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

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A new \emph{ab initio} theoretical formulation to calculate $Z_{\text{eff}}$ and hence the positron annihilation rates is presented using the on-shell and half-offshell T-matrix scattering amplitudes without any explicit use of the scattering wave function. The formulation is exact and universal, as long as the dynamics of the systems can be described by a Lippmann-Schwinger type 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. We also present a basic numerical test of the formulation.

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I. 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].

Until now, the theoretical study of annihilations rate requires the evaluation of the scattering wave function. However, it is of fundamental importance to note that most scattering calculations (T-, K-, S-matrix) yield directly the scattering amplitudes; not the wave function. Thus, the evaluation of \( Z_{eff} \) normally requires a separate calculation for the wave function using these scattering amplitudes (like those in ref. [4]), or need to adopt of a different methodology that will yield the scattering wave function directly. Ryzhikh and Mityoy [4] have used the T-matrix formulation to evaluate the scattering wave function which has subsequently been used to evaluate \( Z_{eff} \). Gribakin [5] has used an approximate form of the T-matrix equation to evaluate \( Z_{eff} \).

Here we present a new \textit{ab-initio} theoretical formulation based on the integral equation formalism, whereby \( Z_{eff} \) and hence the annihilation rates can be exactly calculated using on-shell and half-offshell T-matrix scattering amplitudes \textit{but without any explicit use of the scattering wave function}.

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

\[
\Lambda = \frac{\pi r_0^2 c Z_{eff} N}{\sec}\tag{1.1}
\]

And \( Z_{eff} \) is defined in terms of the scattering wave function \( |\psi^+_{k}| \) as [6–8]

\[
Z_{eff}(k) = \frac{N}{\sqrt{\Delta}} \sum_{j=1}^{N} \delta(|r_j - x|) |\psi^+_{k}| \tag{1.2}
\]

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; \( \delta \) is the Dirac \( \delta \)-function; \( x \) and \( r_j \) are the positron and the electron co-ordinates.

Here we present a new formulation whereby the r.h.s of equation 1.2 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 \textbf{I}) direct (elastic and inelastic) scattering and \textbf{II}) direct plus rearrangement (positronium formation) scattering.

II. POSITRON ANNIHILATION CONSIDERING THE DIRECT SCATTERING CHANNELS

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

\[
\psi^+_k(x, r_1, r_2, \ldots r_N) = \sum_n F_n(x) \phi_n(r_1, r_2, \ldots r_N) \tag{2.1}
\]

where \( F_n \)'s are the expansion coefficients, representing the motion of the positron with momentum \( k \); \( r_j \) is the co-ordinate of the \( j \)-th electron and \( x \) is that of the positron. The total Hamiltonian is partitioned as

\[
H = H^0_k + V_d \tag{2.2}
\]

where \( H^0_k \) 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:

\[
(H^0_k | k \phi_n) = E | k \phi_n \rangle \tag{2.3}
\]

\[
(H^0_d + V_d) | \psi^+_k \rangle = E | \psi^+_k \rangle \tag{2.4}
\]
where $E = k^2 / 2m - E_A$ is the total energy; $E_A$ is the binding energy of the initial target atom ($\phi_n$); $m$ and $k$ are the reduced mass and the onshell momentum of the positron. With the eigen-value equations 2.3 and 2.4 for the unperturbed and the total Hamiltonians, one can write the Lippmann-Schwinger equation for the scattering wave function $\langle \psi^+_k \rangle$ as [9,10]:

$$|\psi^+_k\rangle = |k \phi_n\rangle + \frac{1}{E - H_0^i + i0} V_d |\psi^+_k\rangle \quad (2.5)$$

Using the closure relation $(2\pi)^{-3} \sum_{n''} d^3k'' |k'' \phi_{n''}\rangle \langle k'' \phi_{n''}| = 1$, and using the T-matrix definition: $V_d |\psi^+_k\rangle = T |k \phi_n\rangle$, in eqn(2.5), we arrive at the expression for the total scattering wave function in terms of the T-matrix elements:

$$|\psi^+_k\rangle = |k \phi_n\rangle + \frac{1}{(2\pi)^3} \sum_{n''} \int d^3k'' |k'' \phi_{n''}\rangle \langle k'' \phi_{n''}| T |k \phi_n\rangle \frac{E - E'' + i0}{E - E'' + i0} \quad (2.6)$$

