terms of partial wave Z-matrices, $Z_{eff}(k^2)$ comes out to be:

$$Z_{eff}(k^2) = \sum_J \frac{2J+1}{4\pi} Z_J(nlLk; nlLk). \quad (21)$$

While equation (18) is generally used to study positron-atom scattering, equations (19, 20) are particularly useful to evaluate Z_{eff} from the onshell and half-offshell T-matrix outputs of equation (18). We shall present a simple numerical account on e^+–He scattering to verify the code and compare the numbers, but beforehand we present a general formula for Z_{eff} by inserting equation (19) into equation (20). This latter is of particular interest, as it will explicitly demonstrate how the Z_{eff} is dependent on the T-matrices. For this, we first rewrite equations (18–20) in the following notations:

$$T_{k'k} = V_{k'k} - iV_{k'k'}T_{k'k} + V_{k'k''}G_0(k', k'')T_{k''k} \quad (22)$$

$$D_{k'k} = \Delta_{k'k} - i\Delta_{k'k'}T_{k'k} + \Delta_{k'p''}G_0(k', p'')T_{p''k} \quad (23)$$

$$Z_{k'k} = \bar{D}_{k'k} - i\bar{D}_{k'k'}T_{kk} + \bar{D}_{k'q''}G_0(k', q'')T_{q''k} \quad (24)$$

where summations over intermediate states are implied and off-shell momenta are represented by k'', p'' and q''. In the above, we have used the following relation for the complex Greens function

$$G_0^+(k^2 - k''^2) = \frac{1}{k^2 - k''^2 + i0} = -i\pi\delta(k^2 - k''^2) + \frac{P}{k^2 - k''^2} \quad (25)$$

to expand it into real and imaginary parts; P represents principal value integration; G_0 represents the real (principal value) part of G_0^+. Inserting $\bar{D}_{kk}$ in equation (24) we obtain an explicit relation for $Z_{eff}(k^2) \equiv Z_{kk}$:

$$Z_{kk} = \Delta_{kk} + i\Delta_{kk}[T^*_{kk} - T_{kk}] + T_{kp''}G_0\Delta_{p''k} + \Delta_{kq''}G_0T_{q''k} + \Delta_{kk}|T_{kk}|^2 + T_{kp''}G_0\Delta_{p''q''}G_0T_{q''k} \quad (26)$$

$$= \Delta_{kk} + 2\Delta_{kk}\mathrm{Im}[T_{kk}] + \Delta_{kk}|T_{kk}|^2 + T_{kp''}G_0\Delta_{p''k} + \Delta_{kq''}G_0T_{q''k} + T_{kp''}G_0\Delta_{p''q''}G_0T_{q''k} \quad (27)$$

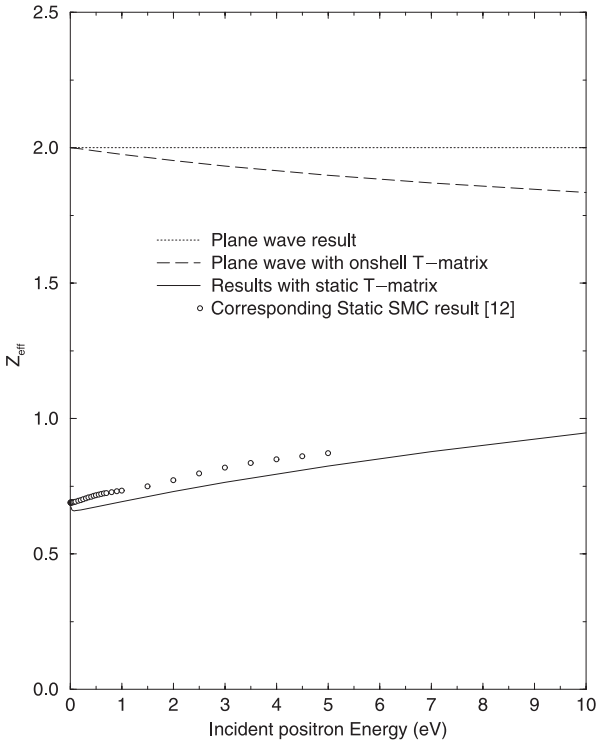

Fig. 1. Theoretical values of Z_{eff} in various approximations as a function of positron energy for the target of atomic helium.

where Δ_{pq} corresponds to plane-wave value of Z_{eff} for the initial and final momenta p and q. Im$[T_{kk}]$ and $|T_{kk}|^2$ are proportional to physical cross-sections (representing the asymptotic behavior of the wave function). Others are interference terms, linear and quadratic in the half-offshell T-matrix elements, and expected to play a crucial role at low and intermediate energies. To understand their role, and to check the normalizations of equations (19, 20), we provide a numerical test below.