The total scattering wave function can be evaluated from this equation [4]. However, we generally solve it for the scattering T-matrix amplitudes obtained by multiplying eqn(2.6) by $V_d$ and projecting with $\langle k' \phi_{n'} |$ and using the T-matrix definition: $V_d |\psi^+_k\rangle = T |k \phi_n\rangle$:

$$\langle k' \phi_{n'}| T |k \phi_n\rangle = \langle k' \phi_{n'}| V_d |k \phi_n\rangle + \frac{1}{(2\pi)^3} \sum_{n''} \int d^3k'' \langle k' \phi_{n'}| V_d |k'' \phi_{n''}\rangle \langle k'' \phi_{n''}| T |k \phi_n\rangle \frac{E - E'' + i0}{E - E'' + i0} \quad (2.7)$$

Eqn.(2.7), in its one-dimensional partial-wave form (eqn.2.16), 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 $k$, $k'$ are on shell momenta and $k''$ 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 off-shell elements can lead to an exact evaluation of the $Z_{eff}$. We multiply eqn.2.6 from left by $\sum_{j=1}^{N} \delta(x - r_j) = \Delta$, (say) and project it by $\langle \psi^+_k |$ to obtain:

$$\langle \psi^+_k | \Delta | \psi^+_k \rangle = \langle \psi^+_k | \Delta | k \phi_n \rangle + \frac{1}{(2\pi)^3} \sum_{n''} \int d^3k'' \langle \psi^+_k | \Delta | k' \phi_{n'} \rangle \langle k'' \phi_{n''}| T |k \phi_n\rangle \frac{E - E'' + i0}{E - E'' + i0} \quad (2.8)$$

At this stage, to calculate $Z_{eff}$, which is equivalent to $\langle \psi^+_k | \Delta | \psi^+_k \rangle$ (see eqn.1.2), we have two options: 1) using equation 2.6, substitute for $\langle \psi^+_k |$ in the r.h.s of (2.8) or 2) evaluate $\langle \psi^+_k | \Delta | k \phi_n \rangle$ separately and substitute in eqn(2.8). The first case leads to a complicated equation as follows:

$$\langle \psi^+_k | \Delta | \psi^+_k \rangle = \langle k \phi_n | \Delta | k \phi_n \rangle + \frac{1}{(2\pi)^3} \sum_{n''} \int d^3k'' \langle k \phi_n | T | k'' \phi_{n''} \rangle \langle k'' \phi_{n''}| \Delta |k \phi_n \rangle \frac{E - E'' - i0}{E - E'' - i0} \quad + \frac{1}{(2\pi)^3} \sum_{n''} \int d^3k'' \langle k \phi_n | \Delta | k'' \phi_{n''} \rangle \langle k'' \phi_{n''}| T |k \phi_n\rangle \frac{E - E'' + i0}{E - E'' + i0} \quad + \frac{1}{(2\pi)^3} \sum_{n''} \int d^3k'' \langle k \phi_n | T | k'' \phi_{n''} \rangle \langle k'' \phi_{n''}| \Delta |k'' \phi_{n''} \rangle \langle k'' \phi_{n''}| T |k \phi_n\rangle \frac{E - E'' - i0)(E - E'' + i0)}{(E - E'' - i0)(E - E'' + i0)} \quad (2.9)$$

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 eqn(2.6) with $\langle k \phi_n | \Delta$:}

3
\[
\langle k'\phi_{n'}|\Delta|\psi_k^+ \rangle = \frac{1}{(2\pi)^3} \int d^3k' \frac{\langle k'\phi_{n'}|\Delta|k''\phi_{n''}\rangle \langle k''\phi_{n''}|T|k\phi_n \rangle}{E - E'' + i\theta} \tag{2.10}
\]

We solve this equation exactly (which is a very straightforward numerical summation) and substitute the complex conjugate of \(\langle k'\phi_{n'}|\Delta|\psi_k^+ \rangle\) in eqn(2.8) 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 (2.10) and (2.8), we define the matrices \(D\) and \(Z\) as:

\[
\Delta|\psi_k^+ \rangle = D|k\phi_n \rangle \tag{2.11}
\]

\[
\langle \psi_k^+|D = \langle k\phi_n|Z \tag{2.12}
\]

and rewrite eqn(2.10) and eqn(2.8) formally in terms of them:

\[
\langle k'\phi_{n'}|D|k\phi_n \rangle = \langle k'\phi_{n'}|\Delta|k\phi_n \rangle \tag{2.13}
\]

\[
\langle k\phi_n|Z|k\phi_n \rangle = \langle k\phi_n|D|k\phi_n \rangle \tag{2.14}
\]