2.1 Implications of the terms of equations (19, 20)

To understand the implications of the various terms of equations (19, 20) (Eq. (18) is well established in literature) we perform two sample calculations with e^+-H and e^+-He systems, considering the first order term of the summation (3), i.e., considering the elastic channel only, and evaluate the Z_{eff} using the resulting onshell and half-onshell T-matrix elements. We use atomic units throughout and use delta-function normalization for the plane wave.

We note that equations (18–20) and (22–24) are equivalent. First, we describe the results on positron-helium system. In Figure 1, we plot the dotted curve which is obtained considering only the plane wave parts (first term of the *r.h.s.*) of equations (22–24). This plane wave approximation gives a value of $Z_{eff} = 2.0\ (= Z)$ as was expected and provides the normalization. Next we consider first two terms of the *r.h.s.* of equations (22–24) and plot the result as dashed curve. This approximation is equivalent of considering the plane wave and the onshell T-matrix contributions of equations (18–20) leaving aside the half-offshell contribution (particular integral part of the Greens function). We obtain a lower value of Z_{eff} with increasing energies, signaling the manifestation of a repulsive potential at higher energies. Now, the solid curve is obtained with all the three terms of equations (22–24). That is, considering both the onshell and the half-offshell contributions together with the plane wave. The static potential in a e^+-He scattering is repulsive and consequently it lowers the value of Z_{eff} (and hence the annihilation rate). We compare the solid curve with the results of a Schwinger Multi-Channel (SMC) calculation on e^+-He with the same physical content (considering static interaction only) [12]. Both the curves agree quite well. The marginal difference in the Z_{eff} value between the present and the SMC calculation is supposed to be acceptable since, the wave functions for helium used in these two calculations are different (we use the Roothaan-Hatree-Fock five-term wave function of Clementi and Roetti [13] for He).

To understand the difference and to make a further check, we employ the equations to e^+-H system, where the target wave function is exact, and evaluate Z_{eff} at $k = 0.1, 0.2, 0.3, 0.4, 0.5$ a.u. in the same static charge distribution approximation. Using thirty two gauss-quadrature points to discretize principal value integration, we obtain the Z_{eff} values of $0.4036, 0.3929, 0.3867, 0.3800, 0.3721$ compared to the values $0.4039, 0.3989, 0.3909, 0.3804, 0.3678$ obtained by Ryzhikh and Mitroy [7] using forty gauss-quadrature points. Studying the convergence we find that 36 or 40 gauss-quadrature points are not sufficient to evaluate Z_{eff} for a discretization of the principal value integration as: $\int_0^\infty dk'' = \int_0^{2k_i} dk'' + \int_{2k_i}^\infty dk''$, where an even number of gauss-quadrature points are used for the $0 \rightarrow 2k_i$ integral so that although we approach to the singularity, we never meet that [14]. We cannot comment upon the convergence pattern in the numerical procedure adopted in reference [7]. In our scheme, we find that the results are very slowly convergent. At very low energies ($k = 0.1, 0.2$) the numerical procedure overestimates the results for low gauss-quadrature points while at $k = 0.3$ and above it underestimates the results. Employing seventy two gauss-quadrature points, we find the results as $0.3982, 0.3951, 0.3911, 0.3855, 0.3784$ which are expected to be convergent within 0.05%.

The results provided in Figure 1 are aimed at understanding the new equations (19, 20) in numerical terms. The results shown for the static interaction only and is nothing to do with the physically converged result. To arrive at a physically converged result for the Z_{eff}, full expansion basis indicated in equations (19, 20) need to be employed which requires the T-matrix amplitudes and is not the goal of this work. In this work, we are interested to stress that available T-matrix elements [17] can be readily employed in equations (19, 20) to calculate the annihilation parameters. For cases where we have K-matrix or S-matrix informations, the matrix elements can be transformed to T-matrix representation and

$$\langle k'\phi_{n'}|T_d|k\phi_n\rangle = \langle k'\phi_{n'}|V_d|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k'' \frac{\langle k'\phi_{n'}|V_d|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T_d|k\phi_n\rangle}{E-E''_n+i0} + \frac{1}{(2\pi)^3}\sum_{\nu''}\int d^3k'' \frac{\langle k'\phi_{n'}|(E''_\nu+V_c-E_{n'})|k''\chi_{\nu''}\rangle\langle k''\chi_{\nu''}|T_c|k\phi_n\rangle}{E-E''_\nu+i0} \quad (36)$$

$$\langle k'\chi_{\nu'}|T_c|k\phi_n\rangle = \langle k'\chi_{\nu'}|V_c|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k'' \frac{\langle k'\chi_{\nu'}|V_c|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T_d|k\phi_n\rangle}{E-E''_n+i0} + \frac{1}{(2\pi)^3}\sum_{\nu''}\int d^3k'' \frac{\langle k'\chi_{\nu'}|V_c|k''\chi_{\nu''}\rangle\langle k''\chi_{\nu''}|T_c|k\phi_n\rangle}{E-E''_\nu+i0} \quad (37)$$

equations (19, 20) be employed to obtain the annihilation parameters.

Regarding convergence, we mention that, in practice, the results for the T-matrix equation (18) do not converge easily unless the continuum effect is fully manifested. Within the coupled channel framework the real and virtual effects of the rearrangement channel of positronium (Ps) formation introduce the continuum effect in the theoretical formulation for positron scattering. This implies that for a convergent description for the Z_{eff}, the above formalism need to be generalized further so that the method accounts for the Ps formation channel explicitly. Before presenting that generalization, we want to mention that when one uses some model short-range and/or polarization potentials alongside the static potential in the T-matrix formalism to arrive at some meaningful results for the positron-atom system, the above formalism can be readily used.

3 Positron annihilation considering the direct and the Ps-formation channels

When the possibility of a real or virtual positronium formation is considered, through the capture of a target electron by the incident positron, the theoretical formulation for a single electron target differs from a multi electron target in the sense that for the latter case the Ps-target(ion) wave function need to be formally antisymmetrized. Here, we discuss them in two different sections (Sects. 3.1 and 3.2).

3.1 Single electron target

For positron scattering from a single electron target, the total wave function (3) can be expanded (considering Ps formation) as [9,15]:

$$\psi_k^+(\mathbf{x},\mathbf{r}_1) = \frac{1}{\sqrt{2}}\left[\sum_n F_n(\mathbf{x})\phi_n(\mathbf{r}_1) + \sum_\nu \mathcal{G}_\nu(\rho_1)\chi_\nu(\mathbf{t}_1)\right] \quad (28)$$

where $\rho_1 = (\mathbf{r}_1+\mathbf{x})/2$ and $\mathbf{t}_1 = \mathbf{r}_1-\mathbf{x}$. $\mathcal{G}_\nu$ and χ_ν represent the moving and the bound-state (νth) positronium atom. The total Hamiltonian is now partitioned as:

$$H = H_d^0 + V_d = H_c^0 + V_c \quad (29)$$

where H_d^0, H_c^0 are the unperturbed Hamiltonians in the direct (d) and capture (c) channels satisfying the eigenvalue equations

$$H_d^0|k\phi_n\rangle = E_n|k\phi_n\rangle \quad (30)$$

$$H_c^0|k\chi_\nu\rangle = E_\nu|k\chi_\nu\rangle \quad (31)$$

and V_d and V_c are the interaction potentials therein. $E_n = k_x^2/2 - \mathcal{E}_A$ and $E_\nu = k_{Ps}^2/4 - \mathcal{E}_{Ps}$; $\mathcal{E}_A$ and $\mathcal{E}_{Ps}$ are the binding energies of the initial target atom and the rearranged positronium atom; k_x and k_{Ps} are the momenta of the positron and the positronium. In terms of the two-cluster channel-Greens-functions $G_d^0 = (E-H_d^0)^{-1}$ and $G_c^0 = (E-H_c^0)^{-1}$, we take the Lippmann-Schwinger integral equation for the wave function as [16]:

$$|\psi_k^+\rangle = |k\phi_n\rangle + G_d^0T_d|k\phi_n\rangle + G_c^0T_c|k\phi_n\rangle \quad (32)$$

where, T_d and T_c are defined as $V_d|\psi_k^+\rangle = T_d|k\phi_n\rangle$ (here $T_d \equiv T$ of Sect. 1) and $V_c|\psi_k^+\rangle = T_c|k\phi_n\rangle$. Using the following closure relations for the direct and the rearrangement channels,