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

\[
\langle k'\phi_{n'}|X|k\phi_n \rangle = \sum_J \sum_M L \sum_{M_L} \sum_{M_{L'}} \sum_{\rho} \sum_{\rho'} \sum_{\rho''} \langle L\rho\rho'|M\rho'\rho''|JM \rangle Y_{M_L}^* (k') Y_{M'_{L'}} (k) X_j (n'\rho' L' k', n\rho L k) \tag{2.15}
\]

where, \(X \equiv T, V, D, \Delta, \text{ or } Z; n, l\) 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:

\[
T_J (\tau', k'; \tau, k) = V_J (\tau', k'; \tau, k) + \frac{m''}{4\pi^3} \sum_{\tau''} \int dk'' k''^2 V_J (\tau', k'; \tau'', k'') T_J (\tau'', k''; \tau, k) \tag{2.16}
\]

\[
D_J (\tau', k'; \tau, k) = \Delta_J (\tau', k'; \tau, k) + \frac{m''}{4\pi^3} \sum_{\tau''} \int dk'' k''^2 \Delta_J (\tau', k'; \tau'', k'') T_J (\tau'', k''; \tau, k) \tag{2.17}
\]

\[
Z_J (\tau', k'; \tau, k) = \bar{D}_J (\tau', k'; \tau, k) + \frac{m''}{4\pi^3} \sum_{\tau''} \int dk'' k''^2 \bar{D}_J (\tau', k'; \tau'', k'') T_J (\tau'', k''; \tau, k) \tag{2.18}
\]

where \(\tau \equiv (nL)\) and \(\tau' \equiv (n'\rho' L')\); \(m''\) 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:

\[
Z_{eff}(k^2) = \sum_j \frac{2J + 1}{4\pi} Z_J (nLk; nLk) \tag{2.19}
\]
While eqn.(2.16) is generally used to study positron-atom scattering, eqs.(2.17) and (2.18) are particularly useful to evaluate $Z_{eff}$ from the onshell and half-offshell T-matrix outputs of eqn.2.16. We shall present a simple numerical account on $e^+\text{-He}$ scattering to verify the code and compare the numbers, but beforehand we present a general formula for $Z_{eff}$ by inserting eqn.(2.17) into eqn.(2.18). 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 eqns.(2.16), (2.17) and (2.18) in the following notations:

$$T_{k'k} = V_{k'k} - i V_{k'k} T_{k'k} + V_{k'k''} G_0(k', k'') T_{k'k}$$
$$D_{k'k} = \Delta_{k'k} - i \Delta_{k'k} T_{k'k} + \Delta_{k''k''} G_0(k', k'') T_{k'k}$$
$$Z_{k'k} = \tilde{D}_{k'k} - i \tilde{D}_{k'k} T_{kk} + \tilde{D}_{k''k''} G_0(k', k'') T_{k'k}$$

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

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

A. Numerical test to equations 2.17, 2.18

To test the formulations of the equations 2.17, 2.18 (Equation 2.16 is well established in literature) we perform sample calculation on $e^+\text{-He}$ elastic scattering, considering only the static interaction [keeping summation over $\tau'' = \text{He}(1\sigma^2)$], and evaluate the $Z_{eff}$ using the resulting onshell and half-offshell T-matrix elements. We use atomic units throughout and use delta-function normalization for the plane wave.

We note that equations \{2.16,2.17,2.18\} and \{2.20,2.21,2.22\} are equivalent. In figure 1, first we plot the dotted curve which is obtained considering only the plane wave parts (first term of the r.h.s) of eqs.(2.20), (2.21) and (2.22). 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 eqs.(2.20), (2.21) and (2.22) and plot the result as dashed curve. This approximation is equivalent of considering the plane wave and the onshell T-matrix contributions of equations (2.16), (2.17) and (2.18) 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 eqs.(2.20), (2.21), and (2.22). That is, considering both the onshell and the half-offshell contributions together with the plane wave. The static potential in a $e^+\text{-He}$ 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 $e^+\text{-He}$ with the same physical content (considering static interaction only) \cite{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 \cite{13} for He) and also the T-matrix and the SMC formulations are different.