$$1 = \frac{1}{(2\pi)^3}\sum_{n''}\int dk''|k''\phi_{n''}\rangle\langle k''\phi_{n''}| \quad (33)$$

$$1 = \frac{1}{(2\pi)^3}\sum_{\nu''}\int dk''|k''\chi_{\nu''}\rangle\langle k''\chi_{\nu''}| \quad (34)$$

we rewrite equation (32) as:

$$|\psi_k^+\rangle = |k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k'' \frac{|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T_d|k\phi_n\rangle}{E-E''_n+i0} + \frac{1}{(2\pi)^3}\sum_{\nu''}\int d^3k'' \frac{|k''\chi_{\nu''}\rangle\langle k''\chi_{\nu''}|T_c|k\phi_n\rangle}{E-E''_\nu+i0}. \quad (35)$$

Here, $E''_n = k''^2/2 - \mathcal{E}_A$ and $E''_\nu = k''^2/4 - \mathcal{E}_{\rm Ps}$ are the off-shell energies in the direct (d) and the capture (c) channels. We construct the coupled equations by (1) multiplying this equation with V_d and projecting out with $\langle k'\phi_{n'}|$ and (2) multiplying this equation with V_c and projecting out with $\langle k'\chi_{\nu'}|$

see equations (36) and (37) above

where in equation (36), we use $V_d = H_c^0 + V_c - H_d^0$ (see Eq. (29)) and also use the eigen-value equations (30, 31). Once the above coupled-equations are solved and we are equipped with the T-matrix amplitudes $\langle p\phi_{n'}|T_d|k\phi_n\rangle$ and $\langle q\chi_{\nu'}|T_c|k\phi_n\rangle$ for on-shell and off-shell values for the momenta p and q, we can get Z_{eff} in terms of them. To deduce Z_{eff}, in terms of T-matrices, we project equation (35) by $\langle\psi_k^+|\Delta$ and arrive at:

$$\langle\psi_k^+|\Delta|\psi_k^+\rangle = \langle\psi_k^+|\Delta|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k''\frac{\langle\psi_k^+|\Delta|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T_d|k\phi_n\rangle}{E-E_n''+i0} + \frac{1}{(2\pi)^3}\sum_{\nu''}\int d^3k''\frac{\langle\psi_k^+|\Delta|k''\chi_{\nu''}\rangle\langle k''\chi_{\nu''}|T_c|k\phi_n\rangle}{E-E_\nu''+i0}. \quad (38)$$

Now, $\langle\psi_k^+|$ from equation (35) may be substituted in the $r.h.s.$ of equation (38) to arrive at a direct expression for Z_{eff}. However, that will lead to a complicated equation like (11). We rather develop simpler equations to evaluate $\langle\psi_k^+|\Delta|k\phi_n\rangle$ and $\langle\psi_k^+|\Delta|k\chi_\nu\rangle$ and substitute them back in equation (38). For this, we project equation (35) from left by $\langle k'\phi_{n'}|\Delta$ and $\langle k'\chi_{\nu'}|\Delta$ and obtain:

$$\langle k'\phi_{n'}|\Delta|\psi_k^+\rangle = \langle k'\phi_{n'}|\Delta|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k''\frac{\langle k'\phi_{n'}|\Delta|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T_d|k\phi_n\rangle}{E-E_n''+i0} + \frac{1}{(2\pi)^3}\sum_{\nu''}\int d^3k''\frac{\langle k'\phi_{n'}|\Delta|k''\chi_{\nu''}\rangle\langle k''\chi_{\nu''}|T_c|k\phi_n\rangle}{E-E_\nu''+i0} \quad (39)$$

$$\langle k'\chi_{\nu'}|\Delta|\psi_k^+\rangle = \langle k'\chi_{\nu'}|\Delta|k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k''\frac{\langle k'\chi_{\nu'}|\Delta|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T_d|k\phi_n\rangle}{E-E_n''+i0} + \frac{1}{(2\pi)^3}\sum_{\nu''}\int d^3k''\frac{\langle k'\chi_{\nu'}|\Delta|k''\chi_{\nu''}\rangle\langle k''\chi_{\nu''}|T_c|k\phi_n\rangle}{E-E_\nu''+i0}. \quad (40)$$

The above two equations are very straight forward to solve as one need to carry only numerical integrations with known values of T_d, T_c and the calculated plane-wave matrix elements concerning Δ as inputs. We are not interested to repeat the calculations for T_d and T_c and rather hope that the existing T-matrix results [17] may be applied to calculate Z_{eff}.