The results provided in figure-1 are aimed at checking the new equations vis-a-vis other methodologies where we considered the static interaction. Formally, to arrive at a physically converged result for the $Z_{eff}$, full expansion basis indicated in equations 2.17 and 2.18 need to be employed like the case for the scattering T-matrix equation 2.16. However, in practice it has been found that the positron-scattering cross sections do not converge easily unless
real and virtual effects of the rearrangement channel of positronium (Ps) formation is considered in the theoretical formulation. So, for a converged description of the scattering and annihilation we need to consider the Ps formation channel explicitly in the theoretical formulation. However, the above formulation is suitable for employing model polarization potentials alongside the static potential so as to arrive at a meaningful physically converged result without being confined in the ab initio framework.

III. 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 A and B.

A. Single Electron Target

For positron scattering from a single electron target, the total wave function (2.1) can be expanded (considering Ps formation) as [9,14]:

$$\psi_k^+ (x, r_1) = \sum_n F_n(x) \phi_n(r_1) + \sum_{\nu} G_{\nu}(\rho_1) \chi_{\nu}(t_1)$$  \hspace{1cm} (3.1)

where $\rho_1 = (r_1 + x)/2$ and $t_1 = r_1 - x$. $G_{\nu}$ and $\chi_{\nu}$ represent the moving and the bound-state ($\nu$-th) positronium atom. The total Hamiltonian is now partitioned as:

$$H = H_d^0 + V_d = H_c^0 + V_c$$  \hspace{1cm} (3.2)

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

$$H_d^0 |k\phi_n\rangle = E_n |k\phi_n\rangle$$  \hspace{1cm} (3.3)

$$H_c^0 |k\chi_{\nu}\rangle = E_{\nu} |k\chi_{\nu}\rangle$$  \hspace{1cm} (3.4)

and $V_d$ and $V_c$ are the interaction potentials therein. $E_n = k^2/2 - \varepsilon_A$ and $E_{\nu} = k^2_{P_s}/2 - \varepsilon_{P_s}$; $\varepsilon_A$ and $\varepsilon_{P_s}$ are the binding energies of the initial target atom and the rearranged positronium atom; $k_x$ and $k_{P_s}$ 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 [15]:

$$|\psi_k^+\rangle = |k\phi_n\rangle + G_d^0 T_d |k\phi_n\rangle + G_c^0 T_c |k\phi_n\rangle$$  \hspace{1cm} (3.5)

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 section-I) and $V_c |\psi_k^+\rangle = T_c |k\phi_n\rangle$. Using the following closure relations for the direct and the rearrangement channels,

$$1 = \frac{1}{(2\pi)^3} \sum_{n''} \int d^3k'' |k''\phi_{n''}\rangle \langle k''\phi_{n''}|$$  \hspace{1cm} (3.6)

$$1 = \frac{1}{(2\pi)^3} \sum_{\nu''} \int d^3k'' |k''\chi_{\nu''}\rangle \langle k''\chi_{\nu''}|$$  \hspace{1cm} (3.7)

we rewrite eqn.(3.5) as:

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

$$+ \frac{1}{(2\pi)^3} \sum_{\nu''} \int d^3k'' |k''\chi_{\nu''}\rangle \langle k''\chi_{\nu''}| \frac{T_c |k\phi_n\rangle}{E - E_{\nu''}'' + i0}$$  \hspace{1cm} (3.8)

6
Here, $E''_n = k''^2/2 - E_A$ and $E'_n = k'^2/2 - E_{P_A}$ 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 $\langle k'\chi_{\nu'} |$

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

(3.9)

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

(3.10)

where in eqn.(3.9), we use $V_d = H_0^0 + V_c - H_0^0$ (see eqn.3.2) and also use the eigen-value equations (3.3.3.4). 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 $Z_{\text{eff}}$ in terms of them. To deduce $Z_{\text{eff}}$ in terms of T-matrices, we project equation (3.8) by $\langle \psi^+_k \Delta |$ and arrive at:

\[
\langle \psi^+_k | \Delta | \psi^+_k \rangle = \langle \psi^+_k | \Delta | \psi^+_k \rangle + \frac{1}{(2\pi)^3} \sum_{n''} \int d^3k'' \frac{\langle \psi^+_k | \Delta | k''\phi_{n''}\rangle \langle k''\phi_{n''}|T_d|k\phi_n\rangle}{E - E''_n + i0} 
+ \frac{1}{(2\pi)^3} \sum_{\nu''} \int d^3k'' \frac{\langle \psi^+_k | \Delta | k''\chi_{\nu''}\rangle \langle k''\chi_{\nu''}|T_c|k\phi_n\rangle}{E - E''_n + i0} \]  

(3.11)

Now, $\langle \psi^+_k |$ from eqn(3.8) may be substituted in the r.h.s of eqn(3.11) to arrive at a direct expression for $Z_{\text{eff}}$. However, that will lead to a complicated equation like (2.9). We rather develop simpler equations to evaluate $\langle \psi^+_k | k\phi_n \rangle$ and $\langle \psi^+_k | k\chi_{\nu} \rangle$ and substitute them back in eqn(3.11). For this, we project eqn(3.8) from left by $\langle k'\phi_{n'} | \Delta |$ and $\langle k'\chi_{\nu'} | \Delta |$ and obtain:

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

(3.12)

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

(3.13)

The above two equations are very straightforward 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 $\Delta$ 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 [16] may be applied to calculate $Z_{\text{eff}}$.

B. Many Electron Target

For multi-electron targets the formulation is very much similar to that of section IIA, 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:

\[
\psi^+_k (x_1, r_2, ..., r_N) = \sum_n F_n(x) \phi_n (r_1, ..., r_N) + A_1 \sum_{\nu\mu} G_{\nu\mu} (r_1, t_1, r_2, ..., r_N) \]  

(14.4)
where $\varphi$ represents the residual target ion and $A_1$ is the antisymmetrization operator, which antisymmetrizes electron 1 with other target electrons. The initial target wave function $\phi$ is supposed to be antisymmetrized implicitly. The total Hamiltonian is now partitioned as: $H = H_0 + V_d = H_0 + V_{c(j)}$, where $H_0$ 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 $j$-th electron being attached to the positron. Accommodating the Pauli exclusion principle for the rearrangement channel, the Lippmann-Schwinger integral equation is now written as:

$$|\psi^+_k⟩ = |kφ_n⟩ + G_0^d T_d |kφ_n⟩ + A_j G_0^c |T_{c(j)} kφ_n⟩$$

(3.15)

where $T_d$ and $T_c$ are defined as $V_d|ψ^+_k⟩ = T_d |kφ_n⟩$ (here $T_d ≡ T$ of section-I) and $V_{c(j)} |ψ^+_k⟩ = T_{c(j)} |kφ_n⟩$. Using following closure relations for the direct and the rearrangement channels:

$$1 = \frac{1}{(2\pi)^3} \sum_{n''=1}^n \int dk'' |k'' φ_{n''}⟩⟨k'' φ_{n''}|$$

(3.16)

$$1 = \frac{1}{(2\pi)^3} \sum_{n''} \sum_{μ''} \int dk'' |k'' j_μ φ_{μ''}⟩⟨k'' j_μ φ_{μ''}|$$

(3.17)

and proceeding in a similar way, we represent the Lippmann-Schwinger equation 3.15 as:

$$|ψ^+_k⟩ = |kφ_n⟩ + \frac{1}{(2\pi)^3} \sum_{n''} \int d^3 k'' |k'' φ_{n''}⟩⟨k'' φ_{n''}|T_d |kφ_n⟩}{E - E''_n + i0} + \frac{1}{(2\pi)^3} \sum_{n''} \sum_{μ''} \int d^3 k'' |A_j k'' χ_{μ''} φ_{μ''}⟩⟨k'' χ_{μ''} φ_{μ''}|T_{c(j)} |kφ_n⟩}{E - E''_n + i0}$$

(3.18)

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

In summary, we present a new *ab initio* methodology to calculate $Z_{eff}$ from physical (onshell) and virtual (half-offshell) scattering T-matrix amplitudes, without any use of the scattering wave function. 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 exact and can act 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. Performing elastic scattering and employing elastic-channel T-matrix amplitudes (on- and off-shell) we reproduce the corresponding $Z_{eff}$ result and demonstrate the utility of the methodology. A similar T-matrix formulation for the pick-off annihilation of ortho-positronium is under way and will be published soon.

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

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Incident positron Energy (eV)

$Z_{\text{eff}}$

- Plane wave result
- Plane wave with onshell T–matrix
- Complete result with static T–matrix
- Corresponding Static SMC result [12]