3.2 Many electron target

For multi-electron targets the formulation is very much similar to that of Section 2.1, except few fundamental changes. Without repeating the whole thing, we thus mention here about the necessary changes. For the positron scattering from a multi-electron target, the capture channel need to be explicitly antisymmetrized and expressed as:

$$\psi_k^+(\mathbf{x},\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = \frac{1}{\sqrt{2}}\left[\sum_n F_n(\mathbf{x})\phi_n(\mathbf{r}_1,...,\mathbf{r}_N) + \mathcal{A}_1\sum_{\nu\mu}\mathcal{G}_{\nu\mu}(\rho_1)\chi_\nu(\mathbf{t}_1)\varphi_\mu(\mathbf{r}_2,...,\mathbf{r}_N)\right] \quad (41)$$

where φ represents the residual target ion and $\mathcal{A}_1$ is the antisymmetrization operator, which antisymmetrizes electron 1 with other target electrons. The initial target wave function ϕ is supposed to be antisymmetrized implicitly. The total Hamiltonian is now partitioned as: $H = H_d^0 + V_d = H_{c(j)}^0 + V_{c(j)}$; where $H_{c(j)}^0$ and $V_{c(j)}$ are the unperturbed Hamiltonian and the Ps-target(ion) interaction potential in the capture channel of the positronium formation, with the jth electron being attached to the positron. Accommodating the Pauli exclusion principle for the rearrangement channel, the Lippmann-Schwinger integral equation is now written as:

$$|\psi_k^+\rangle = |k\phi_n\rangle + G_d^0 T_d|k\phi_n\rangle + \mathcal{A}_j G_{c(j)}^0 T_{c(j)}|k\phi_n\rangle \quad (42)$$

where T_d and T_c are defined as $V_d|\psi_k^+\rangle = T_d|k\phi_n\rangle$ (here $T_d \equiv T$ of Sect. 1) and $V_{c(j)}|\psi_k^+\rangle = T_{c(j)}|k\phi_n\rangle$. Using following closure relations for the direct and the rearrangement channels:

$$1 = \frac{1}{(2\pi)^3}\sum_{n''=1}^{\alpha}\int dk''|k''\phi_{n''}\rangle\langle k''\phi_{n''}| \quad (43)$$

$$1 = \frac{1}{(2\pi)^3}\sum_{\nu''}\sum_{\mu''}\int dk''|k_j''\chi_{\nu''}\varphi_{\mu''}\rangle\langle k_j''\chi_{\nu''}\varphi_{\mu''}| \quad (44)$$

and proceeding in a similar way, we represent the Lippmann-Schwinger equation (42) as:

$$|\psi_k^+\rangle = |k\phi_n\rangle + \frac{1}{(2\pi)^3}\sum_{n''}\int d^3k''\frac{|k''\phi_{n''}\rangle\langle k''\phi_{n''}|T_d|k\phi_n\rangle}{E-E_n''+i0} + \frac{1}{(2\pi)^3}\sum_{\nu''}\sum_{\mu''}\int d^3k''\frac{\mathcal{A}_j|k_j''\chi_{\nu''}\varphi_{\mu''}\rangle\langle k_j''\chi_{\nu''}\varphi_{\mu''}|T_{c(j)}|k\phi_n\rangle}{E-E_{\nu\mu}''+i0}. \quad (45)$$

The rest of the procedures are exactly similar to those described in Section 2.1 and are not repeated here.

In summary, we present a new ab initio methodology to calculate Z_{eff} from physical (onshell) and virtual (half-onshell) scattering T-matrix amplitudes, without any explicit use of the scattering wave function. The methodology is exact within the framework of the Lippmann-Schwinger equation and thus the formalism reveals that the crucial short-range information of a collision process might have been embedded in the half-onshell scattering amplitudes which we generally throw away after the scattering calculation. The formulation presented here is for

positron annihilation in atoms, but it could be universally applied to other annihilation studies as long as the dynamics of the interacting particles (or clusters) can be described by the well-known Lippmann-Schwinger type equation. The methodology is expected to serve as an useful tool for the annihilation studies as most of the scattering theories (T-matrix, K-matrix, S-matrix) yield directly the scattering amplitudes. A similar T-matrix formulation may also be derived for the pick-off annihilation of orthopositronium collisions, which is under consideration.

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